sh2329

Table 1. Crystal data and structure refinement for sh2329.

Identification code	sh2329	
Empirical formula	C122.50 H134 Al4 N6 O16 Si8	
Formula weight	2279.00	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.7882(13) Å	α= 92.329(4)°.
	b = 16.2906(14) Å	β= 100.064(4)°.
	c = 25.664(2) Å	γ = 99.852(4)°.
Volume	5981.9(9) $Å^3$	
Z	2	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.185 mm^{-1}	
F(000)	2406	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.27 to 27.29°.	
Index ranges	-19<=h<=19, -20<=k<=20, -33<=l<=33	
Reflections collected	110504	
Independent reflections	26254 [R(int) = 0.0358]	
Completeness to theta = 27.29°	97.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	26254 / 0 / 1426	
Goodness-of-fit on F^2	1.115	
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1387	
R indices (all data)	R1 = 0.0909, wR2 = 0.1635	
Largest diff. peak and hole	1.114 and -0.666 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2329. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	4760(1)	6547(1)	2965(1)	15(1)
Al(2)	6192(1)	6483(1)	2176(1)	15(1)
Al(3)	7206(1)	8383(1)	2569(1)	15(1)
Al(4)	5532(1)	8537(1)	3183(1)	15(1)
Si(1)	5365(1)	4872(1)	3488(1)	16(1)
Si(2)	6168(1)	4606(1)	2466(1)	16(1)
Si(3)	6361(1)	6923(1)	963(1)	16(1)
Si(4)	7542(1)	8658(1)	1371(1)	17(1)
Si(5)	8677(1)	9388(1)	3567(1)	18(1)
Si(6)	6983(1)	9744(1)	4083(1)	16(1)
Si(7)	3458(1)	8732(1)	2611(1)	16(1)
Si(8)	2840(1)	7048(1)	3051(1)	17(1)
O(1)	5133(1)	6547(1)	2359(1)	18(1)
O(2)	7126(1)	7273(1)	2515(1)	18(1)
O(3)	6189(2)	8668(1)	2686(1)	19(1)
O(4)	5339(1)	7476(1)	3357(1)	18(1)
O(5)	5038(2)	5721(1)	3323(1)	21(1)
O(6)	5948(2)	4510(1)	3066(1)	19(1)
O(7)	6544(2)	5546(1)	2342(1)	19(1)
O(8)	6066(2)	6595(1)	1496(1)	20(1)
O(9)	6763(2)	7933(1)	1002(1)	20(1)
O(10)	7376(2)	8764(1)	1964(1)	21(1)
O(11)	8153(2)	8788(1)	3059(1)	21(1)
O(12)	8012(2)	9608(1)	3977(1)	22(1)
O(13)	6134(2)	9079(1)	3765(1)	21(1)
O(14)	4477(1)	8838(1)	2963(1)	20(1)
O(15)	2749(2)	7916(1)	2757(1)	20(1)
O(16)	3564(1)	6553(1)	2838(1)	19(1)
N(1)	3813(2)	6225(2)	1536(1)	30(1)
C(97)	3055(3)	5540(2)	1606(1)	30(1)
C(98)	2337(3)	5294(3)	1101(2)	40(1)
C(99)	1750(3)	5949(3)	934(2)	53(1)
N(2)	2348(3)	6721(3)	827(2)	62(1)
N(3)	6051(2)	9939(2)	2094(1)	26(1)
C(100)	6464(3)	10758(2)	2389(1)	33(1)
C(101)	6366(3)	11484(2)	2045(2)	39(1)
C(102)	5372(3)	11608(3)	1882(2)	52(1)
N(4)	4794(3)	10853(3)	1566(2)	58(1)
N(5)	8313(3)	6598(3)	3181(2)	58(1)
C(103)	8251(3)	6754(3)	3761(2)	52(1)
C(104)	7336(3)	6993(2)	3799(2)	36(1)
C(105)	7183(3)	7271(3)	4352(2)	40(1)
N(6)	6200(2)	7362(2)	4327(1)	32(1)
C(106)	693(3)	3403(3)	1509(2)	50(1)

Table 3. Bond lengths [Å] and angles [°] for sh2329.

Al(1)-O(5)	1.726(2)
Al(1)-O(1)	1.739(2)
Al(1)-O(16)	1.744(2)
Al(1)-O(4)	1.779(2)
Al(2)-O(1)	1.731(2)
Al(2)-O(7)	1.740(2)
Al(2)-O(8)	1.741(2)
Al(2)-O(2)	1.788(2)
Al(3)-O(3)	1.719(2)
Al(3)-O(11)	1.726(2)
Al(3)-O(10)	1.736(2)
Al(3)-O(2)	1.790(2)
Al(4)-O(13)	1.720(2)
Al(4)-O(14)	1.724(2)
Al(4)-O(3)	1.732(2)
Al(4)-O(4)	1.791(2)
Si(1)-O(5)	1.591(2)
Si(1)-O(6)	1.647(2)
Si(2)-O(7)	1.602(2)
Si(2)-O(6)	1.636(2)
Si(3)-O(8)	1.594(2)
Si(3)-O(9)	1.644(2)
Si(4)-O(10)	1.592(2)
Si(4)-O(9)	1.637(2)
Si(5)-O(11)	1.594(2)
Si(5)-O(12)	1.630(2)
Si(6)-O(13)	1.587(2)
Si(6)-O(12)	1.641(2)
Si(7)-O(14)	1.593(2)
Si(7)-O(15)	1.644(2)
Si(8)-O(16)	1.601(2)
Si(8)-O(15)	1.646(2)
C(99)-N(2)	1.473(6)
N(3)-C(100)	1.485(4)
C(100)-C(101)	1.516(5)
C(101)-C(102)	1.506(6)
C(102)-N(4)	1.489(6)
N(5)-C(103)	1.522(6)
C(103)-C(104)	1.489(6)
C(104)-C(105)	1.538(6)
C(105)-N(6)	1.476(5)
O(5)-Al(1)-O(1)	112.28(11)
O(5)-Al(1)-O(16)	112.64(11)
O(1)-Al(1)-O(16)	107.60(11)
O(5)-Al(1)-O(4)	106.73(11)
O(1)-Al(1)-O(4)	108.87(10)
O(16)-Al(1)-O(4)	108.63(10)
O(1)-Al(2)-O(7)	111.23(10)
O(1)-Al(2)-O(8)	107.61(11)
O(7)-Al(2)-O(8)	111.76(11)
O(1)-Al(2)-O(2)	112.85(10)
O(7)-Al(2)-O(2)	104.50(11)
O(8)-Al(2)-O(2)	108.92(10)
O(3)-Al(3)-O(11)	112.50(11)
O(3)-Al(3)-O(10)	105.91(11)
O(11)-Al(3)-O(10)	110.16(11)
O(3)-Al(3)-O(2)	112.23(11)
O(11)-Al(3)-O(2)	107.48(11)
O(10)-Al(3)-O(2)	108.51(10)
O(13)-Al(4)-O(14)	112.91(11)
O(13)-Al(4)-O(3)	110.67(11)
O(14)-Al(4)-O(3)	108.27(11)
O(13)-Al(4)-O(4)	103.44(11)
O(14)-Al(4)-O(4)	109.82(11)
O(3)-Al(4)-O(4)	111.73(10)
O(5)-Si(1)-O(6)	112.45(11)
O(7)-Si(2)-O(6)	114.24(11)
O(8)-Si(3)-O(9)	113.65(11)
O(8)-Si(3)-C(25)	110.77(13)
O(11)-Si(5)-O(12)	115.02(12)
O(14)-Si(7)-O(15)	112.12(12)
O(16)-Si(8)-O(15)	112.58(11)
Al(2)-O(1)-Al(1)	133.38(13)
Al(2)-O(2)-Al(3)	129.45(12)

Al(3)-O(3)-Al(4)	135.80(13)
Al(1)-O(4)-Al(4)	130.30(12)
Si(1)-O(5)-Al(1)	162.89(15)
Si(2)-O(6)-Si(1)	142.19(14)
Si(2)-O(7)-Al(2)	143.26(14)
Si(3)-O(8)-Al(2)	156.38(15)
Si(4)-O(9)-Si(3)	140.99(14)
Si(4)-O(10)-Al(3)	152.85(14)
Si(5)-O(11)-Al(3)	154.05(15)
Si(5)-O(12)-Si(6)	149.51(15)
Si(6)-O(13)-Al(4)	150.99(15)
Si(7)-O(14)-Al(4)	154.41(15)
Si(7)-O(15)-Si(8)	137.37(14)
Si(8)-O(16)-Al(1)	138.49(14)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2329. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	17(1)	13(1)	17(1)	2(1)	5(1)	4(1)
Al(2)	17(1)	13(1)	15(1)	1(1)	5(1)	3(1)
Al(3)	17(1)	13(1)	17(1)	1(1)	5(1)	2(1)
Al(4)	15(1)	14(1)	17(1)	0(1)	3(1)	4(1)
Si(1)	18(1)	14(1)	18(1)	2(1)	6(1)	3(1)
Si(2)	17(1)	13(1)	18(1)	2(1)	5(1)	5(1)
Si(3)	18(1)	17(1)	15(1)	2(1)	4(1)	4(1)
Si(4)	19(1)	15(1)	18(1)	4(1)	6(1)	4(1)
Si(5)	14(1)	19(1)	21(1)	-1(1)	4(1)	2(1)
Si(6)	16(1)	16(1)	16(1)	-1(1)	4(1)	3(1)
Si(7)	15(1)	16(1)	18(1)	2(1)	4(1)	5(1)
Si(8)	15(1)	16(1)	19(1)	0(1)	5(1)	2(1)
O(1)	18(1)	17(1)	18(1)	1(1)	4(1)	4(1)
O(2)	19(1)	14(1)	21(1)	1(1)	5(1)	3(1)
O(3)	20(1)	18(1)	20(1)	4(1)	6(1)	6(1)
O(4)	21(1)	13(1)	20(1)	0(1)	3(1)	3(1)
O(5)	25(1)	17(1)	22(1)	4(1)	7(1)	7(1)
O(6)	20(1)	18(1)	21(1)	2(1)	7(1)	5(1)
O(7)	20(1)	14(1)	24(1)	5(1)	7(1)	5(1)
O(8)	22(1)	21(1)	17(1)	2(1)	6(1)	4(1)
O(9)	21(1)	18(1)	21(1)	3(1)	4(1)	3(1)
O(10)	26(1)	17(1)	21(1)	3(1)	8(1)	3(1)
O(11)	20(1)	22(1)	23(1)	-1(1)	6(1)	5(1)
O(12)	19(1)	26(1)	21(1)	0(1)	5(1)	6(1)
O(13)	19(1)	21(1)	20(1)	-2(1)	2(1)	2(1)
O(14)	16(1)	21(1)	23(1)	2(1)	4(1)	5(1)
O(15)	19(1)	17(1)	23(1)	3(1)	5(1)	2(1)
O(16)	16(1)	18(1)	23(1)	-1(1)	5(1)	3(1)
N(1)	28(2)	34(2)	26(2)	2(1)	1(1)	3(1)
C(97)	31(2)	28(2)	30(2)	-1(1)	4(1)	3(2)
C(98)	36(2)	43(2)	34(2)	-5(2)	-1(2)	-3(2)
C(99)	28(2)	76(3)	49(3)	-6(2)	-5(2)	9(2)
N(2)	67(3)	53(2)	62(3)	2(2)	-12(2)	23(2)
N(3)	33(2)	22(1)	27(1)	6(1)	9(1)	12(1)
C(100)	34(2)	30(2)	31(2)	-1(2)	5(2)	2(2)
C(101)	49(2)	21(2)	49(2)	2(2)	22(2)	0(2)
C(102)	63(3)	38(2)	74(3)	26(2)	35(3)	32(2)
N(4)	41(2)	72(3)	66(3)	31(2)	3(2)	22(2)
N(5)	44(2)	54(2)	68(3)	-11(2)	-15(2)	17(2)
C(103)	35(2)	39(2)	78(3)	0(2)	2(2)	3(2)
C(104)	34(2)	33(2)	41(2)	9(2)	6(2)	2(2)
C(105)	36(2)	43(2)	35(2)	12(2)	1(2)	-2(2)
N(6)	47(2)	26(2)	24(1)	4(1)	6(1)	7(1)

sh2318

Table 1. Crystal data and structure refinement for sh2318.

Identification code	sh2318	
Empirical formula	C111.50 H121 Al4 N6 O16 Si8	
Formula weight	2133.78	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 27.279(7) Å	α= 90°.
	b = 17.257(4) Å	β= 94.706(8)°.
	c = 23.840(6) Å	γ = 90°.
Volume	11185(5) $Å^3$	
Z	4	
Density (calculated)	1.267 Mg/m^3	
Absorption coefficient	0.193 mm^{-1}	
F(000)	4496	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.40 to 28.33°.	
Index ranges	-33<=h<=36, -22<=k<=20, -31<=l<=31	
Reflections collected	60520	

Independent reflections	25237 [R(int) = 0.0366]
Completeness to theta = 28.33°	98.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	25237 / 1 / 1382
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0617, wR2 = 0.1505
R indices (all data)	R1 = 0.0810, wR2 = 0.1623
Absolute structure parameter	-0.01(8)
Largest diff. peak and hole	0.886 and -0.575 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2318. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	7687(1)	109(1)	7080(1)	21(1)
Al(2)	7386(1)	1656(1)	7746(1)	19(1)
Al(3)	6541(1)	730(1)	8287(1)	19(1)
Al(4)	6934(1)	-841(1)	7717(1)	22(1)
Si(1)	8735(1)	851(1)	7015(1)	26(1)
Si(2)	8513(1)	2134(1)	7899(1)	24(1)
Si(3)	6643(1)	3118(1)	7435(1)	22(1)
Si(4)	5813(1)	2177(1)	7909(1)	23(1)
Si(5)	6236(1)	-347(1)	9279(1)	19(1)
Si(6)	6816(1)	-1753(1)	8897(1)	23(1)
Si(7)	6566(1)	-1802(1)	6577(1)	27(1)
Si(8)	7312(1)	-841(1)	5949(1)	24(1)
O(1)	7402(1)	1036(2)	7155(1)	22(1)
O(2)	7122(1)	1172(2)	8304(1)	21(1)
O(3)	6532(1)	-31(2)	7784(1)	22(1)
O(4)	7516(1)	-515(2)	7596(1)	24(1)
O(5)	8321(1)	242(2)	7148(1)	29(1)
O(6)	8768(1)	1575(2)	7457(1)	31(1)
O(7)	7970(1)	1875(2)	8017(1)	26(1)
O(8)	7042(1)	2451(2)	7536(1)	26(1)
O(9)	6087(1)	2796(2)	7526(1)	26(1)
O(10)	6100(1)	1381(2)	8030(1)	26(1)
O(11)	6461(1)	359(2)	8943(1)	21(1)
O(12)	6605(1)	-1099(2)	9314(1)	24(1)
O(13)	6993(1)	-1365(2)	8339(1)	29(1)
O(14)	6645(1)	-1353(2)	7162(1)	30(1)
O(15)	6838(1)	-1373(2)	6079(1)	31(1)
O(16)	7461(1)	-193(2)	6413(1)	26(1)
C(1)	8619(1)	1272(3)	6289(2)	30(1)
C(2)	8364(2)	1960(3)	6188(2)	38(1)
C(3)	8268(2)	2265(3)	5650(2)	48(1)
C(4)	8427(2)	1864(4)	5189(2)	50(1)
C(5)	8678(2)	1189(4)	5276(2)	52(1)
C(6)	8776(2)	880(3)	5816(2)	42(1)
C(7)	9352(1)	367(3)	7100(2)	33(1)
C(8)	9765(2)	738(4)	6942(4)	84(2)
C(9)	10226(2)	399(5)	7039(4)	81(2)
C(10)	10271(2)	-280(6)	7302(3)	86(3)
C(11A)	9893(3)	-504(6)	7594(6)	47(3)
C(12A)	9428(3)	-175(6)	7481(5)	37(2)
C(11B)	9833(4)	-880(9)	7210(5)	62(3)
C(12B)	9391(4)	-478(7)	7138(6)	51(3)
C(13)	8501(1)	3131(3)	7605(2)	29(1)
C(14)	8139(2)	3672(3)	7740(2)	33(1)
C(15)	8130(2)	4428(3)	7541(2)	40(1)
C(16)	8486(2)	4668(3)	7201(2)	49(1)
C(17)	8845(2)	4164(3)	7059(2)	47(1)
C(18)	8853(2)	3407(3)	7257(2)	40(1)
C(19)	8879(1)	2103(3)	8601(2)	30(1)
C(20)	8719(2)	2539(3)	9046(2)	33(1)
C(21)	8948(2)	2506(3)	9586(2)	42(1)
C(22)	9346(2)	2008(4)	9682(2)	53(1)
C(23)	9515(2)	1590(4)	9260(2)	62(2)
C(24)	9283(2)	1640(3)	8703(2)	48(1)
C(25)	6796(1)	3932(2)	7943(2)	26(1)
C(26)	7018(2)	3774(3)	8481(2)	34(1)
C(27)	7136(2)	4370(3)	8865(2)	45(1)
C(28)	7018(2)	5121(3)	8722(2)	55(1)
C(29)	6797(2)	5296(3)	8201(2)	49(1)
C(30)	6688(2)	4696(3)	7816(2)	37(1)
C(31)	6645(1)	3484(2)	6696(2)	25(1)
C(32)	6224(2)	3660(3)	6350(2)	30(1)
C(33)	6254(2)	3904(3)	5793(2)	35(1)
C(34)	6708(2)	3975(3)	5577(2)	33(1)
C(35)	7128(2)	3817(3)	5918(2)	33(1)
C(36)	7098(2)	3561(3)	6472(2)	29(1)
C(37)	5710(1)	2647(3)	8598(2)	31(1)
C(38)	5715(2)	3449(3)	8670(2)	41(1)
C(39)	5626(2)	3786(4)	9180(2)	56(2)
C(40)	5542(2)	3312(4)	9635(2)	64(2)
C(41)	5545(2)	2526(4)	9580(2)	60(2)

C(42)	5628(2)	2193(3)	9063(2)	46(1)
C(43)	5219(1)	1936(3)	7504(2)	35(1)
C(44A)	4964(4)	2525(7)	7182(4)	43(2)
C(45A)	4513(4)	2363(7)	6908(5)	52(3)
C(46A)	4278(4)	1662(9)	7005(5)	51(3)
C(44B)	5115(4)	2140(6)	6904(4)	41(2)
C(45B)	4713(4)	1913(6)	6585(4)	44(2)
C(46B)	4386(4)	1432(9)	6803(5)	49(3)
C(47)	4496(2)	1138(4)	7365(2)	62(2)
C(48)	4936(2)	1327(3)	7651(2)	50(1)
C(49)	6171(1)	-69(2)	10025(1)	25(1)
C(50)	6502(2)	-322(3)	10468(2)	36(1)
C(51)	6449(2)	-117(3)	11015(2)	51(1)
C(52)	6063(2)	334(3)	11149(2)	56(2)
C(53)	5740(2)	607(4)	10725(2)	62(2)
C(54)	5784(2)	402(3)	10166(2)	46(1)
C(55)	5623(1)	-647(2)	8939(2)	27(1)
C(56)	5310(2)	-1077(4)	9247(2)	72(2)
C(57)	4857(2)	-1328(5)	9013(3)	89(3)
C(58)	4713(2)	-1159(3)	8448(2)	50(1)
C(59)	5023(2)	-773(4)	8138(2)	59(2)
C(60)	5468(2)	-493(4)	8389(2)	55(2)
C(61)	6345(2)	-2521(3)	8714(2)	31(1)
C(62)	6285(2)	-3147(3)	9086(2)	39(1)
C(63)	5936(2)	-3706(3)	8970(2)	50(1)
C(64)	5626(2)	-3666(4)	8471(3)	66(2)
C(65)	5683(3)	-3073(5)	8119(3)	100(3)
C(66)	6045(3)	-2501(4)	8235(2)	75(2)
C(67)	7355(2)	-2224(3)	9313(2)	35(1)
C(68)	7598(3)	-1883(5)	9786(2)	86(3)
C(69)	8005(3)	-2232(6)	10074(3)	112(4)
C(70)	8159(3)	-2955(5)	9906(3)	90(3)
C(71)	7964(2)	-3253(3)	9412(2)	54(1)
C(72)	7565(2)	-2888(3)	9121(2)	37(1)
C(73)	6813(2)	-2809(3)	6657(2)	34(1)
C(74)	6585(2)	-3470(3)	6424(2)	43(1)
C(75)	6790(2)	-4189(3)	6469(2)	50(1)
C(76)	7232(2)	-4285(3)	6770(2)	54(1)
C(77)	7469(3)	-3666(4)	7016(3)	68(2)
C(78)	7268(2)	-2936(3)	6955(2)	54(1)
C(79)	5895(2)	-1851(3)	6345(2)	38(1)
C(80)	5562(2)	-1985(5)	6711(3)	76(2)
C(81)	5062(2)	-2076(4)	6564(3)	73(2)
C(82A)	4861(4)	-1794(10)	6065(5)	55(3)
C(83A)	5164(4)	-1379(7)	5736(4)	51(3)
C(84A)	5670(4)	-1402(7)	5874(4)	48(3)
C(82B)	4919(5)	-2248(8)	6034(7)	60(4)
C(83B)	5260(4)	-2259(6)	5626(5)	53(3)
C(84B)	5731(3)	-2096(6)	5786(4)	40(2)
C(85)	7129(1)	-336(3)	5271(2)	30(1)
C(86)	7425(2)	245(3)	5079(2)	35(1)
C(87)	7308(2)	624(3)	4569(2)	43(1)
C(88)	6896(2)	419(4)	4237(2)	57(2)
C(89)	6599(2)	-160(4)	4409(2)	53(1)
C(90)	6706(2)	-541(3)	4919(2)	42(1)
C(91)	7856(1)	-1465(3)	5850(2)	28(1)
C(92)	8328(2)	-1178(3)	6021(2)	42(1)
C(93)	8746(2)	-1575(4)	5885(2)	55(2)
C(94)	8695(2)	-2275(3)	5575(2)	50(1)
C(95)	8241(2)	-2552(3)	5415(2)	42(1)
C(96)	7827(2)	-2158(3)	5546(2)	36(1)
N(1)	7042(1)	1480(2)	6157(1)	37(1)
C(97)	6160(2)	410(3)	6437(2)	42(1)
C(98)	6216(2)	1264(3)	6453(2)	49(1)
C(99)	6531(2)	1601(4)	6011(2)	48(1)
N(2)	5893(1)	113(2)	6921(1)	39(1)
N(3)	7678(2)	1180(4)	9210(2)	86(2)
C(100)	7938(4)	428(7)	9228(7)	215(9)
C(101)	8407(4)	385(6)	9530(5)	119(3)
C(102)	8707(6)	-304(6)	9496(5)	182(7)
N(4)	8877(3)	-370(5)	8872(4)	130(3)
N(5)	8173(2)	-1257(3)	8227(2)	59(1)
C(103)	8429(2)	-1809(5)	7891(4)	90(2)
C(104)	8634(3)	-2521(5)	8206(4)	103(3)
C(105)	8966(3)	-2338(6)	8685(5)	114(3)
N(6)	9385(2)	-1889(6)	8526(4)	122(3)
C(106)	4957(4)	430(6)	5273(4)	48(2)

C(107)	4644(4)	427(7)	5008(5)	56(3)
C(108)	4589(4)	976(6)	5267(4)	112(3)
C(109)	4927(4)	1540(7)	5576(5)	56(3)
C(110)	4657(4)	1568(7)	4726(4)	49(2)
C(111)	4887(5)	-162(8)	5724(5)	63(3)
C(112)	5003(4)	5276(11)	5240(5)	177(7)
C(113)	4954(2)	4537(8)	5542(4)	104(3)
C(114)	4974(2)	3797(7)	5308(4)	106(3)

Table 3. Bond lengths [Å] and angles [°] for sh2318.

Al(1)-O(4)	1.728(3)
Al(1)-O(5)	1.738(3)
Al(1)-O(16)	1.738(3)
Al(1)-O(1)	1.795(3)
Al(2)-O(7)	1.713(3)
Al(2)-O(8)	1.712(3)
Al(2)-O(2)	1.772(3)
Al(2)-O(1)	1.774(3)
Al(3)-O(11)	1.722(2)
Al(3)-O(10)	1.722(3)
Al(3)-O(2)	1.757(3)
Al(3)-O(3)	1.777(3)
Al(4)-O(14)	1.727(3)
Al(4)-O(4)	1.732(3)
Al(4)-O(13)	1.735(3)
Al(4)-O(3)	1.791(3)
Si(1)-O(5)	1.595(3)
Si(1)-O(6)	1.633(3)
Si(1)-C(7)	1.874(4)
Si(1)-C(1)	1.878(4)
Si(2)-O(7)	1.594(3)
Si(2)-O(6)	1.626(3)
Si(2)-C(13)	1.858(5)
Si(2)-C(19)	1.878(4)
Si(3)-O(8)	1.589(3)
Si(3)-O(9)	1.646(3)
Si(3)-C(31)	1.872(4)
Si(3)-C(25)	1.879(4)
Si(4)-O(10)	1.594(3)
Si(4)-O(9)	1.627(3)
Si(4)-C(43)	1.866(4)
Si(4)-C(37)	1.874(4)
Si(5)-O(11)	1.606(3)
Si(5)-O(12)	1.641(3)
Si(5)-C(49)	1.863(4)
Si(5)-C(55)	1.870(4)
Si(6)-O(13)	1.597(3)
Si(6)-O(12)	1.639(3)
Si(6)-C(61)	1.872(4)
Si(6)-C(67)	1.889(4)
Si(7)-O(14)	1.594(3)
Si(7)-O(15)	1.628(3)
Si(7)-C(73)	1.869(5)
Si(7)-C(79)	1.869(4)
Si(8)-O(16)	1.602(3)
Si(8)-O(15)	1.636(3)
Si(8)-C(91)	1.863(4)
Si(8)-C(85)	1.870(4)
C(1)-C(2)	1.387(6)
C(1)-C(6)	1.412(6)
C(2)-C(3)	1.390(6)
C(3)-C(4)	1.397(7)
C(4)-C(5)	1.360(8)
C(5)-C(6)	1.396(6)
C(7)-C(12A)	1.307(11)
C(7)-C(8)	1.376(7)
C(7)-C(12B)	1.465(12)
C(8)-C(9)	1.390(8)
C(9)-C(10)	1.330(11)
C(10)-C(11A)	1.347(12)
C(10)-C(11B)	1.581(17)
C(11A)-C(12A)	1.395(12)
C(11B)-C(12B)	1.389(15)
C(13)-C(18)	1.404(6)
C(13)-C(14)	1.415(6)
C(14)-C(15)	1.388(6)
C(15)-C(16)	1.378(7)
C(16)-C(17)	1.373(8)
C(17)-C(18)	1.388(7)
C(19)-C(24)	1.368(6)
C(19)-C(20)	1.400(6)
C(20)-C(21)	1.386(6)
C(21)-C(22)	1.389(7)
C(22)-C(23)	1.351(8)
C(23)-C(24)	1.426(7)

C(25)-C(30)	1.380(6)
C(25)-C(26)	1.401(6)
C(26)-C(27)	1.396(6)
C(27)-C(28)	1.372(8)
C(28)-C(29)	1.368(8)
C(29)-C(30)	1.399(7)
C(31)-C(32)	1.393(5)
C(31)-C(36)	1.391(5)
C(32)-C(33)	1.401(6)
C(33)-C(34)	1.386(6)
C(34)-C(35)	1.376(6)
C(35)-C(36)	1.400(5)
C(37)-C(42)	1.390(6)
C(37)-C(38)	1.396(7)
C(38)-C(39)	1.386(7)
C(39)-C(40)	1.393(9)
C(40)-C(41)	1.363(9)
C(41)-C(42)	1.395(7)
C(43)-C(48)	1.367(7)
C(43)-C(44A)	1.421(11)
C(43)-C(44B)	1.477(10)
C(44A)-C(45A)	1.374(13)
C(45A)-C(46A)	1.397(18)
C(46A)-C(47)	1.351(16)
C(44B)-C(45B)	1.342(13)
C(45B)-C(46B)	1.352(16)
C(46B)-C(47)	1.439(13)
C(47)-C(48)	1.372(7)
C(49)-C(54)	1.394(6)
C(49)-C(50)	1.404(6)
C(50)-C(51)	1.370(6)
C(51)-C(52)	1.369(8)
C(52)-C(53)	1.369(8)
C(53)-C(54)	1.394(6)
C(55)-C(60)	1.370(6)
C(55)-C(56)	1.387(7)
C(56)-C(57)	1.382(8)
C(57)-C(58)	1.403(8)
C(58)-C(59)	1.346(7)
C(59)-C(60)	1.394(6)
C(61)-C(66)	1.350(7)
C(61)-C(62)	1.414(6)
C(62)-C(63)	1.369(7)
C(63)-C(64)	1.403(8)
C(64)-C(65)	1.341(9)
C(65)-C(66)	1.407(8)
C(67)-C(72)	1.376(6)
C(67)-C(68)	1.391(8)
C(68)-C(69)	1.396(8)
C(69)-C(70)	1.386(11)
C(70)-C(71)	1.352(9)
C(71)-C(72)	1.394(7)
C(73)-C(74)	1.392(6)
C(73)-C(78)	1.397(7)
C(74)-C(75)	1.362(8)
C(75)-C(76)	1.361(8)
C(76)-C(77)	1.359(8)
C(77)-C(78)	1.377(9)
C(79)-C(80)	1.331(7)
C(79)-C(84B)	1.435(10)
C(79)-C(84A)	1.458(11)
C(80)-C(81)	1.389(8)
C(81)-C(82B)	1.324(17)
C(81)-C(82A)	1.357(14)
C(82A)-C(83A)	1.385(18)
C(83A)-C(84A)	1.393(14)
C(82B)-C(83B)	1.40(2)
C(83B)-C(84B)	1.338(14)
C(85)-C(86)	1.388(6)
C(85)-C(90)	1.415(6)
C(86)-C(87)	1.394(6)
C(87)-C(88)	1.368(8)
C(88)-C(89)	1.371(9)
C(89)-C(90)	1.392(7)
C(91)-C(96)	1.396(6)
C(91)-C(92)	1.409(6)
C(92)-C(93)	1.390(7)

C(93)-C(94)	1.416(8)
C(94)-C(95)	1.354(7)
C(95)-C(96)	1.377(6)
N(1)-C(99)	1.425(6)
C(97)-C(98)	1.483(8)
C(97)-N(2)	1.505(6)
C(98)-C(99)	1.527(7)
N(3)-C(100)	1.480(15)
C(100)-C(101)	1.416(13)
C(101)-C(102)	1.450(15)
C(102)-N(4)	1.598(16)
N(5)-C(103)	1.460(9)
C(103)-C(104)	1.524(11)
C(104)-C(105)	1.433(13)
C(105)-N(6)	1.456(12)
C(106)-C(107)	1.018(14)
C(106)-C(107)#1	1.325(15)
C(106)-C(106)#1	1.34(2)
C(106)-C(108)	1.375(15)
C(106)-C(111)	1.506(16)
C(107)-C(108)	1.146(14)
C(107)-C(106)#1	1.325(15)
C(107)-C(107)#1	1.94(2)
C(108)-C(109)	1.492(15)
C(108)-C(110)	1.665(14)
C(109)-C(110)#1	1.395(15)
C(110)-C(109)#1	1.395(15)
C(112)-C(112)#1	1.14(2)
C(112)-C(113)	1.476(17)
C(113)-C(114)	1.396(13)
C(114)-C(114)#1	1.488(19)

O(4)-Al(1)-O(5)	109.87(14)
O(4)-Al(1)-O(16)	111.65(14)
O(5)-Al(1)-O(16)	113.62(13)
O(4)-Al(1)-O(1)	109.96(12)
O(5)-Al(1)-O(1)	107.98(14)
O(16)-Al(1)-O(1)	103.50(13)
O(7)-Al(2)-O(8)	113.83(15)
O(7)-Al(2)-O(2)	104.09(13)
O(8)-Al(2)-O(2)	110.54(13)
O(7)-Al(2)-O(1)	110.48(13)
O(8)-Al(2)-O(1)	107.40(13)
O(2)-Al(2)-O(1)	110.50(13)
O(11)-Al(3)-O(10)	115.35(13)
O(11)-Al(3)-O(2)	108.75(12)
O(10)-Al(3)-O(2)	109.14(14)
O(11)-Al(3)-O(3)	110.05(13)
O(10)-Al(3)-O(3)	105.82(13)
O(2)-Al(3)-O(3)	107.44(12)
O(14)-Al(4)-O(4)	114.00(13)
O(14)-Al(4)-O(13)	113.11(15)
O(4)-Al(4)-O(13)	106.80(14)
O(14)-Al(4)-O(3)	102.93(14)
O(4)-Al(4)-O(3)	109.79(14)
O(13)-Al(4)-O(3)	110.19(13)
O(5)-Si(1)-O(6)	112.20(15)
O(5)-Si(1)-C(7)	109.23(19)
O(6)-Si(1)-C(7)	105.63(17)
O(5)-Si(1)-C(1)	111.72(16)
O(6)-Si(1)-C(1)	107.14(18)
C(7)-Si(1)-C(1)	110.75(18)
O(7)-Si(2)-O(6)	113.71(15)
O(7)-Si(2)-C(13)	109.67(17)
O(6)-Si(2)-C(13)	107.47(17)
O(7)-Si(2)-C(19)	105.60(16)
O(6)-Si(2)-C(19)	109.71(17)
C(13)-Si(2)-C(19)	110.71(18)
O(8)-Si(3)-O(9)	111.33(15)
O(8)-Si(3)-C(31)	109.35(16)
O(9)-Si(3)-C(31)	108.16(15)
O(8)-Si(3)-C(25)	109.29(16)
O(9)-Si(3)-C(25)	109.00(15)
C(31)-Si(3)-C(25)	109.68(17)
O(10)-Si(4)-O(9)	115.34(14)
O(10)-Si(4)-C(43)	107.15(19)
O(9)-Si(4)-C(43)	105.93(16)

O(10)-Si(4)-C(37)	108.67(17)
O(9)-Si(4)-C(37)	108.45(18)
C(43)-Si(4)-C(37)	111.31(19)
O(11)-Si(5)-O(12)	111.48(14)
O(11)-Si(5)-C(49)	110.57(16)
O(12)-Si(5)-C(49)	105.20(15)
O(11)-Si(5)-C(55)	110.98(16)
O(12)-Si(5)-C(55)	108.98(17)
C(49)-Si(5)-C(55)	109.45(17)
O(13)-Si(6)-O(12)	111.16(15)
O(13)-Si(6)-C(61)	110.55(16)
O(12)-Si(6)-C(61)	111.13(17)
O(13)-Si(6)-C(67)	110.06(18)
O(12)-Si(6)-C(67)	105.93(16)
C(61)-Si(6)-C(67)	107.9(2)
O(14)-Si(7)-O(15)	112.32(16)
O(14)-Si(7)-C(73)	109.94(17)
O(15)-Si(7)-C(73)	108.41(17)
O(14)-Si(7)-C(79)	109.83(17)
O(15)-Si(7)-C(79)	107.38(18)
C(73)-Si(7)-C(79)	108.9(2)
O(16)-Si(8)-O(15)	114.85(14)
O(16)-Si(8)-C(91)	109.43(16)
O(15)-Si(8)-C(91)	110.51(18)
O(16)-Si(8)-C(85)	107.79(18)
O(15)-Si(8)-C(85)	105.38(17)
C(91)-Si(8)-C(85)	108.62(16)
Al(2)-O(1)-Al(1)	130.97(15)
Al(3)-O(2)-Al(2)	127.43(14)
Al(3)-O(3)-Al(4)	131.44(15)
Al(1)-O(4)-Al(4)	128.65(16)
Si(1)-O(5)-Al(1)	141.66(19)
Si(2)-O(6)-Si(1)	150.28(19)
Si(2)-O(7)-Al(2)	147.68(17)
Si(3)-O(8)-Al(2)	167.45(18)
Si(4)-O(9)-Si(3)	139.89(17)
Si(4)-O(10)-Al(3)	160.83(19)
Si(5)-O(11)-Al(3)	144.81(17)
Si(6)-O(12)-Si(5)	139.38(16)
Si(6)-O(13)-Al(4)	156.58(19)
Si(7)-O(14)-Al(4)	159.92(19)
Si(7)-O(15)-Si(8)	143.86(18)
Si(8)-O(16)-Al(1)	153.09(19)
C(2)-C(1)-C(6)	116.8(4)
C(2)-C(1)-Si(1)	122.4(3)
C(6)-C(1)-Si(1)	120.8(3)
C(1)-C(2)-C(3)	122.6(4)
C(2)-C(3)-C(4)	119.4(5)
C(5)-C(4)-C(3)	119.3(4)
C(4)-C(5)-C(6)	121.6(5)
C(5)-C(6)-C(1)	120.4(5)
C(12A)-C(7)-C(8)	115.8(6)
C(12A)-C(7)-C(12B)	40.4(6)
C(8)-C(7)-C(12B)	115.0(6)
C(12A)-C(7)-Si(1)	119.0(5)
C(8)-C(7)-Si(1)	120.7(4)
C(12B)-C(7)-Si(1)	120.7(5)
C(7)-C(8)-C(9)	120.6(7)
C(10)-C(9)-C(8)	119.8(6)
C(9)-C(10)-C(11A)	116.9(7)
C(9)-C(10)-C(11B)	118.2(6)
C(11A)-C(10)-C(11B)	44.2(7)
C(10)-C(11A)-C(12A)	120.3(9)
C(7)-C(12A)-C(11A)	121.1(8)
C(12B)-C(11B)-C(10)	109.2(11)
C(11B)-C(12B)-C(7)	124.3(11)
C(18)-C(13)-C(14)	115.8(4)
C(18)-C(13)-Si(2)	123.0(4)
C(14)-C(13)-Si(2)	121.2(3)
C(15)-C(14)-C(13)	122.4(4)
C(16)-C(15)-C(14)	119.4(5)
C(17)-C(16)-C(15)	120.4(5)
C(16)-C(17)-C(18)	120.2(4)
C(17)-C(18)-C(13)	121.9(5)
C(24)-C(19)-C(20)	118.5(4)
C(24)-C(19)-Si(2)	122.4(3)
C(20)-C(19)-Si(2)	119.0(3)

C(21)-C(20)-C(19)	122.5(4)
C(20)-C(21)-C(22)	117.8(4)
C(23)-C(22)-C(21)	121.2(4)
C(22)-C(23)-C(24)	120.6(5)
C(19)-C(24)-C(23)	119.4(5)
C(30)-C(25)-C(26)	117.1(4)
C(30)-C(25)-Si(3)	122.7(3)
C(26)-C(25)-Si(3)	120.1(3)
C(27)-C(26)-C(25)	121.0(4)
C(28)-C(27)-C(26)	119.8(4)
C(29)-C(28)-C(27)	120.7(5)
C(28)-C(29)-C(30)	119.2(5)
C(25)-C(30)-C(29)	122.2(4)
C(32)-C(31)-C(36)	117.8(3)
C(32)-C(31)-Si(3)	124.4(3)
C(36)-C(31)-Si(3)	117.8(3)
C(31)-C(32)-C(33)	121.1(4)
C(34)-C(33)-C(32)	120.1(4)
C(35)-C(34)-C(33)	119.3(4)
C(34)-C(35)-C(36)	120.6(4)
C(31)-C(36)-C(35)	121.0(4)
C(42)-C(37)-C(38)	117.5(4)
C(42)-C(37)-Si(4)	120.0(4)
C(38)-C(37)-Si(4)	122.5(3)
C(39)-C(38)-C(37)	121.5(5)
C(40)-C(39)-C(38)	119.3(5)
C(41)-C(40)-C(39)	120.4(5)
C(40)-C(41)-C(42)	119.9(5)
C(37)-C(42)-C(41)	121.3(5)
C(48)-C(43)-C(44A)	115.4(5)
C(48)-C(43)-C(44B)	111.5(5)
C(44A)-C(43)-C(44B)	42.3(5)
C(48)-C(43)-Si(4)	121.5(3)
C(44A)-C(43)-Si(4)	119.1(5)
C(44B)-C(43)-Si(4)	122.5(4)
C(45A)-C(44A)-C(43)	119.4(10)
C(44A)-C(45A)-C(46A)	120.2(10)
C(47)-C(46A)-C(45A)	120.0(9)
C(45B)-C(44B)-C(43)	124.1(8)
C(44B)-C(45B)-C(46B)	119.7(9)
C(45B)-C(46B)-C(47)	118.8(9)
C(46A)-C(47)-C(48)	118.7(8)
C(46A)-C(47)-C(46B)	29.1(6)
C(48)-C(47)-C(46B)	119.1(7)
C(43)-C(48)-C(47)	122.9(5)
C(54)-C(49)-C(50)	116.9(4)
C(54)-C(49)-Si(5)	121.0(3)
C(50)-C(49)-Si(5)	122.2(3)
C(51)-C(50)-C(49)	121.7(5)
C(50)-C(51)-C(52)	120.8(5)
C(53)-C(52)-C(51)	118.9(4)
C(52)-C(53)-C(54)	121.2(5)
C(53)-C(54)-C(49)	120.4(5)
C(60)-C(55)-C(56)	117.0(4)
C(60)-C(55)-Si(5)	123.8(3)
C(56)-C(55)-Si(5)	119.1(3)
C(57)-C(56)-C(55)	121.6(5)
C(56)-C(57)-C(58)	119.5(6)
C(59)-C(58)-C(57)	119.3(5)
C(58)-C(59)-C(60)	120.1(5)
C(55)-C(60)-C(59)	122.2(4)
C(66)-C(61)-C(62)	117.1(4)
C(66)-C(61)-Si(6)	122.4(4)
C(62)-C(61)-Si(6)	120.5(3)
C(63)-C(62)-C(61)	121.8(4)
C(62)-C(63)-C(64)	119.8(5)
C(65)-C(64)-C(63)	118.4(5)
C(64)-C(65)-C(66)	121.8(6)
C(61)-C(66)-C(65)	121.1(5)
C(72)-C(67)-C(68)	116.1(4)
C(72)-C(67)-Si(6)	120.7(3)
C(68)-C(67)-Si(6)	122.8(4)
C(67)-C(68)-C(69)	121.6(6)
C(70)-C(69)-C(68)	119.6(7)
C(71)-C(70)-C(69)	119.2(5)
C(70)-C(71)-C(72)	119.9(5)
C(67)-C(72)-C(71)	122.6(5)

C(74)-C(73)-C(78)	115.1(5)
C(74)-C(73)-Si(7)	125.2(4)
C(78)-C(73)-Si(7)	119.7(4)
C(75)-C(74)-C(73)	123.2(5)
C(74)-C(75)-C(76)	119.6(5)
C(77)-C(76)-C(75)	120.1(6)
C(76)-C(77)-C(78)	120.1(6)
C(77)-C(78)-C(73)	121.9(5)
C(80)-C(79)-C(84B)	112.3(6)
C(80)-C(79)-C(84A)	109.2(6)
C(84B)-C(79)-C(84A)	50.2(6)
C(80)-C(79)-Si(7)	121.3(4)
C(84B)-C(79)-Si(7)	120.8(4)
C(84A)-C(79)-Si(7)	123.0(5)
C(79)-C(80)-C(81)	124.3(6)
C(82B)-C(81)-C(82A)	34.9(7)
C(82B)-C(81)-C(80)	118.2(8)
C(82A)-C(81)-C(80)	119.9(7)
C(81)-C(82A)-C(83A)	117.7(10)
C(84A)-C(83A)-C(82A)	118.5(10)
C(83A)-C(84A)-C(79)	123.0(9)
C(81)-C(82B)-C(83B)	120.2(10)
C(84B)-C(83B)-C(82B)	118.5(11)
C(83B)-C(84B)-C(79)	123.1(9)
C(86)-C(85)-C(90)	116.9(4)
C(86)-C(85)-Si(8)	120.1(3)
C(90)-C(85)-Si(8)	122.9(4)
C(85)-C(86)-C(87)	122.0(4)
C(88)-C(87)-C(86)	120.0(5)
C(87)-C(88)-C(89)	119.6(5)
C(88)-C(89)-C(90)	121.3(5)
C(89)-C(90)-C(85)	120.1(5)
C(96)-C(91)-C(92)	117.5(4)
C(96)-C(91)-Si(8)	123.3(3)
C(92)-C(91)-Si(8)	118.6(3)
C(93)-C(92)-C(91)	120.5(5)
C(92)-C(93)-C(94)	119.6(5)
C(95)-C(94)-C(93)	119.8(4)
C(94)-C(95)-C(96)	120.6(5)
C(95)-C(96)-C(91)	121.9(4)
C(98)-C(97)-N(2)	111.9(4)
C(97)-C(98)-C(99)	115.0(5)
N(1)-C(99)-C(98)	111.8(4)
C(101)-C(100)-N(3)	118.1(10)
C(100)-C(101)-C(102)	120.3(11)
C(101)-C(102)-N(4)	108.6(8)
N(5)-C(103)-C(104)	115.3(7)
C(105)-C(104)-C(103)	113.4(8)
C(104)-C(105)-N(6)	111.5(10)
C(107)-C(106)-C(107)#1	111.5(12)
C(107)-C(106)-C(106)#1	66.6(11)
C(107)#1-C(106)-C(106)#1	44.8(8)
C(107)-C(106)-C(108)	54.8(9)
C(107)#1-C(106)-C(108)	128.6(11)
C(106)#1-C(106)-C(108)	100.1(10)
C(107)-C(106)-C(111)	106.9(12)
C(107)#1-C(106)-C(111)	121.1(11)
C(106)#1-C(106)-C(111)	137.3(6)
C(108)-C(106)-C(111)	109.8(9)
C(106)-C(107)-C(108)	78.7(12)
C(106)-C(107)-C(106)#1	68.5(12)
C(108)-C(107)-C(106)#1	114.8(12)
C(106)-C(107)-C(107)#1	39.4(8)
C(108)-C(107)-C(107)#1	100.7(10)
C(106)#1-C(107)-C(107)#1	29.2(6)
C(107)-C(108)-C(106)	46.5(8)
C(107)-C(108)-C(109)	134.5(12)
C(106)-C(108)-C(109)	91.2(9)
C(107)-C(108)-C(110)	93.6(10)
C(106)-C(108)-C(110)	107.6(9)
C(109)-C(108)-C(110)	83.1(8)
C(110)#1-C(109)-C(108)	105.3(10)
C(109)#1-C(110)-C(108)	121.6(10)
C(112)#1-C(112)-C(113)	119.7(8)
C(114)-C(113)-C(112)	125.9(10)
C(113)-C(114)-C(114)#1	113.9(6)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2318. 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}
Al(1)	17(1)	32(1)	15(1)	-3(1)	3(1)	0(1)
Al(2)	16(1)	26(1)	16(1)	0(1)	3(1)	-3(1)
Al(3)	17(1)	26(1)	15(1)	2(1)	4(1)	1(1)
Al(4)	23(1)	28(1)	18(1)	-4(1)	7(1)	-3(1)
Si(1)	15(1)	38(1)	24(1)	-2(1)	4(1)	2(1)
Si(2)	18(1)	36(1)	19(1)	-1(1)	0(1)	-6(1)
Si(3)	21(1)	25(1)	20(1)	3(1)	3(1)	-1(1)
Si(4)	16(1)	29(1)	23(1)	6(1)	2(1)	2(1)
Si(5)	17(1)	25(1)	15(1)	2(1)	3(1)	1(1)
Si(6)	26(1)	23(1)	18(1)	1(1)	1(1)	5(1)
Si(7)	26(1)	33(1)	24(1)	-9(1)	7(1)	-5(1)
Si(8)	22(1)	34(1)	15(1)	-4(1)	4(1)	-1(1)
O(1)	19(1)	30(1)	17(1)	0(1)	2(1)	1(1)
O(2)	19(1)	27(1)	17(1)	-1(1)	4(1)	-3(1)
O(3)	21(1)	30(1)	15(1)	-3(1)	3(1)	-2(1)
O(4)	20(1)	32(2)	20(1)	0(1)	7(1)	0(1)
O(5)	18(1)	43(2)	25(1)	-2(1)	4(1)	0(1)
O(6)	23(1)	41(2)	29(1)	-7(1)	5(1)	-4(1)
O(7)	21(1)	34(2)	23(1)	-2(1)	3(1)	-6(1)
O(8)	25(1)	29(2)	26(1)	2(1)	4(1)	1(1)
O(9)	22(1)	30(2)	25(1)	6(1)	1(1)	0(1)
O(10)	21(1)	31(2)	25(1)	9(1)	4(1)	5(1)
O(11)	19(1)	29(1)	16(1)	2(1)	5(1)	-1(1)
O(12)	25(1)	30(2)	19(1)	2(1)	2(1)	5(1)
O(13)	32(1)	27(2)	28(1)	-1(1)	7(1)	1(1)
O(14)	35(2)	35(2)	23(1)	-8(1)	8(1)	-6(1)
O(15)	31(2)	38(2)	25(1)	-6(1)	6(1)	-3(1)
O(16)	22(1)	40(2)	17(1)	-4(1)	5(1)	-2(1)
C(1)	19(2)	42(2)	31(2)	2(2)	7(2)	-1(2)
C(2)	34(2)	53(3)	26(2)	1(2)	-1(2)	6(2)
C(3)	43(3)	59(3)	42(2)	9(2)	1(2)	12(2)
C(4)	38(3)	82(4)	29(2)	14(2)	5(2)	6(3)
C(5)	44(3)	81(4)	31(2)	7(2)	18(2)	3(3)
C(6)	33(2)	61(3)	33(2)	3(2)	10(2)	10(2)
C(7)	18(2)	52(3)	28(2)	-5(2)	2(2)	4(2)
C(8)	24(2)	54(4)	177(8)	4(5)	19(4)	-2(2)
C(9)	23(3)	100(6)	121(6)	-14(5)	4(3)	-8(3)
C(10)	30(3)	159(8)	68(4)	39(5)	4(3)	27(4)
C(11A)	27(4)	38(6)	77(8)	21(5)	8(5)	4(4)
C(12A)	14(4)	32(5)	66(6)	6(5)	3(4)	4(3)
C(11B)	54(7)	72(9)	61(7)	19(7)	19(6)	27(6)
C(12B)	41(6)	38(6)	76(8)	16(6)	25(6)	9(5)
C(13)	26(2)	37(2)	23(2)	-1(2)	-2(1)	-11(2)
C(14)	34(2)	37(2)	28(2)	-4(2)	0(2)	-8(2)
C(15)	46(3)	39(3)	32(2)	-3(2)	-7(2)	-6(2)
C(16)	58(3)	42(3)	43(3)	13(2)	-11(2)	-20(3)
C(17)	46(3)	56(3)	38(2)	13(2)	2(2)	-18(3)
C(18)	30(2)	57(3)	34(2)	-3(2)	6(2)	-13(2)
C(19)	24(2)	35(2)	32(2)	1(2)	2(2)	-4(2)
C(20)	31(2)	35(2)	32(2)	1(2)	-1(2)	1(2)
C(21)	42(3)	51(3)	31(2)	-6(2)	4(2)	-8(2)
C(22)	48(3)	70(4)	40(3)	7(3)	-10(2)	5(3)
C(23)	45(3)	83(4)	55(3)	-2(3)	-19(2)	23(3)
C(24)	39(3)	63(3)	41(2)	-8(2)	-1(2)	13(2)
C(25)	22(2)	34(2)	24(2)	2(2)	7(1)	-4(2)
C(26)	37(2)	37(2)	27(2)	1(2)	4(2)	-2(2)
C(27)	51(3)	54(3)	30(2)	-7(2)	-6(2)	-5(2)
C(28)	77(4)	40(3)	48(3)	-16(2)	14(3)	-13(3)
C(29)	75(4)	31(3)	42(3)	-3(2)	13(2)	2(3)
C(30)	44(2)	39(2)	29(2)	3(2)	8(2)	-2(2)
C(31)	30(2)	23(2)	22(2)	-1(1)	3(1)	-3(2)
C(32)	27(2)	38(2)	26(2)	5(2)	5(2)	-1(2)
C(33)	33(2)	38(2)	32(2)	4(2)	-1(2)	2(2)
C(34)	46(2)	35(2)	18(2)	3(2)	5(2)	-4(2)
C(35)	32(2)	42(3)	26(2)	2(2)	11(2)	-6(2)
C(36)	26(2)	35(2)	26(2)	2(2)	1(2)	0(2)
C(37)	25(2)	44(3)	27(2)	1(2)	10(2)	5(2)
C(38)	35(2)	45(3)	45(3)	-1(2)	15(2)	-4(2)
C(39)	50(3)	55(3)	67(3)	-25(3)	25(3)	-4(3)
C(40)	47(3)	95(5)	52(3)	-27(3)	22(2)	1(3)
C(41)	75(4)	71(4)	37(3)	1(3)	25(3)	10(3)

C(42)	49(3)	55(3)	38(2)	7(2)	19(2)	15(2)
C(43)	20(2)	48(3)	35(2)	14(2)	-4(2)	-6(2)
C(44A)	35(5)	54(6)	39(5)	14(5)	-12(4)	-7(5)
C(45A)	35(5)	67(7)	51(6)	10(5)	-19(4)	1(5)
C(46A)	25(5)	92(11)	37(6)	-28(6)	-3(4)	-4(6)
C(44B)	44(5)	42(6)	36(5)	9(4)	-3(4)	-13(5)
C(45B)	42(5)	49(6)	38(5)	15(4)	-12(4)	-9(5)
C(46B)	31(6)	82(10)	31(6)	-11(6)	-11(4)	-5(6)
C(47)	37(3)	95(5)	54(3)	-7(3)	2(2)	-32(3)
C(48)	39(3)	66(4)	43(3)	10(2)	-2(2)	-22(2)
C(49)	31(2)	27(2)	17(2)	1(1)	6(1)	-4(2)
C(50)	48(2)	33(2)	25(2)	1(2)	-2(2)	1(2)
C(51)	81(4)	44(3)	26(2)	6(2)	-2(2)	-4(3)
C(52)	87(4)	63(4)	21(2)	-9(2)	23(2)	-12(3)
C(53)	70(4)	78(4)	40(3)	-19(3)	27(3)	15(3)
C(54)	40(2)	71(4)	28(2)	-4(2)	9(2)	9(2)
C(55)	23(2)	29(2)	29(2)	1(2)	0(2)	1(2)
C(56)	48(3)	111(5)	55(3)	38(3)	-17(3)	-42(3)
C(57)	63(4)	128(7)	72(4)	32(4)	-12(3)	-59(4)
C(58)	31(2)	50(3)	68(3)	-3(3)	-9(2)	-14(2)
C(59)	36(3)	100(5)	39(2)	13(3)	-12(2)	-24(3)
C(60)	29(2)	104(5)	30(2)	18(3)	-4(2)	-27(3)
C(61)	37(2)	30(2)	27(2)	1(2)	2(2)	-5(2)
C(62)	46(3)	36(3)	35(2)	4(2)	7(2)	-1(2)
C(63)	55(3)	50(3)	44(3)	4(2)	12(2)	-12(3)
C(64)	70(4)	60(4)	66(4)	-4(3)	2(3)	-28(3)
C(65)	131(7)	93(5)	66(4)	31(4)	-53(4)	-64(5)
C(66)	99(5)	69(4)	52(3)	26(3)	-31(3)	-50(4)
C(67)	36(2)	38(2)	30(2)	-3(2)	-3(2)	15(2)
C(68)	92(5)	106(6)	54(3)	-30(4)	-31(3)	69(5)
C(69)	96(6)	167(9)	64(4)	-42(5)	-38(4)	87(6)
C(70)	78(5)	115(6)	73(4)	-8(4)	-26(4)	71(5)
C(71)	46(3)	46(3)	71(4)	1(3)	11(3)	26(2)
C(72)	34(2)	33(2)	45(2)	0(2)	3(2)	8(2)
C(73)	40(2)	38(2)	24(2)	-8(2)	12(2)	-6(2)
C(74)	56(3)	45(3)	31(2)	-13(2)	14(2)	-11(2)
C(75)	66(3)	41(3)	44(3)	-14(2)	21(2)	-18(3)
C(76)	81(4)	39(3)	42(3)	-1(2)	10(3)	6(3)
C(77)	74(4)	58(4)	71(4)	-2(3)	-10(3)	1(3)
C(78)	59(3)	43(3)	59(3)	-7(3)	-11(3)	1(3)
C(79)	33(2)	47(3)	35(2)	-10(2)	6(2)	-8(2)
C(80)	33(3)	140(7)	56(3)	39(4)	6(2)	-4(3)
C(81)	30(3)	96(5)	98(5)	36(4)	27(3)	4(3)
C(82A)	29(5)	75(9)	63(7)	8(8)	6(5)	6(7)
C(83A)	38(5)	66(7)	49(6)	-5(5)	-2(4)	14(5)
C(84A)	38(5)	76(8)	30(4)	-4(5)	1(4)	-11(5)
C(82B)	34(6)	41(7)	102(11)	21(8)	-17(6)	-6(6)
C(83B)	48(6)	41(6)	68(7)	-9(5)	-9(5)	-9(5)
C(84B)	33(4)	40(5)	48(5)	-18(4)	1(4)	4(4)
C(85)	28(2)	43(2)	18(2)	-4(2)	4(1)	10(2)
C(86)	39(2)	41(3)	26(2)	-3(2)	10(2)	10(2)
C(87)	58(3)	45(3)	27(2)	3(2)	10(2)	16(2)
C(88)	70(4)	70(4)	29(2)	10(2)	-2(2)	31(3)
C(89)	49(3)	78(4)	28(2)	-4(2)	-12(2)	12(3)
C(90)	31(2)	62(3)	30(2)	-9(2)	-4(2)	5(2)
C(91)	29(2)	37(2)	19(2)	2(2)	3(1)	5(2)
C(92)	32(2)	52(3)	41(2)	-15(2)	1(2)	8(2)
C(93)	30(2)	87(4)	47(3)	-18(3)	-8(2)	17(3)
C(94)	43(3)	66(4)	41(3)	-4(2)	4(2)	24(3)
C(95)	55(3)	33(2)	37(2)	-1(2)	11(2)	12(2)
C(96)	35(2)	40(3)	35(2)	-4(2)	9(2)	-4(2)
N(1)	37(2)	51(2)	24(2)	2(2)	2(1)	-4(2)
C(97)	48(3)	46(3)	30(2)	0(2)	-2(2)	-1(2)
C(98)	38(3)	61(3)	48(3)	1(2)	6(2)	-1(2)
C(99)	36(2)	64(3)	43(3)	3(2)	2(2)	0(2)
N(2)	37(2)	49(2)	28(2)	-1(2)	-9(2)	-1(2)
N(3)	81(4)	130(5)	41(2)	33(3)	-28(2)	-52(4)
C(100)	130(9)	158(11)	326(19)	145(12)	-168(12)	-58(8)
C(101)	151(9)	87(7)	116(8)	-14(6)	-11(7)	-1(7)
C(102)	340(20)	80(6)	100(7)	7(6)	-116(10)	16(10)
N(4)	117(6)	106(6)	160(8)	-26(6)	-34(6)	23(5)
N(5)	66(3)	62(3)	50(3)	10(2)	6(2)	31(3)
C(103)	46(3)	89(5)	131(7)	-18(5)	-11(4)	18(4)
C(104)	77(5)	78(5)	154(8)	3(6)	19(6)	14(4)
C(105)	67(5)	100(7)	174(10)	12(7)	4(6)	15(5)
N(6)	45(3)	171(8)	154(7)	23(7)	23(4)	3(4)
C(112)	68(5)	301(17)	165(13)	90(12)	30(9)	45(10)

C(113)	37(3)	185(11)	95(6)	-16(7)	24(4)	4(5)
C(114)	22(3)	159(9)	135(7)	22(7)	1(4)	-1(4)

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sh2330a

Table 2. Crystal data and structure refinement for sh2330a.

Identification code	sh2330a	
Empirical formula	C120 H122 Al4 N4 O16 Si8	
Formula weight	2208.86	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 17.0965(8) Å	α= 90°.
	b = 24.7045(14) Å	β= 92.969(3)°.
	c = 28.0194(13) Å	γ = 90°.
Volume	11818.4(10) $Å^3$	
Z	4	
Density (calculated)	1.241 Mg/m^3	
Absorption coefficient	0.184 mm^{-1}	
F(000)	4648	
Crystal size	0.3 x 0.22 x 0.15 mm^3	
Theta range for data collection	1.36 to 24.33°.	
Index ranges	-19<=h<=19, -28<=k<=28, -32<=l<=32	
Reflections collected	105252	
Independent reflections	19180 [R(int) = 0.0363]	
Completeness to theta = 24.33°	99.5 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19180 / 0 / 1364	
Goodness-of-fit on F^2	1.187	
Final R indices [I>2sigma(I)]	R1 = 0.0653, wR2 = 0.1520	
R indices (all data)	R1 = 0.0844, wR2 = 0.1626	
Largest diff. peak and hole	0.770 and -0.502 e.$Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2330a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	9150(1)	7424(1)	4077(1)	18(1)
Al(2)	7606(1)	7151(1)	4630(1)	19(1)
Al(3)	6668(1)	8046(1)	4010(1)	20(1)
Al(4)	8185(1)	8248(1)	3381(1)	18(1)
Si(1)	10175(1)	7385(1)	5076(1)	22(1)
Si(2)	8723(1)	6776(1)	5456(1)	22(1)
Si(3)	6026(1)	6419(1)	4557(1)	20(1)
Si(4)	5154(1)	7242(1)	3887(1)	22(1)
Si(5)	6233(1)	9310(1)	3912(1)	22(1)
Si(6)	7472(1)	9382(1)	3128(1)	20(1)
Si(7)	9050(1)	7713(1)	2495(1)	23(1)
Si(8)	10008(1)	6909(1)	3157(1)	22(1)
O(1)	8329(1)	7052(1)	4222(1)	21(1)
O(2)	7165(2)	7798(1)	4539(1)	22(1)
O(3)	7272(1)	7960(1)	3520(1)	20(1)
O(4)	8861(2)	8085(1)	3863(1)	20(1)
O(5)	9774(2)	7560(1)	4572(1)	24(1)
O(6)	9582(2)	7055(1)	5412(1)	26(1)
O(7)	8024(2)	7136(1)	5213(1)	24(1)
O(8)	6903(2)	6648(1)	4525(1)	24(1)
O(9)	5439(2)	6669(1)	4135(1)	23(1)
O(10)	5850(2)	7667(1)	3862(1)	29(1)
O(11)	6470(2)	8720(1)	4103(1)	26(1)
O(12)	6788(2)	9522(1)	3492(1)	25(1)
O(13)	8087(2)	8943(1)	3343(1)	22(1)
O(14)	8447(2)	7924(1)	2874(1)	26(1)
O(15)	9580(2)	7200(1)	2690(1)	25(1)
O(16)	9624(2)	7081(1)	3643(1)	24(1)
C(1)	10466(2)	8014(2)	5417(2)	25(1)
C(2)	10922(2)	8410(2)	5211(2)	31(1)
C(3)	11096(3)	8895(2)	5442(2)	39(1)
C(4)	10835(3)	8991(2)	5891(2)	40(1)
C(5)	10387(3)	8605(2)	6105(2)	43(1)
C(6)	10200(3)	8125(2)	5867(2)	33(1)
C(7)	11041(2)	6937(2)	4987(2)	25(1)
C(8)	11580(2)	6820(2)	5367(2)	35(1)
C(9)	12202(3)	6467(2)	5305(2)	46(1)
C(10)	12296(3)	6226(2)	4869(2)	46(1)
C(11)	11775(3)	6342(2)	4489(2)	43(1)
C(12)	11158(2)	6695(2)	4548(2)	32(1)
C(13)	8556(2)	6703(2)	6109(1)	24(1)
C(14)	7982(2)	7005(2)	6324(2)	29(1)
C(15)	7849(3)	6952(2)	6811(2)	34(1)
C(16)	8295(3)	6587(2)	7086(2)	35(1)
C(17)	8871(3)	6286(2)	6882(2)	35(1)
C(18)	8995(3)	6343(2)	6401(2)	31(1)
C(19)	8760(2)	6086(2)	5173(2)	27(1)
C(20)	9380(2)	5912(2)	4912(2)	31(1)
C(21)	9386(3)	5407(2)	4693(2)	32(1)
C(22)	8761(3)	5061(2)	4734(2)	42(1)
C(23)	8121(3)	5228(2)	4974(2)	47(1)
C(24)	8120(3)	5733(2)	5193(2)	42(1)
C(25)	5630(2)	6571(2)	5151(1)	24(1)
C(26)	4832(2)	6671(2)	5202(2)	28(1)
C(27)	4547(3)	6807(2)	5643(2)	33(1)
C(28)	5050(3)	6824(2)	6040(2)	40(1)
C(29)	5836(3)	6716(2)	6005(2)	45(1)
C(30)	6122(3)	6599(2)	5563(2)	34(1)
C(31)	6043(2)	5674(2)	4427(2)	23(1)
C(32)	6173(3)	5501(2)	3965(2)	37(1)
C(33)	6222(3)	4955(2)	3855(2)	47(1)
C(34)	6112(3)	4567(2)	4203(2)	40(1)
C(35)	5953(3)	4732(2)	4656(2)	45(1)
C(36)	5926(3)	5280(2)	4768(2)	35(1)
C(37)	4798(2)	7058(2)	3264(2)	26(1)
C(38)	4768(2)	7446(2)	2895(2)	36(1)
C(39)	4525(3)	7307(2)	2428(2)	44(1)
C(40)	4292(3)	6786(2)	2322(2)	43(1)
C(41)	4314(3)	6398(2)	2679(2)	40(1)
C(42)	4570(2)	6533(2)	3143(2)	29(1)
C(43)	4371(2)	7523(2)	4258(2)	26(1)

C(44)	3603(2)	7341(2)	4218(2)	29(1)
C(45)	3050(3)	7510(2)	4536(2)	35(1)
C(46)	3265(3)	7865(2)	4898(2)	41(1)
C(47)	4028(3)	8051(2)	4947(2)	47(1)
C(48)	4569(3)	7886(2)	4628(2)	40(1)
C(49)	5195(2)	9306(2)	3659(2)	29(1)
C(50A)	4874(4)	9801(3)	3468(2)	35(2)
C(51A)	4109(4)	9808(3)	3267(3)	49(2)
C(52A)	3668(5)	9354(4)	3261(3)	42(2)
C(53A)	3950(4)	8890(3)	3461(3)	39(2)
C(54A)	4726(4)	8875(3)	3657(3)	31(2)
C(50B)	4900(11)	9547(9)	3268(7)	15(4)
C(51B)	4098(14)	9509(11)	3093(9)	29(5)
C(52B)	3600(10)	9134(9)	3317(6)	0(4)
C(53B)	3924(10)	8817(8)	3681(7)	5(4)
C(54B)	4667(10)	8861(7)	3872(8)	3(4)
C(55)	6348(3)	9810(2)	4407(2)	29(1)
C(56)	6773(3)	10285(2)	4379(2)	36(1)
C(57)	6829(3)	10660(2)	4751(2)	46(1)
C(58)	6460(4)	10568(2)	5161(2)	62(2)
C(59)	6034(6)	10108(3)	5200(2)	104(3)
C(60)	5981(5)	9728(3)	4833(2)	78(2)
C(61)	7991(2)	10034(2)	3015(1)	23(1)
C(62)	7659(3)	10539(2)	3081(1)	26(1)
C(63)	8048(3)	11015(2)	2980(2)	34(1)
C(64)	8786(3)	10988(2)	2798(2)	34(1)
C(65)	9126(3)	10495(2)	2723(2)	36(1)
C(66)	8738(3)	10021(2)	2835(2)	33(1)
C(67)	6984(2)	9133(2)	2550(1)	24(1)
C(68)	7219(2)	9306(2)	2105(2)	31(1)
C(69)	6872(3)	9117(2)	1680(2)	39(1)
C(70)	6269(3)	8745(2)	1686(2)	39(1)
C(71)	6017(3)	8566(2)	2124(2)	36(1)
C(72)	6369(2)	8755(2)	2548(2)	27(1)
C(73)	9732(2)	8273(2)	2342(1)	27(1)
C(74)	9437(3)	8776(2)	2187(2)	36(1)
C(75)	9926(3)	9204(2)	2089(2)	44(1)
C(76)	10731(3)	9139(2)	2145(2)	43(1)
C(77)	11042(3)	8652(2)	2299(2)	40(1)
C(78)	10550(2)	8222(2)	2392(2)	33(1)
C(79)	8456(2)	7458(2)	1961(1)	28(1)
C(80)	7682(3)	7633(2)	1873(2)	31(1)
C(81)	7217(3)	7431(2)	1495(2)	37(1)
C(82)	7511(3)	7050(2)	1193(2)	42(1)
C(83)	8279(3)	6873(2)	1269(2)	42(1)
C(84)	8738(3)	7076(2)	1651(2)	33(1)
C(85)	9907(2)	6163(2)	3058(2)	27(1)
C(86)	9521(3)	5945(2)	2650(2)	39(1)
C(87)	9408(3)	5392(2)	2602(2)	47(1)
C(88)	9686(3)	5043(2)	2949(2)	43(1)
C(89)	10084(3)	5242(2)	3355(2)	43(1)
C(90)	10191(3)	5798(2)	3405(2)	37(1)
C(91)	11067(2)	7102(2)	3171(2)	28(1)
C(92)	11358(3)	7526(2)	3457(2)	37(1)
C(93)	12120(3)	7709(2)	3417(2)	50(2)
C(94)	12603(3)	7470(3)	3102(2)	59(2)
C(95)	12338(3)	7044(3)	2825(2)	60(2)
C(96)	11570(3)	6859(2)	2860(2)	43(1)
N(1)	8049(2)	6068(2)	3952(1)	33(1)
C(97)	7988(3)	5967(2)	3433(2)	33(1)
C(98)	7782(3)	6482(2)	3155(2)	32(1)
C(99)	6951(2)	6664(2)	3219(2)	31(1)
N(2)	6808(2)	7192(2)	2957(1)	30(1)
N(3)	7603(3)	8416(2)	5234(2)	70(2)
C(100)	8408(4)	8646(2)	5111(2)	57(2)
C(101)	8295(3)	9058(2)	4720(2)	53(2)
C(102)	9054(3)	9287(2)	4545(2)	62(2)
N(4)	9539(3)	8858(2)	4360(2)	55(1)
C(103)	2145(4)	9603(3)	1337(2)	62(2)
C(104)	1460(5)	9795(3)	1119(2)	73(2)
C(105)	1305(5)	10346(4)	1114(3)	84(2)
C(106)	1866(5)	10688(3)	1326(3)	90(3)
C(107)	2527(4)	10489(3)	1547(3)	93(3)
C(108)	2664(4)	9938(3)	1543(3)	80(2)
C(109)	1504(4)	9698(3)	4248(3)	74(2)
C(110)	1692(4)	9233(3)	4000(2)	73(2)
C(111)	1246(4)	9085(3)	3595(3)	73(2)

C(1A2)	677(4)	9440(3)	3426(3)	53(2)
C(1A3)	501(4)	9898(3)	3673(3)	54(2)
C(1A4)	936(5)	10030(3)	4085(3)	59(2)
C(1B2)	370(15)	9199(11)	3510(9)	41(6)
C(1B3)	84(17)	9635(12)	3778(10)	49(7)
C(1B4)	527(16)	9868(11)	4166(9)	44(6)
C(1A5)	1515(7)	6852(5)	1394(4)	64(3)
C(1A6)	942(7)	6656(5)	1094(4)	65(3)
C(1A7)	1014(7)	6110(5)	936(4)	78(3)
C(1A8)	1691(7)	5813(5)	1067(4)	78(3)
C(1A9)	2266(8)	6039(5)	1373(5)	73(4)
C(12A)	2173(7)	6572(5)	1522(4)	71(3)
C(1B5)	358(12)	6128(9)	894(7)	26(5)
C(1B6)	656(16)	6478(12)	654(10)	52(7)
C(1B7)	833(18)	6872(14)	872(12)	60(8)
C(1B8)	1050(16)	7008(11)	1340(9)	43(6)
C(1B9)	671(19)	6638(14)	1571(12)	65(8)
C(12B)	340(20)	6125(15)	1368(13)	73(9)
C(1C5)	3170(20)	5989(15)	1519(13)	75(10)
C(1C6)	3740(20)	5639(16)	1672(14)	82(10)
C(1C7)	3540(18)	5241(13)	2010(11)	60(8)
C(1C8)	2840(20)	5295(15)	2207(13)	75(10)
C(1C9)	2410(40)	5860(30)	1990(20)	150(20)
C(12C)	2610(30)	6046(19)	1514(17)	88(13)

Table 4. Bond lengths [Å] and angles [°] for sh2330a.

Al(1)-O(16)	1.720(3)
Al(1)-O(5)	1.737(3)
Al(1)-O(1)	1.742(3)
Al(1)-O(4)	1.802(3)
Al(2)-O(8)	1.743(3)
Al(2)-O(1)	1.744(3)
Al(2)-O(7)	1.749(3)
Al(2)-O(2)	1.782(3)
Al(3)-O(10)	1.717(3)
Al(3)-O(11)	1.722(3)
Al(3)-O(3)	1.774(3)
Al(3)-O(2)	1.778(3)
Al(4)-O(14)	1.713(3)
Al(4)-O(13)	1.727(3)
Al(4)-O(3)	1.776(3)
Al(4)-O(4)	1.777(3)
Si(1)-O(5)	1.598(3)
Si(1)-O(6)	1.637(3)
Si(1)-C(7)	1.874(4)
Si(1)-C(1)	1.876(4)
Si(2)-O(7)	1.611(3)
Si(2)-O(6)	1.633(3)
Si(2)-C(13)	1.874(4)
Si(2)-C(19)	1.881(5)
Si(3)-O(8)	1.610(3)
Si(3)-O(9)	1.633(3)
Si(3)-C(25)	1.868(4)
Si(3)-C(31)	1.876(4)
Si(4)-O(10)	1.592(3)
Si(4)-O(9)	1.639(3)
Si(4)-C(43)	1.869(4)
Si(4)-C(37)	1.875(4)
Si(5)-O(11)	1.596(3)
Si(5)-O(12)	1.637(3)
Si(5)-C(55)	1.861(4)
Si(5)-C(49)	1.876(4)
Si(6)-O(13)	1.607(3)
Si(6)-O(12)	1.629(3)
Si(6)-C(61)	1.873(4)
Si(6)-C(67)	1.885(4)
Si(7)-O(14)	1.603(3)
Si(7)-O(15)	1.636(3)
Si(7)-C(79)	1.873(4)
Si(7)-C(73)	1.874(5)
Si(8)-O(16)	1.599(3)
Si(8)-O(15)	1.634(3)
Si(8)-C(85)	1.869(5)
Si(8)-C(91)	1.871(4)
C(1)-C(6)	1.390(6)
C(1)-C(2)	1.397(6)
C(2)-C(3)	1.387(6)
C(3)-C(4)	1.375(7)
C(4)-C(5)	1.379(7)
C(5)-C(6)	1.389(7)
C(7)-C(12)	1.393(6)
C(7)-C(8)	1.402(6)
C(8)-C(9)	1.393(7)
C(9)-C(10)	1.375(8)
C(10)-C(11)	1.382(7)
C(11)-C(12)	1.386(6)
C(13)-C(14)	1.394(6)
C(13)-C(18)	1.400(6)
C(14)-C(15)	1.402(6)
C(15)-C(16)	1.387(6)
C(16)-C(17)	1.381(7)
C(17)-C(18)	1.384(6)
C(19)-C(20)	1.388(6)
C(19)-C(24)	1.403(6)
C(20)-C(21)	1.391(6)
C(21)-C(22)	1.378(7)
C(22)-C(23)	1.377(7)
C(23)-C(24)	1.390(7)
C(25)-C(30)	1.394(6)
C(25)-C(26)	1.401(6)
C(26)-C(27)	1.394(6)

C(27)-C(28)	1.372(7)
C(28)-C(29)	1.379(7)
C(29)-C(30)	1.384(6)
C(31)-C(36)	1.387(6)
C(31)-C(32)	1.393(6)
C(32)-C(33)	1.386(7)
C(33)-C(34)	1.386(7)
C(34)-C(35)	1.374(7)
C(35)-C(36)	1.390(7)
C(37)-C(42)	1.391(6)
C(37)-C(38)	1.409(6)
C(38)-C(39)	1.393(7)
C(39)-C(40)	1.376(8)
C(40)-C(41)	1.383(7)
C(41)-C(42)	1.392(6)
C(43)-C(44)	1.387(6)
C(43)-C(48)	1.399(6)
C(44)-C(45)	1.395(6)
C(45)-C(46)	1.377(7)
C(46)-C(47)	1.383(7)
C(47)-C(48)	1.381(7)
C(49)-C(50B)	1.32(2)
C(49)-C(54A)	1.333(8)
C(49)-C(50A)	1.432(8)
C(49)-C(54B)	1.562(19)
C(50A)-C(51A)	1.396(10)
C(51A)-C(52A)	1.350(12)
C(52A)-C(53A)	1.353(11)
C(53A)-C(54A)	1.411(10)
C(50B)-C(51B)	1.43(3)
C(51B)-C(52B)	1.43(3)
C(52B)-C(53B)	1.38(3)
C(53B)-C(54B)	1.36(3)
C(55)-C(56)	1.385(6)
C(55)-C(60)	1.392(7)
C(56)-C(57)	1.393(7)
C(57)-C(58)	1.359(8)
C(58)-C(59)	1.357(10)
C(59)-C(60)	1.392(9)
C(61)-C(62)	1.386(6)
C(61)-C(66)	1.398(6)
C(62)-C(63)	1.386(6)
C(63)-C(64)	1.387(7)
C(64)-C(65)	1.371(7)
C(65)-C(66)	1.390(6)
C(67)-C(68)	1.398(6)
C(67)-C(72)	1.406(6)
C(68)-C(69)	1.385(6)
C(69)-C(70)	1.383(7)
C(70)-C(71)	1.394(7)
C(71)-C(72)	1.384(6)
C(73)-C(74)	1.400(6)
C(73)-C(78)	1.404(6)
C(74)-C(75)	1.384(7)
C(75)-C(76)	1.385(7)
C(76)-C(77)	1.375(7)
C(77)-C(78)	1.390(7)
C(79)-C(84)	1.386(6)
C(79)-C(80)	1.403(6)
C(80)-C(81)	1.384(6)
C(81)-C(82)	1.380(7)
C(82)-C(83)	1.390(7)
C(83)-C(84)	1.387(6)
C(85)-C(90)	1.397(6)
C(85)-C(86)	1.398(6)
C(86)-C(87)	1.385(7)
C(87)-C(88)	1.366(7)
C(88)-C(89)	1.384(7)
C(89)-C(90)	1.390(7)
C(91)-C(96)	1.392(6)
C(91)-C(92)	1.395(7)
C(92)-C(93)	1.390(6)
C(93)-C(94)	1.373(9)
C(94)-C(95)	1.370(9)
C(95)-C(96)	1.399(7)
N(1)-C(97)	1.472(6)
C(97)-C(98)	1.525(6)

C(98)-C(99)	1.509(6)
C(99)-N(2)	1.511(6)
N(3)-C(100)	1.545(8)
C(100)-C(101)	1.499(8)
C(101)-C(102)	1.519(8)
C(102)-N(4)	1.460(7)
C(103)-C(108)	1.323(9)
C(103)-C(104)	1.377(9)
C(104)-C(105)	1.386(10)
C(105)-C(106)	1.388(11)
C(106)-C(107)	1.353(11)
C(107)-C(108)	1.382(9)
C(109)-C(1A4)	1.334(10)
C(109)-C(110)	1.387(9)
C(109)-C(1B4)	1.73(3)
C(110)-C(111)	1.384(9)
C(111)-C(1A2)	1.375(10)
C(111)-C(1B2)	1.53(3)
C(1A2)-C(1A3)	1.368(10)
C(1A3)-C(1A4)	1.378(10)
C(1B2)-C(1B3)	1.42(4)
C(1B3)-C(1B4)	1.41(4)
C(1A5)-C(1A6)	1.347(15)
C(1A5)-C(12A)	1.354(15)
C(1A6)-C(1A7)	1.426(16)
C(1A7)-C(1A8)	1.405(16)
C(1A8)-C(1A9)	1.388(17)
C(1A9)-C(12A)	1.392(17)
C(1B5)-C(1B6)	1.22(3)
C(1B5)-C(12B)	1.33(4)
C(1B5)-C(1B7)	2.01(4)
C(1B6)-C(1B7)	1.18(4)
C(1B7)-C(1B8)	1.39(4)
C(1B8)-C(1B9)	1.31(4)
C(1B9)-C(12B)	1.49(5)
C(1C5)-C(12C)	0.97(5)
C(1C5)-C(1C6)	1.35(5)
C(1C5)-C(1C9)	1.92(8)
C(1C6)-C(1C7)	1.42(5)
C(1C7)-C(1C8)	1.35(4)
C(1C8)-C(1C9)	1.68(7)
C(1C9)-C(12C)	1.46(7)

O(16)-Al(1)-O(5)	111.51(14)
O(16)-Al(1)-O(1)	108.71(14)
O(5)-Al(1)-O(1)	112.69(14)
O(16)-Al(1)-O(4)	110.01(14)
O(5)-Al(1)-O(4)	103.67(14)
O(1)-Al(1)-O(4)	110.17(13)
O(8)-Al(2)-O(1)	107.18(14)
O(8)-Al(2)-O(7)	112.87(14)
O(1)-Al(2)-O(7)	109.94(13)
O(8)-Al(2)-O(2)	109.37(13)
O(1)-Al(2)-O(2)	109.89(13)
O(7)-Al(2)-O(2)	107.58(14)
O(10)-Al(3)-O(11)	113.57(15)
O(10)-Al(3)-O(3)	104.24(14)
O(11)-Al(3)-O(3)	111.17(14)
O(10)-Al(3)-O(2)	111.20(14)
O(11)-Al(3)-O(2)	107.24(14)
O(3)-Al(3)-O(2)	109.41(13)
O(14)-Al(4)-O(13)	116.27(15)
O(14)-Al(4)-O(3)	105.34(14)
O(13)-Al(4)-O(3)	109.20(13)
O(14)-Al(4)-O(4)	109.70(14)
O(13)-Al(4)-O(4)	109.19(14)
O(3)-Al(4)-O(4)	106.68(13)
O(5)-Si(1)-O(6)	113.14(15)
O(5)-Si(1)-C(7)	110.36(17)
O(6)-Si(1)-C(7)	107.42(17)
O(5)-Si(1)-C(1)	108.43(17)
O(6)-Si(1)-C(1)	105.97(17)
C(7)-Si(1)-C(1)	111.47(18)
O(7)-Si(2)-O(6)	112.61(15)
O(7)-Si(2)-C(13)	108.51(17)
O(6)-Si(2)-C(13)	107.28(16)
O(7)-Si(2)-C(19)	111.27(17)

O(6)-Si(2)-C(19)	107.51(17)
C(13)-Si(2)-C(19)	109.55(19)
O(8)-Si(3)-O(9)	111.40(15)
O(8)-Si(3)-C(25)	111.20(17)
O(9)-Si(3)-C(25)	109.41(17)
O(8)-Si(3)-C(31)	108.10(16)
O(9)-Si(3)-C(31)	104.12(16)
C(25)-Si(3)-C(31)	112.41(18)
O(10)-Si(4)-O(9)	112.47(15)
O(10)-Si(4)-C(43)	109.76(18)
O(9)-Si(4)-C(43)	106.93(17)
O(10)-Si(4)-C(37)	108.95(17)
O(9)-Si(4)-C(37)	105.12(17)
C(43)-Si(4)-C(37)	113.59(18)
O(11)-Si(5)-O(12)	112.83(15)
O(11)-Si(5)-C(55)	109.91(17)
O(12)-Si(5)-C(55)	106.24(18)
O(11)-Si(5)-C(49)	109.96(18)
O(12)-Si(5)-C(49)	107.54(17)
C(55)-Si(5)-C(49)	110.26(19)
O(13)-Si(6)-O(12)	112.68(15)
O(13)-Si(6)-C(61)	109.74(17)
O(12)-Si(6)-C(61)	106.52(17)
O(13)-Si(6)-C(67)	110.74(16)
O(12)-Si(6)-C(67)	107.82(17)
C(61)-Si(6)-C(67)	109.21(18)
O(14)-Si(7)-O(15)	113.24(15)
O(14)-Si(7)-C(79)	107.30(17)
O(15)-Si(7)-C(79)	105.88(18)
O(14)-Si(7)-C(73)	109.97(17)
O(15)-Si(7)-C(73)	107.89(17)
C(79)-Si(7)-C(73)	112.59(19)
O(16)-Si(8)-O(15)	112.24(15)
O(16)-Si(8)-C(85)	110.52(17)
O(15)-Si(8)-C(85)	106.33(17)
O(16)-Si(8)-C(91)	110.71(17)
O(15)-Si(8)-C(91)	107.24(17)
C(85)-Si(8)-C(91)	109.65(19)
Al(1)-O(1)-Al(2)	133.32(17)
Al(3)-O(2)-Al(2)	127.55(16)
Al(3)-O(3)-Al(4)	132.42(16)
Al(4)-O(4)-Al(1)	127.94(16)
Si(1)-O(5)-Al(1)	150.51(19)
Si(2)-O(6)-Si(1)	147.18(19)
Si(2)-O(7)-Al(2)	131.54(18)
Si(3)-O(8)-Al(2)	151.34(19)
Si(3)-O(9)-Si(4)	142.33(18)
Si(4)-O(10)-Al(3)	162.0(2)
Si(5)-O(11)-Al(3)	151.6(2)
Si(6)-O(12)-Si(5)	147.62(19)
Si(6)-O(13)-Al(4)	138.87(18)
Si(7)-O(14)-Al(4)	154.97(19)
Si(8)-O(15)-Si(7)	145.77(18)
Si(8)-O(16)-Al(1)	164.3(2)
C(6)-C(1)-C(2)	116.8(4)
C(6)-C(1)-Si(1)	122.4(3)
C(2)-C(1)-Si(1)	120.6(3)
C(3)-C(2)-C(1)	121.6(4)
C(4)-C(3)-C(2)	120.2(5)
C(3)-C(4)-C(5)	119.5(4)
C(4)-C(5)-C(6)	120.0(5)
C(5)-C(6)-C(1)	121.8(4)
C(12)-C(7)-C(8)	117.6(4)
C(12)-C(7)-Si(1)	121.4(3)
C(8)-C(7)-Si(1)	120.9(3)
C(9)-C(8)-C(7)	120.7(5)
C(10)-C(9)-C(8)	120.4(5)
C(9)-C(10)-C(11)	119.7(5)
C(10)-C(11)-C(12)	120.2(5)
C(11)-C(12)-C(7)	121.3(4)
C(14)-C(13)-C(18)	117.1(4)
C(14)-C(13)-Si(2)	121.1(3)
C(18)-C(13)-Si(2)	121.8(3)
C(13)-C(14)-C(15)	121.6(4)
C(16)-C(15)-C(14)	119.3(4)
C(17)-C(16)-C(15)	120.3(4)
C(16)-C(17)-C(18)	119.7(4)

C(17)-C(18)-C(13)	122.0(4)
C(20)-C(19)-C(24)	116.5(4)
C(20)-C(19)-Si(2)	123.1(3)
C(24)-C(19)-Si(2)	120.2(3)
C(19)-C(20)-C(21)	122.3(4)
C(22)-C(21)-C(20)	119.7(4)
C(23)-C(22)-C(21)	119.6(5)
C(22)-C(23)-C(24)	120.3(5)
C(23)-C(24)-C(19)	121.4(5)
C(30)-C(25)-C(26)	117.2(4)
C(30)-C(25)-Si(3)	121.1(3)
C(26)-C(25)-Si(3)	121.7(3)
C(27)-C(26)-C(25)	121.3(4)
C(28)-C(27)-C(26)	119.6(4)
C(27)-C(28)-C(29)	120.5(4)
C(28)-C(29)-C(30)	119.7(5)
C(29)-C(30)-C(25)	121.7(4)
C(36)-C(31)-C(32)	117.4(4)
C(36)-C(31)-Si(3)	123.4(3)
C(32)-C(31)-Si(3)	119.2(3)
C(33)-C(32)-C(31)	121.3(5)
C(32)-C(33)-C(34)	120.4(5)
C(35)-C(34)-C(33)	119.0(5)
C(34)-C(35)-C(36)	120.4(5)
C(31)-C(36)-C(35)	121.5(5)
C(42)-C(37)-C(38)	117.2(4)
C(42)-C(37)-Si(4)	121.6(3)
C(38)-C(37)-Si(4)	121.1(4)
C(39)-C(38)-C(37)	121.2(5)
C(40)-C(39)-C(38)	120.2(5)
C(39)-C(40)-C(41)	119.6(5)
C(40)-C(41)-C(42)	120.5(5)
C(37)-C(42)-C(41)	121.3(4)
C(44)-C(43)-C(48)	117.2(4)
C(44)-C(43)-Si(4)	122.5(3)
C(48)-C(43)-Si(4)	119.8(3)
C(43)-C(44)-C(45)	121.5(4)
C(46)-C(45)-C(44)	119.8(4)
C(45)-C(46)-C(47)	119.9(4)
C(48)-C(47)-C(46)	119.8(5)
C(47)-C(48)-C(43)	121.7(4)
C(50B)-C(49)-C(54A)	98.8(10)
C(50B)-C(49)-C(50A)	35.3(9)
C(54A)-C(49)-C(50A)	117.5(5)
C(50B)-C(49)-C(54B)	115.5(12)
C(54A)-C(49)-C(54B)	22.9(7)
C(50A)-C(49)-C(54B)	121.7(7)
C(50B)-C(49)-Si(5)	128.6(9)
C(54A)-C(49)-Si(5)	124.2(4)
C(50A)-C(49)-Si(5)	118.3(4)
C(54B)-C(49)-Si(5)	114.4(7)
C(51A)-C(50A)-C(49)	119.6(6)
C(52A)-C(51A)-C(50A)	120.3(8)
C(51A)-C(52A)-C(53A)	120.8(8)
C(52A)-C(53A)-C(54A)	119.4(7)
C(49)-C(54A)-C(53A)	122.2(6)
C(49)-C(50B)-C(51B)	124.8(19)
C(52B)-C(51B)-C(50B)	118(2)
C(53B)-C(52B)-C(51B)	117.9(18)
C(54B)-C(53B)-C(52B)	125.4(19)
C(53B)-C(54B)-C(49)	116.9(16)
C(56)-C(55)-C(60)	115.7(5)
C(56)-C(55)-Si(5)	123.9(3)
C(60)-C(55)-Si(5)	120.4(4)
C(55)-C(56)-C(57)	122.5(5)
C(58)-C(57)-C(56)	120.3(5)
C(59)-C(58)-C(57)	118.9(5)
C(58)-C(59)-C(60)	121.4(6)
C(59)-C(60)-C(55)	121.3(6)
C(62)-C(61)-C(66)	117.2(4)
C(62)-C(61)-Si(6)	123.4(3)
C(66)-C(61)-Si(6)	119.3(3)
C(61)-C(62)-C(63)	122.1(4)
C(62)-C(63)-C(64)	119.4(4)
C(65)-C(64)-C(63)	119.9(4)
C(64)-C(65)-C(66)	120.2(4)
C(65)-C(66)-C(61)	121.2(4)

C(68)-C(67)-C(72)	116.6(4)
C(68)-C(67)-Si(6)	122.1(3)
C(72)-C(67)-Si(6)	121.3(3)
C(69)-C(68)-C(67)	122.4(4)
C(70)-C(69)-C(68)	119.9(4)
C(69)-C(70)-C(71)	119.3(4)
C(72)-C(71)-C(70)	120.4(4)
C(71)-C(72)-C(67)	121.4(4)
C(74)-C(73)-C(78)	116.9(4)
C(74)-C(73)-Si(7)	120.5(3)
C(78)-C(73)-Si(7)	122.6(4)
C(75)-C(74)-C(73)	121.8(4)
C(74)-C(75)-C(76)	119.7(5)
C(77)-C(76)-C(75)	120.2(5)
C(76)-C(77)-C(78)	120.0(5)
C(77)-C(78)-C(73)	121.4(5)
C(84)-C(79)-C(80)	117.1(4)
C(84)-C(79)-Si(7)	122.6(3)
C(80)-C(79)-Si(7)	120.2(3)
C(81)-C(80)-C(79)	121.5(4)
C(82)-C(81)-C(80)	120.2(4)
C(81)-C(82)-C(83)	119.4(4)
C(84)-C(83)-C(82)	119.8(5)
C(79)-C(84)-C(83)	121.9(4)
C(90)-C(85)-C(86)	116.9(4)
C(90)-C(85)-Si(8)	120.5(3)
C(86)-C(85)-Si(8)	122.6(4)
C(87)-C(86)-C(85)	121.2(5)
C(88)-C(87)-C(86)	120.8(5)
C(87)-C(88)-C(89)	119.9(5)
C(88)-C(89)-C(90)	119.4(5)
C(89)-C(90)-C(85)	121.9(5)
C(96)-C(91)-C(92)	118.1(4)
C(96)-C(91)-Si(8)	120.4(4)
C(92)-C(91)-Si(8)	121.3(3)
C(93)-C(92)-C(91)	120.4(5)
C(94)-C(93)-C(92)	120.6(6)
C(95)-C(94)-C(93)	120.1(5)
C(94)-C(95)-C(96)	119.8(5)
C(91)-C(96)-C(95)	121.0(5)
N(1)-C(97)-C(98)	111.4(4)
C(99)-C(98)-C(97)	112.5(4)
C(98)-C(99)-N(2)	109.2(4)
C(101)-C(100)-N(3)	109.3(5)
C(100)-C(101)-C(102)	114.1(5)
N(4)-C(102)-C(101)	110.7(5)
C(108)-C(103)-C(104)	120.9(7)
C(103)-C(104)-C(105)	120.1(8)
C(104)-C(105)-C(106)	117.7(7)
C(107)-C(106)-C(105)	121.1(7)
C(106)-C(107)-C(108)	119.5(8)
C(103)-C(108)-C(107)	120.6(8)
C(1A4)-C(109)-C(110)	121.4(7)
C(1A4)-C(109)-C(1B4)	28.6(9)
C(110)-C(109)-C(1B4)	112.5(11)
C(111)-C(110)-C(109)	119.7(7)
C(1A2)-C(111)-C(110)	117.7(7)
C(1A2)-C(111)-C(1B2)	32.9(10)
C(110)-C(111)-C(1B2)	124.9(11)
C(1A3)-C(1A2)-C(111)	121.6(7)
C(1A2)-C(1A3)-C(1A4)	119.6(7)
C(109)-C(1A4)-C(1A3)	119.6(8)
C(1B3)-C(1B2)-C(111)	115(2)
C(1B4)-C(1B3)-C(1B2)	122(3)
C(1B3)-C(1B4)-C(109)	119(2)
C(1A6)-C(1A5)-C(12A)	123.3(12)
C(1A5)-C(1A6)-C(1A7)	117.5(12)
C(1A8)-C(1A7)-C(1A6)	119.8(12)
C(1A9)-C(1A8)-C(1A7)	119.9(12)
C(1A8)-C(1A9)-C(12A)	118.6(13)
C(1A5)-C(12A)-C(1A9)	120.7(12)
C(1B6)-C(1B5)-C(12B)	126(3)
C(1B6)-C(1B5)-C(1B7)	32.5(17)
C(12B)-C(1B5)-C(1B7)	94(2)
C(1B7)-C(1B6)-C(1B5)	114(3)
C(1B6)-C(1B7)-C(1B8)	138(4)
C(1B6)-C(1B7)-C(1B5)	33.8(18)

C(1B8)-C(1B7)-C(1B5)	106(2)
C(1B9)-C(1B8)-C(1B7)	101(3)
C(1B8)-C(1B9)-C(12B)	126(3)
C(1B5)-C(12B)-C(1B9)	110(3)
C(12C)-C(1C5)-C(1C6)	142(5)
C(12C)-C(1C5)-C(1C9)	48(4)
C(1C6)-C(1C5)-C(1C9)	100(3)
C(1C5)-C(1C6)-C(1C7)	118(3)
C(1C8)-C(1C7)-C(1C6)	117(3)
C(1C7)-C(1C8)-C(1C9)	108(4)
C(12C)-C(1C9)-C(1C8)	118(5)
C(12C)-C(1C9)-C(1C5)	29(3)
C(1C8)-C(1C9)-C(1C5)	95(4)
C(1C5)-C(12C)-C(1C9)	103(6)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2330a. 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}
Al(1)	15(1)	20(1)	19(1)	-1(1)	0(1)	-1(1)
Al(2)	17(1)	20(1)	19(1)	1(1)	0(1)	-2(1)
Al(3)	17(1)	18(1)	24(1)	3(1)	2(1)	0(1)
Al(4)	18(1)	18(1)	19(1)	-1(1)	1(1)	-1(1)
Si(1)	18(1)	27(1)	22(1)	0(1)	-3(1)	-4(1)
Si(2)	21(1)	24(1)	22(1)	3(1)	0(1)	-3(1)
Si(3)	19(1)	19(1)	22(1)	2(1)	2(1)	-3(1)
Si(4)	17(1)	24(1)	27(1)	4(1)	-1(1)	-2(1)
Si(5)	23(1)	20(1)	23(1)	0(1)	6(1)	3(1)
Si(6)	21(1)	19(1)	19(1)	1(1)	3(1)	-2(1)
Si(7)	21(1)	30(1)	19(1)	-5(1)	0(1)	2(1)
Si(8)	17(1)	27(1)	23(1)	-4(1)	1(1)	2(1)
O(1)	18(1)	20(2)	24(1)	2(1)	0(1)	-1(1)
O(2)	21(1)	21(2)	24(2)	3(1)	3(1)	-1(1)
O(3)	18(1)	20(2)	23(1)	1(1)	-1(1)	-1(1)
O(4)	20(1)	23(2)	19(1)	1(1)	1(1)	0(1)
O(5)	20(1)	28(2)	23(2)	-1(1)	0(1)	-3(1)
O(6)	24(2)	29(2)	24(2)	1(1)	-1(1)	-4(1)
O(7)	25(1)	24(2)	23(2)	2(1)	1(1)	-2(1)
O(8)	22(1)	23(2)	27(2)	2(1)	0(1)	-2(1)
O(9)	20(1)	23(2)	26(2)	1(1)	0(1)	-3(1)
O(10)	20(1)	27(2)	40(2)	8(1)	-3(1)	-3(1)
O(11)	25(2)	23(2)	29(2)	2(1)	7(1)	2(1)
O(12)	30(2)	22(2)	23(2)	1(1)	6(1)	0(1)
O(13)	23(1)	21(2)	22(2)	0(1)	1(1)	-2(1)
O(14)	22(1)	32(2)	23(2)	-4(1)	-1(1)	4(1)
O(15)	23(1)	30(2)	22(2)	-7(1)	2(1)	5(1)
O(16)	20(1)	26(2)	26(2)	-2(1)	1(1)	0(1)
C(1)	20(2)	28(2)	26(2)	0(2)	-9(2)	-1(2)
C(2)	29(2)	35(3)	29(2)	4(2)	-7(2)	-5(2)
C(3)	35(3)	29(3)	49(3)	6(2)	-15(2)	-9(2)
C(4)	45(3)	29(3)	45(3)	-10(2)	-16(2)	-2(2)
C(5)	44(3)	48(3)	36(3)	-15(2)	-1(2)	-1(2)
C(6)	30(2)	39(3)	28(2)	-1(2)	-1(2)	-5(2)
C(7)	19(2)	23(2)	33(2)	4(2)	-2(2)	-5(2)
C(8)	28(2)	44(3)	32(3)	8(2)	-1(2)	-4(2)
C(9)	28(3)	48(3)	61(4)	18(3)	-8(2)	3(2)
C(10)	26(2)	31(3)	80(4)	5(3)	7(3)	4(2)
C(11)	27(2)	42(3)	60(3)	-11(3)	3(2)	1(2)
C(12)	22(2)	42(3)	32(2)	-3(2)	0(2)	-1(2)
C(13)	24(2)	24(2)	25(2)	4(2)	-1(2)	-6(2)
C(14)	28(2)	31(3)	26(2)	4(2)	-1(2)	-1(2)
C(15)	34(2)	40(3)	29(2)	2(2)	4(2)	-1(2)
C(16)	39(3)	44(3)	22(2)	6(2)	-2(2)	-12(2)
C(17)	37(3)	36(3)	30(2)	10(2)	-8(2)	0(2)
C(18)	29(2)	35(3)	29(2)	5(2)	1(2)	2(2)
C(19)	24(2)	27(2)	28(2)	4(2)	-4(2)	-1(2)
C(20)	25(2)	30(3)	36(3)	5(2)	-1(2)	-2(2)
C(21)	34(2)	29(3)	34(3)	1(2)	-2(2)	9(2)
C(22)	40(3)	27(3)	58(3)	-5(2)	-6(2)	5(2)
C(23)	38(3)	31(3)	72(4)	5(3)	2(3)	-4(2)
C(24)	34(3)	28(3)	64(3)	2(2)	10(2)	-2(2)
C(25)	26(2)	18(2)	26(2)	1(2)	3(2)	-3(2)
C(26)	27(2)	29(2)	30(2)	4(2)	3(2)	-3(2)
C(27)	32(2)	33(3)	36(3)	4(2)	14(2)	1(2)
C(28)	53(3)	42(3)	27(3)	0(2)	14(2)	6(2)
C(29)	50(3)	63(4)	23(2)	2(2)	1(2)	2(3)
C(30)	30(2)	40(3)	30(2)	0(2)	2(2)	1(2)
C(31)	15(2)	22(2)	32(2)	0(2)	-1(2)	-4(2)
C(32)	38(3)	34(3)	40(3)	-2(2)	4(2)	-7(2)
C(33)	43(3)	41(3)	58(3)	-17(3)	8(3)	-9(2)
C(34)	36(3)	19(2)	66(4)	-6(2)	2(2)	-3(2)
C(35)	44(3)	32(3)	57(3)	11(3)	1(2)	-2(2)
C(36)	35(2)	30(3)	40(3)	3(2)	2(2)	-3(2)
C(37)	13(2)	37(3)	28(2)	9(2)	2(2)	1(2)
C(38)	24(2)	46(3)	39(3)	12(2)	-2(2)	1(2)
C(39)	24(2)	69(4)	38(3)	18(3)	4(2)	10(2)
C(40)	26(2)	79(4)	25(2)	-5(3)	2(2)	15(3)
C(41)	27(2)	54(3)	39(3)	-15(2)	1(2)	10(2)
C(42)	22(2)	37(3)	27(2)	-2(2)	5(2)	4(2)
C(43)	25(2)	20(2)	32(2)	2(2)	-1(2)	2(2)

C(44)	26(2)	29(2)	34(2)	1(2)	5(2)	-1(2)
C(45)	28(2)	36(3)	42(3)	3(2)	7(2)	0(2)
C(46)	42(3)	36(3)	47(3)	-3(2)	16(2)	9(2)
C(47)	47(3)	40(3)	54(3)	-18(3)	5(3)	6(2)
C(48)	30(2)	31(3)	58(3)	-12(2)	-1(2)	-1(2)
C(49)	28(2)	39(3)	21(2)	0(2)	8(2)	5(2)
C(55)	38(2)	24(2)	25(2)	2(2)	4(2)	11(2)
C(56)	37(3)	35(3)	38(3)	-10(2)	2(2)	1(2)
C(57)	45(3)	38(3)	52(3)	-17(3)	-9(2)	4(2)
C(58)	103(5)	46(4)	37(3)	-16(3)	-5(3)	14(3)
C(59)	217(10)	60(5)	41(4)	-14(3)	60(5)	-12(6)
C(60)	154(7)	44(4)	41(3)	-6(3)	47(4)	-20(4)
C(61)	26(2)	23(2)	20(2)	2(2)	-3(2)	-4(2)
C(62)	32(2)	24(2)	22(2)	0(2)	0(2)	-1(2)
C(63)	50(3)	22(2)	29(2)	4(2)	-7(2)	-2(2)
C(64)	41(3)	29(3)	30(2)	11(2)	-11(2)	-14(2)
C(65)	30(2)	38(3)	42(3)	9(2)	2(2)	-10(2)
C(66)	31(2)	26(2)	40(3)	6(2)	2(2)	-3(2)
C(67)	23(2)	22(2)	26(2)	-1(2)	-1(2)	3(2)
C(68)	26(2)	41(3)	25(2)	3(2)	1(2)	-1(2)
C(69)	37(3)	59(3)	20(2)	5(2)	1(2)	6(2)
C(70)	36(3)	52(3)	28(3)	-12(2)	-11(2)	13(2)
C(71)	29(2)	34(3)	44(3)	-6(2)	-9(2)	0(2)
C(72)	24(2)	26(2)	32(2)	3(2)	-1(2)	-1(2)
C(73)	28(2)	36(3)	16(2)	-7(2)	2(2)	0(2)
C(74)	36(3)	41(3)	32(3)	2(2)	2(2)	1(2)
C(75)	53(3)	38(3)	41(3)	5(2)	8(2)	0(2)
C(76)	46(3)	48(3)	35(3)	-4(2)	16(2)	-13(3)
C(77)	31(3)	55(3)	33(3)	-8(2)	9(2)	-8(2)
C(78)	29(2)	45(3)	25(2)	-4(2)	4(2)	2(2)
C(79)	28(2)	35(3)	20(2)	-1(2)	-1(2)	-2(2)
C(80)	34(2)	33(3)	25(2)	-2(2)	-4(2)	0(2)
C(81)	34(3)	43(3)	32(3)	4(2)	-12(2)	-4(2)
C(82)	46(3)	55(3)	25(2)	-5(2)	-7(2)	-17(3)
C(83)	46(3)	53(3)	27(3)	-13(2)	5(2)	-9(2)
C(84)	32(2)	45(3)	21(2)	-9(2)	3(2)	-2(2)
C(85)	20(2)	31(2)	31(2)	-5(2)	6(2)	2(2)
C(86)	44(3)	34(3)	37(3)	-8(2)	-1(2)	0(2)
C(87)	53(3)	37(3)	49(3)	-17(3)	-3(3)	-1(2)
C(88)	38(3)	26(3)	64(4)	-14(3)	9(2)	-1(2)
C(89)	38(3)	30(3)	60(3)	1(2)	-1(2)	6(2)
C(90)	32(2)	32(3)	47(3)	-6(2)	-5(2)	2(2)
C(91)	19(2)	38(3)	27(2)	7(2)	-1(2)	4(2)
C(92)	24(2)	48(3)	38(3)	6(2)	-3(2)	-6(2)
C(93)	29(3)	64(4)	56(3)	21(3)	-13(2)	-15(3)
C(94)	20(3)	91(5)	67(4)	45(4)	-5(3)	-10(3)
C(95)	28(3)	91(5)	61(4)	23(4)	15(3)	18(3)
C(96)	26(2)	56(3)	48(3)	5(3)	6(2)	14(2)
N(1)	30(2)	23(2)	44(2)	-1(2)	-12(2)	2(2)
C(97)	35(2)	30(3)	34(3)	-6(2)	1(2)	2(2)
C(98)	31(2)	40(3)	26(2)	-7(2)	1(2)	-4(2)
C(99)	28(2)	35(3)	29(2)	-8(2)	0(2)	-5(2)
N(2)	27(2)	31(2)	32(2)	-7(2)	-6(2)	0(2)
N(3)	104(4)	67(4)	38(3)	-21(3)	-5(3)	4(3)
C(100)	63(4)	56(4)	51(3)	-16(3)	-17(3)	-6(3)
C(101)	55(3)	39(3)	62(4)	-22(3)	-17(3)	10(3)
C(102)	55(4)	45(3)	82(4)	-21(3)	-20(3)	4(3)
N(4)	52(3)	43(3)	68(3)	-20(2)	-22(2)	0(2)
C(103)	86(5)	43(4)	62(4)	6(3)	39(4)	7(3)
C(104)	113(6)	64(5)	43(4)	-3(3)	10(4)	15(4)
C(105)	91(6)	98(6)	66(5)	28(4)	32(4)	30(5)
C(106)	78(5)	44(4)	156(8)	25(5)	79(5)	15(4)
C(107)	56(4)	57(5)	170(9)	-10(5)	42(5)	-15(4)
C(108)	60(4)	53(4)	129(7)	4(4)	33(4)	4(3)

sh2155

Table 1. Crystal data and structure refinement for sh2155.

Identification code	sh2155	
Empirical formula	C118 H136 Al4 N4 O20 Si8	
Formula weight	2262.95	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.251(3) Å	a= 86.90(3)°.
	b = 17.560(4) Å	b= 79.95(3)°.
	c = 22.629(5) Å	g = 77.38(3)°.
Volume	6586(2) $Å^3$	
Z	2	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	0.169 mm^{-1}	
F(000)	2392	
Crystal size	0.34 x 0.22 x 0.2 mm^3	
Theta range for data collection	1.88 to 24.10°.	
Index ranges	-19<=h<=19, -19<=k<=18, -25<=l<=25	
Reflections collected	38321	
Independent reflections	18906 [R(int) = 0.0886]	
Completeness to theta = 24.10°	90.4 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18906 / 0 / 1499	
Goodness-of-fit on F^2	1.536	
Final R indices [I>2sigma(I)]	R1 = 0.0970, wR2 = 0.2529	
R indices (all data)	R1 = 0.1592, wR2 = 0.2818	
Largest diff. peak and hole	0.753 and -0.474 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2155. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	8986(1)	8647(1)	2872(1)	42(1)
Al(2)	8973(1)	6940(1)	2522(1)	41(1)
Al(3)	7587(1)	7671(1)	1717(1)	45(1)
Al(4)	7489(1)	9377(1)	2154(1)	45(1)
Si(1)	10859(1)	8129(1)	2853(1)	47(1)
Si(2)	10894(1)	6439(1)	2527(1)	45(1)
Si(3)	8237(1)	5420(1)	2771(1)	45(1)
Si(4)	6884(1)	6108(1)	2032(1)	47(1)
Si(5)	7117(1)	8398(1)	478(1)	61(1)
Si(6)	6928(1)	10101(1)	935(1)	66(1)
Si(7)	6768(1)	10603(1)	3232(1)	53(1)
Si(8)	8238(1)	9993(1)	3846(1)	49(1)
O(1)	8725(2)	7740(2)	2994(2)	40(1)
O(2)	8606(2)	7242(3)	1828(2)	43(1)
O(3)	7179(2)	8503(2)	2145(2)	46(1)
O(4)	8531(2)	9170(3)	2255(2)	46(1)
O(5)	10016(2)	8577(3)	2663(2)	50(1)
O(6)	11165(2)	7255(3)	2578(2)	52(1)
O(7)	10004(2)	6575(3)	2367(2)	47(1)
O(8)	8521(2)	6203(2)	2871(2)	46(1)
O(9)	7353(2)	5642(3)	2564(2)	50(1)
O(10)	7007(2)	6983(3)	1936(2)	49(1)
O(11)	7638(2)	7893(3)	947(2)	53(1)
O(12)	7017(3)	9324(3)	543(2)	71(2)
O(13)	7410(2)	9922(3)	1488(2)	59(1)
O(14)	6926(2)	9916(3)	2764(2)	49(1)
O(15)	7280(2)	10324(3)	3782(2)	52(1)
O(16)	8610(2)	9192(3)	3506(2)	50(1)
C(1)	10755(4)	8044(4)	3694(3)	50(2)
C(2)	10261(4)	7590(4)	4037(3)	58(2)
C(3)	10193(4)	7504(5)	4639(4)	66(2)
C(4)	10611(4)	7895(5)	4952(4)	66(2)
C(5)	11074(5)	8357(6)	4638(4)	80(3)
C(6)	11156(4)	8430(5)	4018(4)	69(2)
C(7)	11712(4)	8615(4)	2547(3)	52(2)
C(8)	11634(4)	9424(5)	2520(4)	72(2)
C(9)	12298(5)	9749(6)	2301(4)	85(3)
C(10)	13036(5)	9293(6)	2120(4)	80(3)
C(11)	13131(4)	8509(6)	2155(4)	79(3)
C(12)	12480(4)	8154(5)	2361(3)	64(2)
C(13)	10990(4)	5884(4)	3252(3)	50(2)
C(14)	10377(4)	5574(5)	3604(4)	62(2)
C(15)	10466(5)	5195(5)	4147(4)	77(3)
C(16)	11189(5)	5103(6)	4365(4)	82(3)
C(17)	11787(6)	5410(6)	4047(5)	95(3)
C(18)	11703(4)	5795(5)	3495(4)	79(3)
C(19)	11651(4)	5879(4)	1937(3)	50(2)
C(20)	11587(5)	5152(6)	1815(4)	85(3)
C(21)	12166(7)	4697(6)	1374(5)	110(4)
C(22)	12791(6)	4986(8)	1088(5)	103(4)
C(23)	12863(5)	5709(8)	1201(5)	102(4)
C(24)	12300(4)	6143(5)	1619(3)	68(2)
C(25)	8976(4)	4783(4)	2202(3)	55(2)
C(26)	9360(6)	5073(6)	1678(5)	104(4)
C(27)	9877(7)	4590(7)	1251(5)	119(4)
C(28)	10023(6)	3809(6)	1339(5)	94(3)
C(29)	9595(9)	3513(7)	1808(6)	149(6)
C(30)	9094(8)	4000(6)	2240(6)	147(6)
C(31)	8107(4)	4818(4)	3474(3)	49(2)
C(32)	7389(5)	4603(5)	3704(4)	85(3)
C(33)	7308(6)	4129(6)	4217(5)	103(4)
C(34)	7938(7)	3830(6)	4512(4)	87(3)
C(35)	8648(7)	4026(5)	4297(5)	89(3)
C(36)	8735(5)	4518(5)	3786(4)	77(3)
C(37)	5799(4)	6080(4)	2288(4)	60(2)
C(38)	5242(4)	6315(6)	1895(5)	82(3)
C(39)	4445(5)	6289(7)	2032(6)	99(3)
C(40)	4169(6)	6014(7)	2586(8)	125(5)
C(41)	4685(6)	5774(7)	3008(6)	132(5)
C(42)	5505(5)	5808(6)	2849(5)	89(3)
C(43)	7254(4)	5537(5)	1334(4)	58(2)

C(44)	7145(6)	4790(6)	1339(5)	98(3)
C(45)	7455(10)	4334(7)	825(8)	153(6)
C(46)	7845(8)	4647(11)	318(6)	131(6)
C(47)	7925(7)	5380(9)	313(5)	114(4)
C(48)	7657(5)	5824(6)	811(4)	89(3)
C(49)	7643(4)	8202(5)	-318(3)	57(2)
C(50)	8280(5)	8556(6)	-565(4)	80(3)
C(51)	8678(6)	8452(6)	-1153(4)	90(3)
C(52)	8443(6)	7986(6)	-1515(5)	94(3)
C(53)	7808(6)	7619(6)	-1291(5)	98(3)
C(54)	7415(5)	7720(5)	-694(5)	77(3)
C(55)	6096(5)	8166(8)	567(4)	96(4)
C(56)	5384(5)	8796(10)	682(5)	155(7)
C(57)	4614(11)	8770(20)	697(9)	280(20)
C(58)	4513(10)	8110(20)	659(8)	205(14)
C(59)	5173(12)	7311(14)	500(8)	219(11)
C(60)	5992(7)	7440(11)	492(7)	171(8)
C(61)	7286(4)	10818(6)	381(4)	78(3)
C(62)	7487(5)	10716(6)	-230(4)	83(3)
C(63)	7716(5)	11287(8)	-635(5)	105(4)
C(64)	7737(6)	11991(9)	-430(7)	113(4)
C(65)	7560(7)	12122(7)	171(7)	122(4)
C(66)	7313(6)	11549(8)	592(5)	110(4)
C(67)	5824(4)	10492(5)	1193(4)	69(2)
C(68)	5423(4)	10406(5)	1755(4)	64(2)
C(69)	4593(4)	10635(5)	1911(4)	72(2)
C(70)	4124(5)	10932(6)	1494(5)	94(3)
C(71)	4501(7)	11006(11)	914(6)	197(9)
C(72)	5309(6)	10795(9)	778(5)	179(8)
C(73)	5679(4)	10829(4)	3608(4)	57(2)
C(74)	5089(4)	11227(6)	3279(4)	82(3)
C(75)	4282(5)	11382(7)	3512(5)	100(4)
C(76)	4059(5)	11179(6)	4096(6)	108(4)
C(77)	4617(6)	10807(7)	4447(5)	123(5)
C(78)	5432(5)	10637(5)	4188(5)	87(3)
C(79)	7004(4)	11523(5)	2873(4)	68(2)
C(80)	6680(6)	12236(5)	3176(5)	95(3)
C(81)	6885(8)	12917(7)	2923(8)	128(5)
C(82)	7388(11)	12917(10)	2408(9)	143(6)
C(83)	7706(9)	12223(11)	2090(7)	150(6)
C(84)	7513(6)	11564(7)	2330(5)	105(4)
C(85)	8805(4)	10753(4)	3548(3)	54(2)
C(86)	8503(4)	11539(5)	3705(4)	65(2)
C(87)	8886(5)	12124(5)	3471(4)	78(3)
C(88)	9590(5)	11956(6)	3076(4)	80(3)
C(89)	9904(5)	11200(6)	2910(5)	92(3)
C(90)	9513(4)	10598(5)	3143(4)	76(3)
C(91)	8260(4)	9851(4)	4673(3)	54(2)
C(92)	7559(5)	10048(5)	5100(4)	76(3)
C(93)	7611(7)	9954(7)	5714(5)	96(3)
C(94)	8354(7)	9669(6)	5899(5)	90(3)
C(95)	9037(6)	9480(6)	5486(5)	85(3)
C(96)	8990(5)	9571(5)	4875(4)	71(2)
N(1)	7904(3)	7409(3)	4049(3)	53(2)
N(2)	5777(3)	8428(3)	2843(3)	55(2)
C(97)	6682(4)	7999(4)	3600(4)	57(2)
C(98)	7128(4)	7281(4)	3900(3)	54(2)
C(99)	6075(4)	7800(5)	3255(4)	58(2)
C(100)	5275(4)	8181(5)	2431(4)	75(3)
C(101)	8348(4)	6678(5)	4303(4)	65(2)
C(102)	7768(5)	8060(5)	4471(4)	70(2)
C(103)	5313(4)	9139(4)	3160(4)	68(2)
N(3)	9669(3)	7084(5)	797(3)	76(2)
N(4)	9521(4)	9769(5)	1358(3)	79(2)
C(104)	9836(5)	8423(6)	1005(4)	86(3)
C(105)	9624(5)	7923(5)	564(4)	80(3)
C(106)	9511(5)	9291(6)	870(5)	85(3)
C(107)	10505(5)	6731(6)	890(4)	92(3)
C(108)	9413(5)	6689(7)	350(5)	95(3)
C(109)	10337(5)	9734(6)	1470(4)	94(3)
C(110)	9178(5)	10613(6)	1190(5)	106(4)
O(17)	4667(5)	5579(7)	405(5)	166(4)
C(111)	4561(9)	5658(12)	-254(7)	171(7)
C(112)	5354(11)	5050(12)	501(8)	186(8)
O(18)	5473(7)	3578(9)	1594(7)	87(4)
C(113)	5140(13)	3902(14)	2070(11)	101(7)
C(114)	4280(10)	3991(12)	2218(9)	81(5)

O(19)	4151(8)	3296(13)	2316(9)	129(7)
C(115)	4450(20)	2879(15)	1850(20)	210(20)
C(116)	5378(13)	2921(17)	1612(13)	131(10)
O(20)	4029(7)	8158(9)	4043(7)	80(4)
C(117)	4113(12)	7989(17)	4523(12)	116(10)
C(118)	3630(20)	7460(30)	4931(12)	202(18)
O(21)	3529(15)	6850(16)	4524(18)	190(16)
C(119)	3251(13)	7160(17)	4169(17)	128(13)
C(120)	3590(20)	7810(20)	3882(11)	172(14)
O(22)	1392(13)	2781(12)	2966(7)	143(7)
C(121)	1640(30)	3362(17)	2938(11)	155(14)
C(122)	2231(14)	3314(16)	3270(20)	159(16)
O(23)	2198(12)	2941(13)	3821(11)	150(8)
C(123)	1759(16)	2520(20)	3888(10)	148(12)
C(124)	1190(18)	2595(19)	3570(15)	159(11)
Q(1)	4121(8)	3353(9)	4928(7)	74(4)
Q(2)	3755(14)	4175(15)	5033(11)	118(7)
Q(3)	4050(20)	3910(20)	3872(16)	137(12)
Q(4)	3395(13)	3743(15)	4676(11)	112(7)
Q(5)	4104(15)	4685(16)	4626(12)	124(8)
Q(6)	4028(17)	3190(19)	4365(14)	118(9)
Q(7)	4714(19)	4336(19)	4356(14)	120(10)
Q(8)	4680(20)	3660(20)	4004(16)	100(10)
Q(9)	4081(17)	4430(20)	3967(14)	76(8)

Table 3. Bond lengths [Å] and angles [°] for sh2155.

Al(1)-O(16)	1.716(5)
Al(1)-O(5)	1.736(4)
Al(1)-O(1)	1.744(4)
Al(1)-O(4)	1.826(5)
Al(2)-O(7)	1.734(4)
Al(2)-O(8)	1.739(5)
Al(2)-O(1)	1.742(4)
Al(2)-O(2)	1.807(5)
Al(3)-O(10)	1.731(4)
Al(3)-O(3)	1.743(5)
Al(3)-O(11)	1.756(5)
Al(3)-O(2)	1.809(4)
Al(4)-O(3)	1.734(5)
Al(4)-O(14)	1.737(5)
Al(4)-O(13)	1.749(5)
Al(4)-O(4)	1.808(4)
Si(1)-O(5)	1.614(5)
Si(1)-O(6)	1.630(5)
Si(1)-C(7)	1.871(7)
Si(1)-C(1)	1.881(8)
Si(2)-O(7)	1.602(4)
Si(2)-O(6)	1.619(5)
Si(2)-C(19)	1.852(6)
Si(2)-C(13)	1.876(8)
Si(3)-O(8)	1.597(5)
Si(3)-O(9)	1.633(5)
Si(3)-C(25)	1.869(7)
Si(3)-C(31)	1.869(8)
Si(4)-O(10)	1.595(5)
Si(4)-O(9)	1.648(5)
Si(4)-C(43)	1.855(8)
Si(4)-C(37)	1.871(7)
Si(5)-O(12)	1.609(6)
Si(5)-O(11)	1.614(5)
Si(5)-C(55)	1.867(9)
Si(5)-C(49)	1.883(8)
Si(6)-O(13)	1.602(5)
Si(6)-O(12)	1.632(6)
Si(6)-C(61)	1.853(9)
Si(6)-C(67)	1.877(7)
Si(7)-O(14)	1.594(5)
Si(7)-O(15)	1.644(5)
Si(7)-C(79)	1.862(8)
Si(7)-C(73)	1.887(6)
Si(8)-O(16)	1.592(5)
Si(8)-O(15)	1.656(5)
Si(8)-C(85)	1.853(7)
Si(8)-C(91)	1.881(8)
C(1)-C(6)	1.383(10)
C(1)-C(2)	1.400(10)
C(2)-C(3)	1.350(10)
C(3)-C(4)	1.393(11)
C(4)-C(5)	1.351(11)
C(5)-C(6)	1.386(11)
C(7)-C(8)	1.397(10)
C(7)-C(12)	1.400(9)
C(8)-C(9)	1.392(10)
C(9)-C(10)	1.356(11)
C(10)-C(11)	1.350(12)
C(11)-C(12)	1.399(10)
C(13)-C(14)	1.399(9)
C(13)-C(18)	1.408(10)
C(14)-C(15)	1.381(11)
C(15)-C(16)	1.395(11)
C(16)-C(17)	1.346(12)
C(17)-C(18)	1.404(12)
C(19)-C(20)	1.352(11)
C(19)-C(24)	1.378(9)
C(20)-C(21)	1.422(12)
C(21)-C(22)	1.341(14)
C(22)-C(23)	1.346(14)
C(23)-C(24)	1.361(12)
C(25)-C(30)	1.346(12)
C(25)-C(26)	1.382(12)
C(26)-C(27)	1.380(12)

C(27)-C(28)	1.350(14)
C(28)-C(29)	1.332(14)
C(29)-C(30)	1.379(14)
C(31)-C(32)	1.381(10)
C(31)-C(36)	1.388(11)
C(32)-C(33)	1.396(12)
C(33)-C(34)	1.366(13)
C(34)-C(35)	1.346(13)
C(35)-C(36)	1.413(12)
C(37)-C(42)	1.383(12)
C(37)-C(38)	1.404(12)
C(38)-C(39)	1.365(11)
C(39)-C(40)	1.363(17)
C(40)-C(41)	1.404(17)
C(41)-C(42)	1.410(12)
C(43)-C(44)	1.365(12)
C(43)-C(48)	1.393(12)
C(44)-C(45)	1.406(16)
C(45)-C(46)	1.376(19)
C(46)-C(47)	1.323(18)
C(47)-C(48)	1.359(13)
C(49)-C(54)	1.391(11)
C(49)-C(50)	1.398(10)
C(50)-C(51)	1.389(11)
C(51)-C(52)	1.356(13)
C(52)-C(53)	1.397(14)
C(53)-C(54)	1.405(13)
C(55)-C(60)	1.351(18)
C(55)-C(56)	1.458(16)
C(56)-C(57)	1.332(18)
C(57)-C(58)	1.23(4)
C(58)-C(59)	1.61(3)
C(59)-C(60)	1.476(17)
C(61)-C(62)	1.377(12)
C(61)-C(66)	1.407(14)
C(62)-C(63)	1.395(13)
C(63)-C(64)	1.353(16)
C(64)-C(65)	1.363(17)
C(65)-C(66)	1.429(15)
C(67)-C(68)	1.356(10)
C(67)-C(72)	1.409(13)
C(68)-C(69)	1.386(9)
C(69)-C(70)	1.359(12)
C(70)-C(71)	1.372(14)
C(71)-C(72)	1.346(14)
C(73)-C(78)	1.356(12)
C(73)-C(74)	1.405(12)
C(74)-C(75)	1.373(11)
C(75)-C(76)	1.362(15)
C(76)-C(77)	1.385(15)
C(77)-C(78)	1.398(11)
C(79)-C(84)	1.387(12)
C(79)-C(80)	1.416(11)
C(80)-C(81)	1.386(15)
C(81)-C(82)	1.325(19)
C(82)-C(83)	1.404(19)
C(83)-C(84)	1.336(16)
C(85)-C(90)	1.378(9)
C(85)-C(86)	1.405(10)
C(86)-C(87)	1.373(11)
C(87)-C(88)	1.363(11)
C(88)-C(89)	1.366(12)
C(89)-C(90)	1.405(11)
C(91)-C(96)	1.393(10)
C(91)-C(92)	1.401(10)
C(92)-C(93)	1.406(13)
C(93)-C(94)	1.397(13)
C(94)-C(95)	1.360(12)
C(95)-C(96)	1.399(12)
N(1)-C(102)	1.482(9)
N(1)-C(101)	1.486(9)
N(1)-C(98)	1.500(8)
N(2)-C(99)	1.468(10)
N(2)-C(103)	1.475(9)
N(2)-C(100)	1.517(10)
C(97)-C(99)	1.518(10)
C(97)-C(98)	1.519(10)

N(3)-C(108)	1.435(10)
N(3)-C(107)	1.487(10)
N(3)-C(105)	1.528(11)
N(4)-C(106)	1.427(11)
N(4)-C(109)	1.461(10)
N(4)-C(110)	1.525(11)
C(104)-C(105)	1.506(13)
C(104)-C(106)	1.537(13)
O(17)-C(112)	1.379(16)
O(17)-C(111)	1.530(16)
C(111)-C(112)#1	1.36(2)
C(112)-C(111)#1	1.36(2)
O(18)-C(116)	1.20(3)
O(18)-C(113)	1.23(2)
C(113)-C(114)	1.44(2)
C(114)-O(19)	1.29(2)
O(19)-C(115)	1.29(4)
C(115)-C(116)	1.61(4)
O(20)-C(117)	1.14(3)
O(20)-C(120)	1.18(3)
C(117)-C(118)	1.54(4)
C(117)-C(120)	1.91(4)
C(118)-O(21)	1.51(4)
O(21)-C(119)	1.07(4)
C(119)-C(120)	1.47(4)
O(22)-C(121)	1.18(2)
O(22)-C(124)	1.39(3)
C(121)-C(122)	1.36(4)
C(122)-O(23)	1.37(4)
O(23)-C(123)	1.16(3)
C(123)-C(124)	1.30(3)
Q(1)-Q(6)	1.36(3)
Q(1)-Q(2)	1.46(3)
Q(1)-Q(4)	1.48(3)
Q(2)-Q(5)	1.40(3)
Q(2)-Q(4)	1.43(3)
Q(3)-Q(9)	0.98(4)
Q(3)-Q(8)	1.16(4)
Q(3)-Q(6)	1.64(5)
Q(3)-Q(7)	1.99(5)
Q(3)-Q(4)	2.01(4)
Q(4)-Q(6)	1.40(3)
Q(5)-Q(7)	1.18(3)
Q(5)-Q(9)	1.59(4)
Q(6)-Q(8)	1.62(4)
Q(7)-Q(8)	1.48(4)
Q(7)-Q(9)	1.49(4)
Q(8)-Q(9)	1.52(5)

O(16)-Al(1)-O(5)	111.6(2)
O(16)-Al(1)-O(1)	108.6(2)
O(5)-Al(1)-O(1)	112.9(2)
O(16)-Al(1)-O(4)	107.6(2)
O(5)-Al(1)-O(4)	105.6(2)
O(1)-Al(1)-O(4)	110.4(2)
O(7)-Al(2)-O(8)	108.1(2)
O(7)-Al(2)-O(1)	112.1(2)
O(8)-Al(2)-O(1)	108.8(2)
O(7)-Al(2)-O(2)	109.1(2)
O(8)-Al(2)-O(2)	110.1(2)
O(1)-Al(2)-O(2)	108.5(2)
O(10)-Al(3)-O(3)	108.7(2)
O(10)-Al(3)-O(11)	111.2(2)
O(3)-Al(3)-O(11)	111.0(2)
O(10)-Al(3)-O(2)	107.7(2)
O(3)-Al(3)-O(2)	111.8(2)
O(11)-Al(3)-O(2)	106.3(2)
O(3)-Al(4)-O(14)	109.1(2)
O(3)-Al(4)-O(13)	112.7(3)
O(14)-Al(4)-O(13)	110.4(2)
O(3)-Al(4)-O(4)	108.9(2)
O(14)-Al(4)-O(4)	107.5(2)
O(13)-Al(4)-O(4)	108.2(2)
O(5)-Si(1)-O(6)	112.4(2)
O(5)-Si(1)-C(7)	112.9(3)
O(6)-Si(1)-C(7)	103.1(3)
O(5)-Si(1)-C(1)	110.1(3)

O(6)-Si(1)-C(1)	108.3(3)
C(7)-Si(1)-C(1)	109.8(3)
O(7)-Si(2)-O(6)	111.7(2)
O(7)-Si(2)-C(19)	111.4(3)
O(6)-Si(2)-C(19)	106.2(3)
O(7)-Si(2)-C(13)	112.6(3)
O(6)-Si(2)-C(13)	107.6(3)
C(19)-Si(2)-C(13)	107.0(3)
O(8)-Si(3)-O(9)	109.3(2)
O(8)-Si(3)-C(25)	111.8(3)
O(9)-Si(3)-C(25)	110.3(3)
O(8)-Si(3)-C(31)	112.6(3)
O(9)-Si(3)-C(31)	105.7(3)
C(25)-Si(3)-C(31)	106.8(3)
O(10)-Si(4)-O(9)	112.1(3)
O(10)-Si(4)-C(43)	111.8(3)
O(9)-Si(4)-C(43)	107.9(3)
O(10)-Si(4)-C(37)	111.4(3)
O(9)-Si(4)-C(37)	104.9(3)
C(43)-Si(4)-C(37)	108.5(3)
O(12)-Si(5)-O(11)	112.9(3)
O(12)-Si(5)-C(55)	109.0(5)
O(11)-Si(5)-C(55)	110.9(4)
O(12)-Si(5)-C(49)	103.9(3)
O(11)-Si(5)-C(49)	110.9(3)
C(55)-Si(5)-C(49)	109.0(4)
O(13)-Si(6)-O(12)	112.1(3)
O(13)-Si(6)-C(61)	114.0(4)
O(12)-Si(6)-C(61)	104.4(4)
O(13)-Si(6)-C(67)	111.6(3)
O(12)-Si(6)-C(67)	107.5(4)
C(61)-Si(6)-C(67)	106.7(4)
O(14)-Si(7)-O(15)	110.2(2)
O(14)-Si(7)-C(79)	112.6(3)
O(15)-Si(7)-C(79)	110.7(3)
O(14)-Si(7)-C(73)	110.8(3)
O(15)-Si(7)-C(73)	104.7(3)
C(79)-Si(7)-C(73)	107.5(3)
O(16)-Si(8)-O(15)	112.0(2)
O(16)-Si(8)-C(85)	111.0(3)
O(15)-Si(8)-C(85)	108.3(3)
O(16)-Si(8)-C(91)	110.3(3)
O(15)-Si(8)-C(91)	106.1(3)
C(85)-Si(8)-C(91)	109.0(3)
Al(2)-O(1)-Al(1)	129.0(2)
Al(2)-O(2)-Al(3)	128.5(2)
Al(4)-O(3)-Al(3)	131.2(2)
Al(4)-O(4)-Al(1)	128.9(2)
Si(1)-O(5)-Al(1)	140.6(3)
Si(2)-O(6)-Si(1)	143.4(3)
Si(2)-O(7)-Al(2)	152.3(3)
Si(3)-O(8)-Al(2)	145.1(3)
Si(3)-O(9)-Si(4)	141.8(3)
Si(4)-O(10)-Al(3)	152.8(3)
Si(5)-O(11)-Al(3)	141.2(3)
Si(5)-O(12)-Si(6)	152.4(4)
Si(6)-O(13)-Al(4)	144.3(3)
Si(7)-O(14)-Al(4)	152.5(3)
Si(7)-O(15)-Si(8)	136.5(3)
Si(8)-O(16)-Al(1)	152.9(3)
C(6)-C(1)-C(2)	115.3(7)
C(6)-C(1)-Si(1)	122.3(6)
C(2)-C(1)-Si(1)	122.4(6)
C(3)-C(2)-C(1)	123.4(7)
C(2)-C(3)-C(4)	119.9(8)
C(5)-C(4)-C(3)	118.3(8)
C(4)-C(5)-C(6)	121.6(8)
C(1)-C(6)-C(5)	121.5(7)
C(8)-C(7)-C(12)	117.4(6)
C(8)-C(7)-Si(1)	123.2(5)
C(12)-C(7)-Si(1)	119.3(6)
C(9)-C(8)-C(7)	120.4(8)
C(10)-C(9)-C(8)	121.3(9)
C(11)-C(10)-C(9)	119.4(7)
C(10)-C(11)-C(12)	121.4(8)
C(11)-C(12)-C(7)	120.0(8)
C(14)-C(13)-C(18)	115.3(7)

C(14)-C(13)-Si(2)	124.8(6)
C(18)-C(13)-Si(2)	119.8(5)
C(15)-C(14)-C(13)	122.7(7)
C(14)-C(15)-C(16)	120.2(8)
C(17)-C(16)-C(15)	119.0(9)
C(16)-C(17)-C(18)	121.3(9)
C(17)-C(18)-C(13)	121.5(7)
C(20)-C(19)-C(24)	116.8(7)
C(20)-C(19)-Si(2)	118.8(5)
C(24)-C(19)-Si(2)	124.3(6)
C(19)-C(20)-C(21)	120.5(9)
C(22)-C(21)-C(20)	119.5(11)
C(21)-C(22)-C(23)	120.8(9)
C(22)-C(23)-C(24)	119.1(9)
C(23)-C(24)-C(19)	123.2(9)
C(30)-C(25)-C(26)	115.0(8)
C(30)-C(25)-Si(3)	121.5(7)
C(26)-C(25)-Si(3)	123.0(7)
C(27)-C(26)-C(25)	122.1(10)
C(28)-C(27)-C(26)	120.0(10)
C(29)-C(28)-C(27)	118.8(9)
C(28)-C(29)-C(30)	120.3(12)
C(25)-C(30)-C(29)	123.2(11)
C(32)-C(31)-C(36)	114.8(8)
C(32)-C(31)-Si(3)	122.4(6)
C(36)-C(31)-Si(3)	122.7(6)
C(31)-C(32)-C(33)	121.9(9)
C(34)-C(33)-C(32)	122.3(9)
C(35)-C(34)-C(33)	117.3(9)
C(34)-C(35)-C(36)	121.1(10)
C(31)-C(36)-C(35)	122.6(8)
C(42)-C(37)-C(38)	116.5(7)
C(42)-C(37)-Si(4)	123.4(7)
C(38)-C(37)-Si(4)	120.0(6)
C(39)-C(38)-C(37)	124.3(10)
C(40)-C(39)-C(38)	118.2(11)
C(39)-C(40)-C(41)	121.0(9)
C(40)-C(41)-C(42)	119.1(11)
C(37)-C(42)-C(41)	120.8(10)
C(44)-C(43)-C(48)	118.2(8)
C(44)-C(43)-Si(4)	118.3(7)
C(48)-C(43)-Si(4)	123.4(7)
C(43)-C(44)-C(45)	119.3(12)
C(46)-C(45)-C(44)	120.1(14)
C(47)-C(46)-C(45)	120.0(12)
C(46)-C(47)-C(48)	121.0(12)
C(47)-C(48)-C(43)	121.2(10)
C(54)-C(49)-C(50)	116.4(7)
C(54)-C(49)-Si(5)	122.7(6)
C(50)-C(49)-Si(5)	120.8(6)
C(51)-C(50)-C(49)	123.6(9)
C(52)-C(51)-C(50)	119.1(9)
C(51)-C(52)-C(53)	119.7(9)
C(52)-C(53)-C(54)	120.8(9)
C(49)-C(54)-C(53)	120.4(8)
C(60)-C(55)-C(56)	118.4(10)
C(60)-C(55)-Si(5)	122.2(10)
C(56)-C(55)-Si(5)	119.3(10)
C(57)-C(56)-C(55)	129.0(19)
C(58)-C(57)-C(56)	113(3)
C(57)-C(58)-C(59)	129.2(18)
C(60)-C(59)-C(58)	110.5(17)
C(55)-C(60)-C(59)	119.6(17)
C(62)-C(61)-C(66)	116.4(9)
C(62)-C(61)-Si(6)	125.6(9)
C(66)-C(61)-Si(6)	117.8(8)
C(61)-C(62)-C(63)	123.8(11)
C(64)-C(63)-C(62)	119.6(12)
C(63)-C(64)-C(65)	119.3(11)
C(64)-C(65)-C(66)	121.8(13)
C(61)-C(66)-C(65)	119.0(11)
C(68)-C(67)-C(72)	113.1(8)
C(68)-C(67)-Si(6)	125.2(6)
C(72)-C(67)-Si(6)	120.9(7)
C(67)-C(68)-C(69)	123.3(8)
C(70)-C(69)-C(68)	121.1(8)
C(69)-C(70)-C(71)	117.7(8)

C(72)-C(71)-C(70)	119.9(11)
C(71)-C(72)-C(67)	124.8(10)
C(78)-C(73)-C(74)	117.6(7)
C(78)-C(73)-Si(7)	123.3(7)
C(74)-C(73)-Si(7)	119.1(6)
C(75)-C(74)-C(73)	122.6(10)
C(76)-C(75)-C(74)	117.8(10)
C(75)-C(76)-C(77)	122.0(9)
C(76)-C(77)-C(78)	118.5(10)
C(73)-C(78)-C(77)	121.4(9)
C(84)-C(79)-C(80)	116.1(9)
C(84)-C(79)-Si(7)	124.6(7)
C(80)-C(79)-Si(7)	119.2(7)
C(81)-C(80)-C(79)	119.4(12)
C(82)-C(81)-C(80)	121.7(14)
C(81)-C(82)-C(83)	120.4(14)
C(84)-C(83)-C(82)	118.3(14)
C(83)-C(84)-C(79)	124.1(12)
C(90)-C(85)-C(86)	116.0(7)
C(90)-C(85)-Si(8)	123.0(6)
C(86)-C(85)-Si(8)	120.8(5)
C(87)-C(86)-C(85)	122.6(7)
C(88)-C(87)-C(86)	120.4(8)
C(87)-C(88)-C(89)	119.0(8)
C(88)-C(89)-C(90)	121.0(8)
C(85)-C(90)-C(89)	121.0(7)
C(96)-C(91)-C(92)	118.4(8)
C(96)-C(91)-Si(8)	120.0(5)
C(92)-C(91)-Si(8)	121.5(6)
C(91)-C(92)-C(93)	119.4(9)
C(94)-C(93)-C(92)	120.5(8)
C(95)-C(94)-C(93)	120.4(10)
C(94)-C(95)-C(96)	119.4(9)
C(91)-C(96)-C(95)	121.9(8)
C(102)-N(1)-C(101)	110.5(6)
C(102)-N(1)-C(98)	111.9(5)
C(101)-N(1)-C(98)	109.7(6)
C(99)-N(2)-C(103)	112.6(6)
C(99)-N(2)-C(100)	113.0(6)
C(103)-N(2)-C(100)	109.1(6)
C(99)-C(97)-C(98)	111.8(6)
N(1)-C(98)-C(97)	111.5(6)
N(2)-C(99)-C(97)	113.2(6)
C(108)-N(3)-C(107)	112.7(7)
C(108)-N(3)-C(105)	105.7(8)
C(107)-N(3)-C(105)	109.6(6)
C(106)-N(4)-C(109)	112.2(7)
C(106)-N(4)-C(110)	107.9(9)
C(109)-N(4)-C(110)	107.1(7)
C(105)-C(104)-C(106)	110.1(9)
C(104)-C(105)-N(3)	111.7(8)
N(4)-C(106)-C(104)	111.5(9)
C(112)-O(17)-C(111)	113.3(10)
C(112)#1-C(111)-O(17)	111.5(15)
C(111)#1-C(112)-O(17)	114.0(17)
C(116)-O(18)-C(113)	109.5(19)
O(18)-C(113)-C(114)	117(2)
O(19)-C(114)-C(113)	106.0(16)
C(115)-O(19)-C(114)	110(2)
O(19)-C(115)-C(116)	112(2)
O(18)-C(116)-C(115)	111.8(17)
C(117)-O(20)-C(120)	110.9(19)
O(20)-C(117)-C(118)	124(2)
O(20)-C(117)-C(120)	35.3(11)
C(118)-C(117)-C(120)	88.7(19)
O(21)-C(118)-C(117)	105(2)
C(119)-O(21)-C(118)	106(4)
O(21)-C(119)-C(120)	117(3)
O(20)-C(120)-C(119)	130(3)
O(20)-C(120)-C(117)	33.8(14)
C(119)-C(120)-C(117)	97(2)
C(121)-O(22)-C(124)	108(2)
O(22)-C(121)-C(122)	112(2)
C(121)-C(122)-O(23)	121.4(19)
C(123)-O(23)-C(122)	113(2)
O(23)-C(123)-C(124)	121(2)
C(123)-C(124)-O(22)	116(3)

Q(6)-Q(1)-Q(2)	107(2)
Q(6)-Q(1)-Q(4)	58.9(15)
Q(2)-Q(1)-Q(4)	58.4(13)
Q(5)-Q(2)-Q(4)	105(2)
Q(5)-Q(2)-Q(1)	114(2)
Q(4)-Q(2)-Q(1)	61.6(15)
Q(9)-Q(3)-Q(8)	91(4)
Q(9)-Q(3)-Q(6)	124(4)
Q(8)-Q(3)-Q(6)	68(3)
Q(9)-Q(3)-Q(7)	46(3)
Q(8)-Q(3)-Q(7)	47(2)
Q(6)-Q(3)-Q(7)	88(2)
Q(9)-Q(3)-Q(4)	93(3)
Q(8)-Q(3)-Q(4)	97(3)
Q(6)-Q(3)-Q(4)	43.8(15)
Q(7)-Q(3)-Q(4)	83.9(18)
Q(6)-Q(4)-Q(2)	106(2)
Q(6)-Q(4)-Q(1)	56.4(16)
Q(2)-Q(4)-Q(1)	59.9(15)
Q(6)-Q(4)-Q(3)	53.9(18)
Q(2)-Q(4)-Q(3)	98.5(19)
Q(1)-Q(4)-Q(3)	92.3(16)
Q(7)-Q(5)-Q(2)	109(3)
Q(7)-Q(5)-Q(9)	63(2)
Q(2)-Q(5)-Q(9)	108(2)
Q(1)-Q(6)-Q(4)	64.7(18)
Q(1)-Q(6)-Q(8)	97(2)
Q(4)-Q(6)-Q(8)	107(3)
Q(1)-Q(6)-Q(3)	116(3)
Q(4)-Q(6)-Q(3)	82(2)
Q(8)-Q(6)-Q(3)	41.7(17)
Q(5)-Q(7)-Q(8)	118(3)
Q(5)-Q(7)-Q(9)	72(2)
Q(8)-Q(7)-Q(9)	62(2)
Q(5)-Q(7)-Q(3)	87(3)
Q(8)-Q(7)-Q(3)	35.2(17)
Q(9)-Q(7)-Q(3)	28.1(16)
Q(3)-Q(8)-Q(7)	97(3)
Q(3)-Q(8)-Q(9)	40(2)
Q(7)-Q(8)-Q(9)	60(2)
Q(3)-Q(8)-Q(6)	70(3)
Q(7)-Q(8)-Q(6)	110(3)
Q(9)-Q(8)-Q(6)	96(3)
Q(3)-Q(9)-Q(7)	106(4)
Q(3)-Q(9)-Q(8)	50(3)
Q(7)-Q(9)-Q(8)	59(2)
Q(3)-Q(9)-Q(5)	123(4)
Q(7)-Q(9)-Q(5)	44.9(16)
Q(8)-Q(9)-Q(5)	94(3)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2155. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	27(1)	33(1)	64(1)	0(1)	-2(1)	-5(1)
Al(2)	27(1)	35(1)	59(1)	0(1)	-4(1)	-7(1)
Al(3)	32(1)	39(1)	63(1)	4(1)	-8(1)	-8(1)
Al(4)	29(1)	38(1)	65(1)	6(1)	-4(1)	-5(1)
Si(1)	28(1)	42(1)	69(1)	2(1)	-3(1)	-10(1)
Si(2)	27(1)	39(1)	64(1)	-1(1)	-3(1)	-2(1)
Si(3)	41(1)	35(1)	60(1)	3(1)	-6(1)	-12(1)
Si(4)	35(1)	40(1)	66(1)	-1(1)	-8(1)	-10(1)
Si(5)	38(1)	81(2)	63(1)	14(1)	-10(1)	-13(1)
Si(6)	50(1)	61(2)	71(2)	20(1)	0(1)	11(1)
Si(7)	33(1)	39(1)	82(2)	-4(1)	-2(1)	-3(1)
Si(8)	38(1)	37(1)	71(1)	-5(1)	-2(1)	-9(1)
O(1)	33(2)	28(3)	57(3)	-2(2)	-1(2)	-9(2)
O(2)	27(2)	48(3)	56(3)	5(2)	-14(2)	-6(2)
O(3)	31(2)	38(3)	67(3)	2(2)	-4(2)	-10(2)
O(4)	31(2)	43(3)	60(3)	-1(2)	-4(2)	-5(2)
O(5)	35(2)	45(3)	67(3)	4(2)	-2(2)	-12(2)
O(6)	33(2)	45(3)	74(3)	-2(2)	-2(2)	-10(2)
O(7)	30(2)	46(3)	62(3)	-3(2)	-6(2)	-6(2)
O(8)	43(2)	33(3)	63(3)	1(2)	-9(2)	-12(2)
O(9)	41(2)	44(3)	65(3)	5(2)	-12(2)	-13(2)
O(10)	39(2)	34(3)	75(3)	3(2)	-7(2)	-15(2)
O(11)	44(2)	60(3)	54(3)	13(2)	-13(2)	-14(2)
O(12)	61(3)	59(4)	75(4)	10(3)	0(3)	15(2)
O(13)	44(2)	53(3)	68(3)	17(2)	-2(2)	3(2)
O(14)	35(2)	39(3)	69(3)	-2(2)	2(2)	-6(2)
O(15)	41(2)	39(3)	72(3)	-2(2)	-4(2)	-3(2)
O(16)	41(2)	33(3)	69(3)	-6(2)	-1(2)	-2(2)
C(1)	36(3)	41(5)	70(5)	2(4)	-4(3)	-8(3)
C(2)	52(4)	61(6)	60(5)	-4(4)	-3(4)	-14(4)
C(3)	55(4)	74(6)	68(6)	6(4)	-10(4)	-14(4)
C(4)	65(5)	76(7)	55(5)	1(4)	-13(4)	-9(4)
C(5)	82(6)	83(8)	82(7)	-4(5)	-18(5)	-31(5)
C(6)	62(5)	67(6)	85(7)	1(5)	-12(4)	-31(4)
C(7)	37(4)	50(5)	73(5)	2(4)	-12(3)	-16(3)
C(8)	53(4)	52(6)	114(7)	2(5)	-10(4)	-20(4)
C(9)	69(5)	65(7)	128(8)	19(5)	-11(5)	-40(5)
C(10)	51(5)	75(8)	116(8)	4(6)	9(5)	-35(4)
C(11)	32(4)	101(9)	104(7)	-7(6)	-1(4)	-21(4)
C(12)	38(4)	77(6)	78(6)	-4(4)	-6(4)	-22(4)
C(13)	37(4)	46(5)	63(5)	2(3)	-5(3)	-2(3)
C(14)	48(4)	64(6)	74(6)	10(4)	-12(4)	-14(4)
C(15)	73(6)	91(7)	70(6)	17(5)	-13(5)	-28(5)
C(16)	82(6)	96(8)	69(6)	16(5)	-17(5)	-24(5)
C(17)	72(6)	126(10)	88(7)	16(6)	-40(5)	-8(6)
C(18)	49(4)	94(7)	92(7)	32(5)	-17(4)	-16(4)
C(19)	38(4)	44(5)	60(5)	1(4)	-4(3)	4(3)
C(20)	81(6)	68(7)	89(7)	-1(5)	20(5)	-2(5)
C(21)	145(10)	58(7)	102(8)	-19(6)	14(7)	9(6)
C(22)	59(6)	139(11)	82(7)	-16(7)	17(5)	24(6)
C(23)	55(5)	158(12)	96(8)	-35(8)	5(5)	-36(6)
C(24)	42(4)	87(7)	70(5)	-16(5)	13(4)	-18(4)
C(25)	51(4)	43(5)	66(5)	-1(4)	-8(4)	-2(3)
C(26)	130(8)	58(7)	107(8)	-20(6)	35(7)	-20(6)
C(27)	136(9)	94(10)	103(8)	-24(7)	46(7)	-22(7)
C(28)	104(7)	60(8)	93(8)	-8(5)	9(6)	17(5)
C(29)	205(14)	65(9)	126(10)	-5(7)	39(10)	28(8)
C(30)	188(12)	50(8)	146(11)	6(7)	71(9)	16(7)
C(31)	63(4)	26(4)	62(5)	-2(3)	-17(4)	-10(3)
C(32)	59(5)	84(7)	102(7)	39(5)	1(5)	-17(4)
C(33)	88(7)	100(9)	105(8)	43(7)	13(6)	-21(6)
C(34)	125(8)	63(7)	68(6)	10(5)	-6(6)	-17(6)
C(35)	129(8)	58(7)	98(8)	26(5)	-58(6)	-29(6)
C(36)	87(6)	56(6)	100(7)	23(5)	-34(5)	-32(4)
C(37)	42(4)	36(5)	98(6)	-8(4)	-1(4)	-11(3)
C(38)	53(5)	94(8)	109(8)	-2(6)	-20(5)	-32(4)
C(39)	44(5)	117(9)	141(10)	-11(7)	-17(6)	-24(5)
C(40)	38(5)	114(10)	221(16)	-13(10)	-1(8)	-24(5)
C(41)	71(7)	140(12)	164(12)	39(9)	32(8)	-29(7)
C(42)	56(5)	97(8)	104(8)	24(6)	4(5)	-13(4)
C(43)	48(4)	44(5)	80(6)	-15(4)	-20(4)	3(3)

C(44)	140(9)	52(7)	98(8)	-19(6)	-19(6)	-5(6)
C(45)	232(17)	57(9)	163(14)	-36(9)	-70(13)	20(9)
C(46)	128(10)	144(14)	92(9)	-52(10)	-26(8)	49(9)
C(47)	114(9)	128(12)	94(9)	-36(8)	8(6)	-27(8)
C(48)	74(6)	119(9)	79(7)	-38(6)	14(5)	-44(5)
C(49)	42(4)	62(6)	66(5)	8(4)	-15(3)	-7(3)
C(50)	67(5)	99(8)	74(6)	-8(5)	3(5)	-29(5)
C(51)	102(7)	78(8)	84(7)	-10(6)	17(6)	-28(5)
C(52)	103(7)	68(8)	92(8)	-3(6)	15(6)	0(6)
C(53)	100(7)	80(8)	108(9)	-34(6)	-23(6)	6(6)
C(54)	65(5)	57(6)	110(8)	-2(5)	-20(5)	-11(4)
C(55)	64(6)	167(12)	70(6)	26(6)	-25(5)	-50(7)
C(56)	40(5)	287(19)	133(11)	-91(11)	3(6)	-17(8)
C(57)	77(10)	620(60)	169(18)	-160(30)	25(10)	-130(20)
C(58)	68(9)	480(40)	85(10)	96(18)	-36(8)	-99(16)
C(59)	212(18)	350(30)	185(17)	128(19)	-101(15)	-220(20)
C(60)	110(9)	250(20)	205(15)	140(14)	-106(10)	-129(12)
C(61)	50(4)	77(7)	85(7)	27(5)	1(4)	16(4)
C(62)	61(5)	81(7)	88(7)	25(5)	6(5)	6(4)
C(63)	66(6)	118(11)	108(9)	40(8)	16(5)	-2(6)
C(64)	74(6)	117(11)	130(11)	62(9)	4(7)	-12(6)
C(65)	125(9)	78(9)	150(13)	31(8)	-10(9)	-11(6)
C(66)	125(9)	95(10)	91(8)	26(7)	-5(6)	1(7)
C(67)	57(4)	69(6)	68(6)	13(4)	-6(4)	10(4)
C(68)	46(4)	59(6)	87(6)	5(4)	-15(4)	-8(3)
C(69)	46(4)	83(7)	81(6)	2(5)	-4(4)	-8(4)
C(70)	46(5)	106(8)	113(8)	17(6)	-13(5)	18(5)
C(71)	74(7)	340(20)	104(10)	53(11)	-12(7)	97(10)
C(72)	88(8)	278(19)	98(9)	76(10)	6(7)	81(10)
C(73)	41(4)	39(5)	86(6)	-10(4)	8(4)	-8(3)
C(74)	44(4)	97(8)	95(7)	-33(6)	1(4)	4(4)
C(75)	42(5)	131(10)	116(9)	-37(7)	-14(5)	15(5)
C(76)	49(5)	96(9)	158(12)	-27(8)	16(7)	6(5)
C(77)	61(6)	153(11)	126(10)	42(8)	21(6)	-1(6)
C(78)	49(5)	83(7)	116(8)	11(6)	-2(5)	1(4)
C(79)	57(4)	36(5)	115(7)	8(4)	-32(5)	-8(3)
C(80)	94(7)	36(7)	161(10)	-5(6)	-42(6)	-8(5)
C(81)	139(10)	40(8)	225(17)	28(8)	-71(11)	-38(7)
C(82)	165(14)	121(15)	185(16)	69(12)	-82(12)	-93(12)
C(83)	176(13)	125(15)	162(14)	35(11)	-5(10)	-86(11)
C(84)	129(8)	83(9)	102(8)	15(6)	18(7)	-54(6)
C(85)	41(4)	44(5)	77(5)	-2(4)	-9(3)	-11(3)
C(86)	55(4)	67(6)	73(6)	-9(4)	-6(4)	-18(4)
C(87)	82(6)	58(7)	99(7)	-6(5)	-21(5)	-21(5)
C(88)	84(6)	63(7)	99(7)	4(5)	-5(5)	-38(5)
C(89)	80(6)	61(7)	124(8)	-9(6)	29(6)	-29(5)
C(90)	61(5)	49(6)	111(7)	-8(5)	19(5)	-18(4)
C(91)	61(4)	39(5)	62(5)	-5(3)	0(4)	-14(3)
C(92)	65(5)	85(7)	80(7)	-20(5)	-6(5)	-22(4)
C(93)	101(8)	117(9)	71(7)	-24(6)	16(6)	-41(6)
C(94)	121(8)	81(8)	78(7)	2(5)	-28(7)	-37(6)
C(95)	84(6)	76(7)	94(8)	-2(5)	-22(6)	-9(5)
C(96)	64(5)	70(6)	75(6)	-9(5)	-12(4)	-1(4)
N(1)	46(3)	49(4)	62(4)	-5(3)	9(3)	-20(3)
N(2)	36(3)	43(4)	82(5)	0(3)	1(3)	-9(3)
C(97)	50(4)	41(5)	80(6)	-5(4)	1(4)	-16(3)
C(98)	44(4)	38(5)	81(5)	-9(4)	3(4)	-19(3)
C(99)	40(4)	50(5)	81(6)	-4(4)	4(4)	-12(3)
C(100)	47(4)	57(6)	130(8)	-6(5)	-27(5)	-16(4)
C(101)	58(4)	57(6)	79(6)	3(4)	-7(4)	-17(4)
C(102)	72(5)	58(6)	82(6)	-13(5)	8(4)	-29(4)
C(103)	43(4)	54(6)	95(6)	1(4)	14(4)	-4(3)
N(3)	49(4)	99(6)	70(5)	-6(4)	5(3)	-7(3)
N(4)	50(4)	90(6)	87(6)	16(5)	8(4)	-14(4)
C(104)	70(5)	93(8)	80(7)	14(6)	-1(5)	-2(5)
C(105)	63(5)	63(7)	103(8)	14(5)	2(5)	-11(4)
C(106)	67(5)	91(8)	95(7)	10(6)	1(5)	-27(5)
C(107)	62(5)	107(8)	90(7)	5(6)	-2(5)	6(5)
C(108)	75(6)	116(9)	99(8)	-28(7)	-7(5)	-32(6)
C(109)	60(5)	119(9)	106(8)	13(6)	-11(5)	-29(5)
C(110)	84(6)	73(8)	150(10)	17(7)	-21(6)	4(5)
O(17)	87(5)	210(11)	158(9)	8(8)	34(6)	13(6)
C(111)	151(13)	210(20)	101(12)	38(11)	-6(10)	39(13)
C(112)	163(15)	194(19)	156(15)	-14(13)	-30(11)	63(14)
O(18)	89(9)	43(9)	117(12)	24(8)	6(8)	-15(6)
C(113)	99(16)	108(19)	100(17)	38(14)	-18(13)	-41(13)
C(114)	79(12)	64(15)	102(15)	-3(11)	-27(10)	-13(10)

O(19)	86(9)	92(17)	200(20)	49(13)	4(11)	-41(10)
C(115)	230(40)	3(17)	440(70)	30(20)	-150(40)	-69(18)
C(116)	85(15)	100(20)	180(30)	5(18)	-5(15)	32(14)
O(20)	68(7)	93(10)	93(11)	37(8)	-4(8)	-63(7)
C(117)	69(12)	180(30)	103(18)	-83(19)	28(14)	-43(14)
C(118)	240(40)	260(50)	74(19)	70(20)	30(20)	-40(40)
O(21)	140(20)	100(20)	280(40)	87(19)	60(20)	-28(15)
C(119)	44(11)	80(20)	260(40)	-50(20)	17(16)	-45(12)
C(120)	230(30)	220(40)	76(17)	90(20)	4(19)	-110(30)
O(22)	270(20)	144(17)	77(10)	37(10)	-113(12)	-112(15)
C(121)	320(50)	110(20)	78(16)	62(15)	-70(20)	-130(30)
C(122)	93(16)	90(20)	300(50)	40(30)	10(20)	-70(15)
O(23)	145(15)	170(20)	200(20)	42(15)	-116(15)	-99(14)
C(123)	150(20)	250(40)	76(15)	117(19)	-75(15)	-90(20)

sh2315

Tabelle x. Kristalldaten und Strukturverfeinerung für **17**.

Identifizierungscode	sh2315	
Summenformel	C_{131} H_{158} Al_4 N_2 O_{28} Si_8	
Molmasse	2541.23	
Temperatur	103(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem	Monoclinic	
Raumgruppe	P2(1)	
Gitterkonstanten	a = 14.5990(6) Å	α= 90°.
	b = 27.9082(11) Å	β= 107.067(2)°.
	c = 16.8743(7) Å	γ = 90°.
Zellvolumen	6572.4(5) $Å^3$	
Anzahl der Formeleinheiten	2	
Density (calculated)	1.284 Mg/m^3	
Röntgenographische Dichte	0.181 mm^{-1}	
F(000)	2692	
Kristallgröße	0.3 x 0.25 x 0.2 mm^3	
Gemessener Theta-Bereich	1.26 to 29.57°.	
Indexbereich	-20<=h<=20, -38<=k<=38, -23<=l<=17	
Anzahl gemessener Reflexe	84867	
Unabhängige Reflexe	34913 [R(int) = 0.0398]	
Datenvollständigkeit bis Theta = 29.57°	99.5 %	
Absorptionskorrektur	N/A	
Verfeinerung	Full-matrix-block least-squares on F^2	
Daten / Restraints / Parameters	34913 / 1 / 1623	
Goodness-of-fit on F^2	1.022	
Endgültige R-Werte [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1102	
R-Werte (alle Daten)	R1 = 0.0630, wR2 = 0.1197	
Absolute structure parameter	0.02(5)	
Restelektronendichte	0.546 and -0.331 e.$Å^{-3}$	

Tabelle x Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$x 10^3) für **17**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalisierten U_{ij}-Tensors.

	x	y	z	U(eq)
Al(1)	1690(1)	2833(1)	-1654(1)	14(1)
Al(2)	-210(1)	3515(1)	-1869(1)	15(1)
Al(3)	644(1)	3920(1)	-68(1)	16(1)
Al(4)	2360(1)	3086(1)	219(1)	14(1)
Si(1)	455(1)	2178(1)	-3141(1)	17(1)
Si(2)	-1412(1)	2724(1)	-3093(1)	16(1)
Si(3)	-867(1)	4574(1)	-2582(1)	19(1)
Si(4)	126(1)	4978(1)	-801(1)	18(1)
Si(5)	1058(1)	3889(1)	1866(1)	18(1)
Si(6)	2199(1)	2919(1)	2076(1)	17(1)
Si(7)	4504(1)	3330(1)	105(1)	16(1)
Si(8)	3899(1)	2844(1)	-1613(1)	16(1)
N(1)	-1417(1)	3102(1)	-232(1)	18(1)
N(2)	1070(1)	1917(1)	-262(1)	17(1)

O(1)	963(1)	3367(1)	-1964(1)	16(1)
O(2)	-154(1)	3585(1)	-828(1)	17(1)
O(3)	1853(1)	3692(1)	44(1)	17(1)
O(4)	1760(1)	2737(1)	-617(1)	16(1)
O(5)	1123(1)	2360(1)	-2263(1)	19(1)
O(6)	-629(1)	2378(1)	-3327(1)	21(1)
O(7)	-942(1)	3032(1)	-2269(1)	19(1)
O(8)	-502(1)	4034(1)	-2443(1)	23(1)
O(9)	-286(1)	4917(1)	-1802(1)	23(1)
O(10)	672(1)	4516(1)	-326(1)	20(1)
O(11)	477(1)	3829(1)	902(1)	21(1)
O(12)	1720(1)	3424(1)	2243(1)	22(1)
O(13)	2168(1)	2872(1)	1120(1)	19(1)
O(14)	3556(1)	3171(1)	328(1)	20(1)
O(15)	4571(1)	3106(1)	-771(1)	19(1)
O(16)	2786(1)	2963(1)	-1792(1)	19(1)
O(17)	1896(1)	4106(1)	-2380(1)	37(1)
O(18)	3073(2)	4840(1)	-2674(2)	77(1)
O(19)	2210(2)	6669(1)	-3295(2)	59(1)
O(20)	2359(2)	6220(1)	-4754(2)	68(1)
O(21)	5084(2)	6501(1)	-1561(2)	62(1)
O(22)	4894(2)	5999(1)	-3053(2)	59(1)
O(23)	3130(2)	135(1)	-2527(1)	41(1)
O(24)	4103(2)	-446(1)	-3386(1)	37(1)
O(25)	2585(2)	4226(1)	-5164(2)	72(1)
O(26)	3966(2)	4863(1)	-5447(2)	80(1)
O(27A)	3595(3)	812(1)	-4786(3)	51(1)
O(28A)	4677(3)	1636(1)	-4825(3)	50(1)
O(27B)	3977(17)	1262(8)	-5622(8)	259(12)
O(28B)	4455(11)	1197(5)	-3927(6)	154(5)
C(1)	916(2)	2399(1)	-4001(1)	22(1)
C(2)	1064(2)	2891(1)	-4076(2)	25(1)
C(3)	1392(2)	3075(1)	-4711(2)	32(1)
C(4)	1581(2)	2768(1)	-5287(2)	37(1)
C(5)	1444(2)	2281(1)	-5234(2)	41(1)
C(6)	1116(2)	2099(1)	-4595(2)	32(1)
C(7)	338(2)	1510(1)	-3153(1)	20(1)
C(8)	1120(2)	1209(1)	-2805(2)	26(1)
C(9)	1020(2)	715(1)	-2787(2)	31(1)
C(10)	113(2)	508(1)	-3116(2)	33(1)
C(11)	-660(2)	795(1)	-3472(2)	31(1)
C(12)	-554(2)	1292(1)	-3490(2)	26(1)
C(13)	-2349(2)	2320(1)	-2903(1)	19(1)
C(14)	-2089(2)	1909(1)	-2414(2)	25(1)
C(15)	-2767(2)	1627(1)	-2194(2)	31(1)
C(16)	-3726(2)	1750(1)	-2477(2)	34(1)
C(17)	-4008(2)	2146(1)	-2976(2)	37(1)
C(18)	-3326(2)	2426(1)	-3190(2)	27(1)
C(19)	-1928(2)	3116(1)	-4013(1)	21(1)
C(20)	-2488(2)	3517(1)	-3971(2)	24(1)
C(21)	-2909(2)	3789(1)	-4665(2)	33(1)
C(22)	-2775(2)	3674(1)	-5420(2)	37(1)
C(23)	-2199(2)	3287(1)	-5475(2)	35(1)
C(24)	-1775(2)	3013(1)	-4774(2)	28(1)
C(25)	-653(2)	4864(1)	-3507(2)	29(1)
C(26)	-753(3)	5367(1)	-3575(2)	42(1)
C(27)	-630(3)	5619(2)	-4247(2)	58(1)
C(28)	-391(4)	5378(2)	-4856(2)	70(1)
C(29)	-270(4)	4882(2)	-4805(2)	79(2)
C(30)	-417(3)	4627(1)	-4136(2)	51(1)
C(31)	-2169(2)	4615(1)	-2663(2)	24(1)
C(32)	-2498(2)	4385(1)	-2061(2)	29(1)
C(33)	-3438(2)	4427(1)	-2032(2)	39(1)
C(34)	-4072(2)	4689(1)	-2612(2)	49(1)
C(35)	-3805(3)	4908(2)	-3235(3)	61(1)
C(36)	-2845(2)	4874(1)	-3259(2)	45(1)
C(37)	-933(2)	5128(1)	-438(2)	22(1)
C(38)	-1747(2)	5358(1)	-952(2)	29(1)
C(39)	-2531(2)	5459(1)	-680(2)	38(1)
C(40)	-2531(2)	5346(1)	113(2)	40(1)
C(41)	-1730(2)	5122(1)	644(2)	39(1)
C(42)	-951(2)	5015(1)	364(2)	31(1)
C(43)	1008(2)	5485(1)	-621(2)	23(1)
C(44)	1811(2)	5493(1)	74(2)	27(1)
C(45)	2466(2)	5872(1)	213(2)	33(1)
C(46)	2320(2)	6246(1)	-338(2)	42(1)
C(47)	1520(3)	6250(1)	-1010(3)	58(1)

C(48)	874(2)	5872(1)	-1152(2)	47(1)
C(49)	189(2)	3956(1)	2476(2)	21(1)
C(50)	-661(2)	4213(1)	2166(2)	24(1)
C(51)	-1280(2)	4300(1)	2639(2)	28(1)
C(52)	-1079(2)	4113(1)	3425(2)	34(1)
C(53)	-263(2)	3849(1)	3740(2)	45(1)
C(54)	378(2)	3778(1)	3278(2)	37(1)
C(55)	1878(2)	4422(1)	2064(1)	21(1)
C(56)	2867(2)	4375(1)	2218(2)	32(1)
C(57)	3473(2)	4768(1)	2410(2)	39(1)
C(58)	3107(2)	5221(1)	2443(2)	33(1)
C(59)	2137(2)	5280(1)	2290(2)	32(1)
C(60)	1533(2)	4883(1)	2108(2)	28(1)
C(61)	3451(2)	2886(1)	2780(1)	20(1)
C(62)	4224(2)	3065(1)	2540(2)	25(1)
C(63)	5157(2)	3047(1)	3073(2)	31(1)
C(64)	5337(2)	2842(1)	3851(2)	30(1)
C(65)	4587(2)	2654(1)	4099(2)	31(1)
C(66)	3655(2)	2678(1)	3570(2)	26(1)
C(67)	1483(2)	2427(1)	2361(1)	20(1)
C(68)	567(2)	2500(1)	2446(2)	26(1)
C(69)	37(2)	2125(1)	2631(2)	33(1)
C(70)	410(2)	1667(1)	2734(2)	36(1)
C(71)	1312(2)	1581(1)	2656(2)	31(1)
C(72)	1839(2)	1958(1)	2469(2)	24(1)
C(73)	5593(2)	3119(1)	934(1)	19(1)
C(74)	6340(2)	3426(1)	1332(2)	22(1)
C(75)	7158(2)	3258(1)	1929(2)	29(1)
C(76)	7246(2)	2774(1)	2121(2)	32(1)
C(77)	6511(2)	2464(1)	1742(2)	34(1)
C(78)	5691(2)	2636(1)	1168(2)	29(1)
C(79)	4516(2)	3999(1)	17(1)	20(1)
C(80)	4080(2)	4288(1)	485(2)	25(1)
C(81)	4059(2)	4785(1)	411(2)	32(1)
C(82)	4496(3)	5006(1)	-121(2)	42(1)
C(83)	4942(3)	4730(1)	-583(2)	43(1)
C(84)	4946(2)	4234(1)	-520(2)	29(1)
C(85)	4294(2)	3055(1)	-2514(1)	19(1)
C(86)	5126(2)	3323(1)	-2428(2)	22(1)
C(87)	5403(2)	3461(1)	-3117(2)	26(1)
C(88)	4858(2)	3326(1)	-3904(2)	29(1)
C(89)	4025(2)	3064(1)	-4005(2)	31(1)
C(90)	3743(2)	2931(1)	-3314(2)	26(1)
C(91)	4122(2)	2182(1)	-1484(1)	20(1)
C(92)	3583(2)	1859(1)	-2070(2)	29(1)
C(93)	3744(2)	1366(1)	-1991(2)	36(1)
C(94)	4440(2)	1186(1)	-1313(2)	35(1)
C(95)	4985(2)	1494(1)	-723(2)	31(1)
C(96)	4830(2)	1987(1)	-814(2)	24(1)
C(97A)	2219(5)	4957(2)	-2255(5)	50(2)
C(98A)	2162(4)	4506(2)	-1769(4)	29(1)
C(99A)	2734(6)	4505(3)	-3191(4)	54(2)
C(97B)	2669(6)	4860(3)	-2116(6)	55(2)
C(98B)	1781(5)	4599(2)	-2292(6)	51(2)
C(99B)	3293(6)	4267(3)	-2813(6)	58(2)
C(100)	2537(4)	4035(1)	-2847(3)	75(2)
C(101)	401(2)	2075(1)	208(1)	19(1)
C(102)	-402(2)	2386(1)	-329(1)	19(1)
C(103)	-810(2)	2698(1)	229(1)	21(1)
C(104)	-2236(2)	2942(1)	-958(1)	21(1)
C(105)	-2976(2)	2637(1)	-724(2)	30(1)
C(106)	-1720(2)	3401(1)	388(2)	22(1)
C(107)	-2278(2)	3845(1)	20(2)	30(1)
C(108)	1930(2)	1669(1)	306(2)	23(1)
C(109)	2735(2)	1610(1)	-87(2)	31(1)
C(110)	582(2)	1636(1)	-1028(2)	22(1)
C(111)	22(2)	1205(1)	-886(2)	32(1)
C(112)	3970(2)	-599(1)	-2625(2)	33(1)
C(113)	3898(2)	-171(1)	-2096(2)	37(1)
C(114)	3266(3)	289(1)	-3285(2)	44(1)
C(115)	3346(2)	-134(1)	-3821(2)	42(1)
C(116)	2213(3)	5953(2)	-4100(3)	68(1)
C(117)	1741(3)	6240(2)	-3591(3)	68(1)
C(118)	2357(4)	6937(2)	-3958(3)	66(1)
C(119)	2840(3)	6659(2)	-4469(2)	66(1)
C(120)	4710(3)	5771(1)	-2354(3)	55(1)
C(121)	4405(3)	6126(1)	-1838(3)	60(1)

C(122)	5279(3)	6721(1)	-2250(3)	56(1)
C(123)	5572(3)	6372(2)	-2783(3)	70(1)
C(124)	2374(4)	4720(2)	-5359(4)	83(2)
C(125)	3282(4)	5011(2)	-5074(4)	82(2)
C(126)	4155(4)	4367(2)	-5296(3)	70(1)
C(127)	3260(3)	4075(2)	-5566(2)	62(1)
C(128)	3182(4)	1251(2)	-5026(4)	98(2)
C(129)	3805(4)	1631(2)	-4566(4)	107(2)
C(130)	5129(4)	1187(2)	-4546(4)	90(2)
C(131)	4483(6)	814(2)	-5012(4)	129(3)

Tabelle x. Bindungslängen [Å] und Winkel [°] für sh2315.

Al(1)-O(16)	1.7212(16)	O(26)-C(126)	1.420(5)
Al(1)-O(5)	1.7291(17)	O(27A)-C(128)	1.372(6)
Al(1)-O(4)	1.7441(16)	O(27A)-C(131)	1.456(9)
Al(1)-O(1)	1.8149(17)	O(28A)-C(130)	1.431(6)
Al(2)-O(8)	1.7264(18)	O(28A)-C(129)	1.463(8)
Al(2)-O(7)	1.7293(17)	O(27B)-C(131)	1.649(16)
Al(2)-O(2)	1.7442(16)	O(27B)-C(128)	1.745(19)
Al(2)-O(1)	1.8144(17)	O(28B)-C(130)	1.632(12)
Al(3)-O(10)	1.7215(17)	O(28B)-C(129)	1.712(16)
Al(3)-O(2)	1.7328(17)	C(1)-C(6)	1.401(3)
Al(3)-O(11)	1.7430(17)	C(1)-C(2)	1.401(4)
Al(3)-O(3)	1.8343(17)	C(2)-C(3)	1.394(3)
Al(4)-O(14)	1.7183(17)	C(3)-C(4)	1.383(4)
Al(4)-O(4)	1.7256(16)	C(4)-C(5)	1.381(5)
Al(4)-O(13)	1.7315(16)	C(5)-C(6)	1.397(4)
Al(4)-O(3)	1.8350(17)	C(7)-C(12)	1.399(3)
Si(1)-O(5)	1.5988(17)	C(7)-C(8)	1.400(3)
Si(1)-O(6)	1.6200(17)	C(8)-C(9)	1.387(4)
Si(1)-C(7)	1.870(2)	C(9)-C(10)	1.401(4)
Si(1)-C(1)	1.873(2)	C(10)-C(11)	1.371(4)
Si(2)-O(7)	1.6071(17)	C(11)-C(12)	1.396(4)
Si(2)-O(6)	1.6318(17)	C(13)-C(18)	1.396(3)
Si(2)-C(19)	1.868(2)	C(13)-C(14)	1.399(3)
Si(2)-C(13)	1.872(2)	C(14)-C(15)	1.397(4)
Si(3)-O(8)	1.5922(17)	C(15)-C(16)	1.383(4)
Si(3)-O(9)	1.6466(18)	C(16)-C(17)	1.377(4)
Si(3)-C(25)	1.863(3)	C(17)-C(18)	1.394(4)
Si(3)-C(31)	1.868(3)	C(19)-C(24)	1.396(3)
Si(4)-O(10)	1.6030(17)	C(19)-C(20)	1.398(3)
Si(4)-O(9)	1.6271(18)	C(20)-C(21)	1.380(4)
Si(4)-C(37)	1.870(2)	C(21)-C(22)	1.384(4)
Si(4)-C(43)	1.877(2)	C(22)-C(23)	1.389(4)
Si(5)-O(11)	1.6077(18)	C(23)-C(24)	1.392(4)
Si(5)-O(12)	1.6319(18)	C(25)-C(30)	1.377(4)
Si(5)-C(49)	1.862(2)	C(25)-C(26)	1.414(4)
Si(5)-C(55)	1.877(3)	C(26)-C(27)	1.390(4)
Si(6)-O(13)	1.6048(16)	C(27)-C(28)	1.358(6)
Si(6)-O(12)	1.6317(17)	C(28)-C(29)	1.394(7)
Si(6)-C(61)	1.868(2)	C(29)-C(30)	1.402(5)
Si(6)-C(67)	1.872(2)	C(31)-C(36)	1.388(4)
Si(7)-O(14)	1.5987(16)	C(31)-C(32)	1.400(4)
Si(7)-O(15)	1.6351(16)	C(32)-C(33)	1.393(4)
Si(7)-C(79)	1.872(2)	C(33)-C(34)	1.348(5)
Si(7)-C(73)	1.879(2)	C(34)-C(35)	1.369(6)
Si(8)-O(16)	1.5982(16)	C(35)-C(36)	1.417(5)
Si(8)-O(15)	1.6427(17)	C(37)-C(42)	1.398(4)
Si(8)-C(85)	1.873(2)	C(37)-C(38)	1.404(4)
Si(8)-C(91)	1.876(2)	C(38)-C(39)	1.382(4)
N(1)-C(106)	1.503(3)	C(39)-C(40)	1.373(5)
N(1)-C(103)	1.503(3)	C(40)-C(41)	1.395(5)
N(1)-C(104)	1.507(3)	C(41)-C(42)	1.386(4)
N(2)-C(101)	1.493(3)	C(43)-C(48)	1.380(4)
N(2)-C(110)	1.501(3)	C(43)-C(44)	1.394(4)
N(2)-C(108)	1.506(3)	C(44)-C(45)	1.398(4)
O(17)-C(98B)	1.398(7)	C(45)-C(46)	1.373(4)
O(17)-C(100)	1.402(4)	C(46)-C(47)	1.369(5)
O(17)-C(98A)	1.492(6)	C(47)-C(48)	1.389(4)
O(18)-C(97B)	1.251(8)	C(49)-C(54)	1.392(4)
O(18)-C(99A)	1.275(8)	C(49)-C(50)	1.396(3)
O(18)-C(97A)	1.637(8)	C(50)-C(51)	1.392(3)
O(18)-C(99B)	1.659(8)	C(51)-C(52)	1.374(4)
O(19)-C(117)	1.398(5)	C(52)-C(53)	1.369(4)
O(19)-C(118)	1.414(5)	C(53)-C(54)	1.397(4)
O(20)-C(116)	1.400(5)	C(55)-C(60)	1.391(4)
O(20)-C(119)	1.423(5)	C(55)-C(56)	1.395(3)
O(21)-C(122)	1.414(5)	C(56)-C(57)	1.389(4)
O(21)-C(121)	1.423(4)	C(57)-C(58)	1.379(4)
O(22)-C(123)	1.416(5)	C(58)-C(59)	1.373(4)
O(22)-C(120)	1.432(5)	C(59)-C(60)	1.393(4)
O(23)-C(114)	1.415(4)	C(61)-C(62)	1.398(3)
O(23)-C(113)	1.428(4)		
O(24)-C(112)	1.420(4)		
O(24)-C(115)	1.429(4)		
O(25)-C(127)	1.415(5)		
O(25)-C(124)	1.429(5)		
O(26)-C(125)	1.391(6)		

O(6)-Si(1)-C(7) 105.06(10)
O(5)-Si(1)-C(1) 110.68(10)
O(6)-Si(1)-C(1) 106.85(10)
C(7)-Si(1)-C(1) 111.86(11)
O(7)-Si(2)-O(6) 111.97(9)
O(7)-Si(2)-C(19) 111.82(10)
O(6)-Si(2)-C(19) 106.61(10)
O(7)-Si(2)-C(13) 108.82(9)
O(6)-Si(2)-C(13) 106.44(10)
C(19)-Si(2)-C(13) 111.06(11)
O(8)-Si(3)-O(9) 111.09(9)
O(8)-Si(3)-C(25) 113.77(11)
O(9)-Si(3)-C(25) 104.16(11)
O(8)-Si(3)-C(31) 110.94(10)
O(9)-Si(3)-C(31) 107.29(10)
C(25)-Si(3)-C(31) 109.21(12)
O(10)-Si(4)-O(9) 114.36(9)
O(10)-Si(4)-C(37) 110.79(10)
O(9)-Si(4)-C(37) 105.90(10)
O(10)-Si(4)-C(43) 107.99(10)
O(9)-Si(4)-C(43) 105.91(10)
C(37)-Si(4)-C(43) 111.85(11)
O(11)-Si(5)-O(12) 112.74(9)
O(11)-Si(5)-C(49) 109.04(10)
O(12)-Si(5)-C(49) 106.62(10)
O(11)-Si(5)-C(55) 112.51(10)
O(12)-Si(5)-C(55) 106.74(10)
C(49)-Si(5)-C(55) 108.96(11)
O(13)-Si(6)-O(12) 110.96(9)
O(13)-Si(6)-C(61) 111.60(9)
O(12)-Si(6)-C(61) 108.84(10)
O(13)-Si(6)-C(67) 110.15(10)
O(12)-Si(6)-C(67) 106.77(10)
C(61)-Si(6)-C(67) 108.37(11)
O(14)-Si(7)-O(15) 113.07(9)
O(14)-Si(7)-C(79) 108.98(10)
O(15)-Si(7)-C(79) 107.70(10)
O(14)-Si(7)-C(73) 109.85(9)
O(15)-Si(7)-C(73) 106.90(9)
C(79)-Si(7)-C(73) 110.30(11)
O(16)-Si(8)-O(15) 112.71(9)
O(16)-Si(8)-C(85) 108.57(9)
O(15)-Si(8)-C(85) 108.25(10)
O(16)-Si(8)-C(91) 111.11(9)
O(15)-Si(8)-C(91) 107.43(10)
C(85)-Si(8)-C(91) 108.66(10)
C(97A)-O(18)-C(99B) 117.2(3)
C(117)-O(19)-C(118) 110.1(3)
C(116)-O(20)-C(119) 111.5(3)
C(122)-O(21)-C(121) 109.7(3)
C(123)-O(22)-C(120) 110.2(3)
C(114)-O(23)-C(113) 110.1(2)
C(112)-O(24)-C(115) 110.9(2)
C(127)-O(25)-C(124) 108.1(4)
C(125)-O(26)-C(126) 109.7(4)
C(128)-O(27A)-C(131) 105.5(4)
C(130)-O(28A)-C(129) 104.5(4)
C(131)-O(27B)-C(128) 83.1(8)
C(130)-O(28B)-C(129) 86.3(6)
C(6)-C(1)-C(2) 116.8(2)
C(6)-C(1)-Si(1) 123.7(2)
C(2)-C(1)-Si(1) 119.49(18)
C(3)-C(2)-C(1) 121.8(2)
C(4)-C(3)-C(2) 119.8(3)
C(5)-C(4)-C(3) 120.0(3)
C(4)-C(5)-C(6) 119.9(3)
C(5)-C(6)-C(1) 121.6(3)
C(12)-C(7)-C(8) 117.1(2)
C(12)-C(7)-Si(1) 120.62(19)
C(8)-C(7)-Si(1) 122.24(19)
C(9)-C(8)-C(7) 121.9(3)
C(8)-C(9)-C(10) 119.6(3)
C(11)-C(10)-C(9) 119.5(2)
C(10)-C(11)-C(12) 120.5(3)
C(11)-C(12)-C(7) 121.3(2)
C(18)-C(13)-C(14) 116.8(2)
C(18)-C(13)-Si(2) 122.40(19)
C(14)-C(13)-Si(2) 120.64(18)
C(15)-C(14)-C(13) 121.8(2)
C(16)-C(15)-C(14) 119.6(3)
C(17)-C(16)-C(15) 120.0(2)
C(16)-C(17)-C(18) 120.0(3)
C(17)-C(18)-C(13) 121.8(3)
C(24)-C(19)-C(20) 117.7(2)
C(24)-C(19)-Si(2) 120.60(19)
C(20)-C(19)-Si(2) 121.68(18)
C(21)-C(20)-C(19) 121.3(2)
C(20)-C(21)-C(22) 120.3(3)
C(21)-C(22)-C(23) 119.6(3)
C(22)-C(23)-C(24) 119.8(3)
C(23)-C(24)-C(19) 121.1(3)
C(30)-C(25)-C(26) 117.1(3)

C(43)-C(48)-C(47) 121.6(3)	N(1)-C(103)-C(102) 112.73(18)
C(54)-C(49)-C(50) 116.7(2)	N(1)-C(104)-C(105) 114.3(2)
C(54)-C(49)-Si(5) 121.92(19)	N(1)-C(106)-C(107) 113.6(2)
C(50)-C(49)-Si(5) 121.29(18)	N(2)-C(108)-C(109) 112.4(2)
C(51)-C(50)-C(49) 122.0(2)	N(2)-C(110)-C(111) 114.9(2)
C(52)-C(51)-C(50) 119.9(3)	O(24)-C(112)-C(113) 110.4(3)
C(53)-C(52)-C(51) 119.6(2)	O(23)-C(113)-C(112) 110.6(2)
C(52)-C(53)-C(54) 120.6(3)	O(23)-C(114)-C(115) 111.2(3)
C(49)-C(54)-C(53) 121.2(3)	O(24)-C(115)-C(114) 110.6(3)
C(60)-C(55)-C(56) 116.7(2)	O(20)-C(116)-C(117) 111.9(4)
C(60)-C(55)-Si(5) 121.32(19)	O(19)-C(117)-C(116) 114.0(4)
C(56)-C(55)-Si(5) 121.92(19)	O(19)-C(118)-C(119) 113.1(4)
C(57)-C(56)-C(55) 121.5(3)	O(20)-C(119)-C(118) 112.0(4)
C(58)-C(57)-C(56) 120.4(3)	O(22)-C(120)-C(121) 110.5(3)
C(59)-C(58)-C(57) 119.5(3)	O(21)-C(121)-C(120) 112.7(4)
C(58)-C(59)-C(60) 119.8(3)	O(21)-C(122)-C(123) 112.4(3)
C(55)-C(60)-C(59) 122.1(2)	O(22)-C(123)-C(122) 112.4(3)
C(62)-C(61)-C(66) 117.3(2)	O(25)-C(124)-C(125) 109.7(4)
C(62)-C(61)-Si(6) 121.35(18)	O(26)-C(125)-C(124) 112.0(4)
C(66)-C(61)-Si(6) 121.34(18)	O(26)-C(126)-C(127) 111.7(4)
C(63)-C(62)-C(61) 121.3(2)	O(25)-C(127)-C(126) 111.2(4)
C(64)-C(63)-C(62) 120.2(2)	O(27A)-C(128)-C(129) 109.9(5)
C(65)-C(64)-C(63) 119.8(2)	O(27A)-C(128)-O(27B) 82.9(7)
C(64)-C(65)-C(66) 119.9(2)	C(129)-C(128)-O(27B) 83.0(9)
C(65)-C(66)-C(61) 121.6(2)	C(128)-C(129)-O(28A) 107.9(5)
C(72)-C(67)-C(68)	C(128)-C(129)-O(28B) 88.0(6)
	O(28A)-C(129)-O(28B) 79.9(5)
	O(28A)-C(130)-C(131) 106.5(5)
	O(28A)-C(130)-O(28B) 83.6(6)
	C(131)-C(130)-O(28B) 86.7(6)
	O(27A)-C(131)-C(130) 110.0(5)
	O(27A)-C(131)-O(27B) 84.0(8)
	C(88)-C(89)-C(90) 120.0(2)
	C(89)-C(90)-C(85) 121.0(2)
	C(92)-C(91)-C(96) 116.7(2)
	C(92)-C(91)-Si(8) 120.68(19)
	C(96)-C(91)-Si(8) 122.61(18)
	C(93)-C(92)-C(91) 121.6(3)
	C(94)-C(93)-C(92)

116.8(2)
C(72)-C(67)-Si(6)
120.40(18)
C(68)-C(67)-Si(6)
122.74(19)
C(69)-C(68)-C(67)
121.6(3)
C(70)-C(69)-C(68)
120.0(3)
C(71)-C(70)-C(69)
120.0(3)
C(70)-C(71)-C(72)
119.7(3)
C(71)-C(72)-C(67)
121.8(2)
C(74)-C(73)-C(78)
117.1(2)
C(74)-C(73)-Si(7)
122.44(19)
C(78)-C(73)-Si(7)
120.44(19)
C(73)-C(74)-C(75)
121.5(2)
C(76)-C(75)-C(74)
119.8(3)
C(77)-C(76)-C(75)
119.7(2)
C(76)-C(77)-C(78)
120.1(3)
C(77)-C(78)-C(73)
121.8(3)
C(80)-C(79)-C(84)
117.1(2)
C(80)-C(79)-Si(7)
120.63(18)
C(84)-C(79)-Si(7)
122.24(18)
C(81)-C(80)-C(79)
121.5(3)
C(82)-C(81)-C(80)
119.9(3)
C(83)-C(82)-C(81)
119.8(3)
C(84)-C(83)-C(82)
120.1(3)
C(83)-C(84)-C(79)
121.5(3)
C(90)-C(85)-C(86)
117.9(2)
C(90)-C(85)-Si(8)
118.68(18)

120.0(3)
C(95)-C(94)-C(93)
120.0(3)
C(94)-C(95)-C(96)
119.7(3)
C(95)-C(96)-C(91)
122.1(3)
C(98A)-C(97A)-O(18)
103.7(4)
O(17)-C(98A)-C(97A)
106.9(5)
O(18)-C(99A)-C(100)
117.2(5)
O(18)-C(97B)-C(98B)
114.6(7)
O(17)-C(98B)-C(97B)
113.1(6)
C(100)-C(99B)-O(18)
107.3(5)
C(99B)-C(100)-O(17)
128.2(5)
C(99B)-C(100)-C(99A)
46.0(5)
O(17)-C(100)-C(99A)
109.3(4)
N(2)-C(101)-C(102)
111.21(18)
C(101)-C(102)-C(103)
109.25(19)
C(130)-C(131)-O(27B)
84.0(10)

C(86)-C(85)-Si(8) 123.38(18) C(87)-C(86)-C(85) 121.2(2) C(88)-C(87)-C(86) 120.0(2) C(87)-C(88)-C(89) 119.8(2)	

Tabelle x U_{ij}-Werte ($Å^2 x\ 10^3$) des Temperaturfaktors exp $(-2p^2[\ h^2\ a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ])$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	15(1)	13(1)	15(1)	0(1)	5(1)	1(1)
Al(2)	17(1)	12(1)	17(1)	-1(1)	6(1)	1(1)
Al(3)	19(1)	12(1)	17(1)	-1(1)	7(1)	1(1)
Al(4)	16(1)	13(1)	15(1)	-1(1)	5(1)	0(1)
Si(1)	17(1)	16(1)	17(1)	-2(1)	4(1)	2(1)
Si(2)	16(1)	14(1)	19(1)	-1(1)	5(1)	1(1)
Si(3)	24(1)	13(1)	18(1)	2(1)	7(1)	3(1)
Si(4)	22(1)	11(1)	22(1)	-1(1)	7(1)	0(1)
Si(5)	22(1)	17(1)	18(1)	-2(1)	9(1)	2(1)
Si(6)	20(1)	16(1)	16(1)	0(1)	7(1)	1(1)
Si(7)	15(1)	16(1)	17(1)	-1(1)	6(1)	-1(1)
Si(8)	16(1)	16(1)	17(1)	-1(1)	7(1)	0(1)
N(1)	18(1)	19(1)	19(1)	-2(1)	8(1)	1(1)
N(2)	20(1)	13(1)	20(1)	3(1)	7(1)	0(1)
O(1)	17(1)	15(1)	19(1)	2(1)	8(1)	0(1)
O(2)	19(1)	15(1)	20(1)	-2(1)	8(1)	0(1)
O(3)	18(1)	13(1)	22(1)	0(1)	7(1)	-1(1)
O(4)	17(1)	15(1)	17(1)	0(1)	6(1)	0(1)
O(5)	22(1)	19(1)	17(1)	-2(1)	6(1)	1(1)
O(6)	17(1)	22(1)	24(1)	-5(1)	5(1)	2(1)
O(7)	20(1)	17(1)	20(1)	-2(1)	6(1)	-2(1)
O(8)	27(1)	15(1)	25(1)	2(1)	5(1)	5(1)
O(9)	29(1)	16(1)	24(1)	3(1)	9(1)	1(1)
O(10)	26(1)	13(1)	22(1)	0(1)	6(1)	1(1)
O(11)	24(1)	20(1)	20(1)	0(1)	11(1)	3(1)
O(12)	27(1)	22(1)	19(1)	0(1)	9(1)	5(1)
O(13)	21(1)	17(1)	20(1)	1(1)	7(1)	0(1)
O(14)	17(1)	25(1)	20(1)	-2(1)	7(1)	0(1)
O(15)	18(1)	21(1)	21(1)	-2(1)	8(1)	-2(1)
O(16)	17(1)	20(1)	20(1)	0(1)	8(1)	1(1)
O(17)	36(1)	21(1)	64(1)	5(1)	29(1)	-2(1)
O(18)	76(2)	77(2)	75(2)	14(2)	17(2)	-55(2)
O(19)	75(2)	48(2)	50(2)	-4(1)	12(1)	-2(1)
O(20)	76(2)	65(2)	51(2)	-9(1)	-1(1)	13(2)
O(21)	66(2)	41(1)	60(2)	0(1)	-11(1)	-10(1)
O(22)	47(1)	39(1)	87(2)	-12(1)	15(1)	-2(1)
O(23)	33(1)	42(1)	50(1)	-11(1)	14(1)	4(1)
O(24)	38(1)	35(1)	41(1)	-6(1)	17(1)	-1(1)
O(25)	79(2)	56(2)	75(2)	9(2)	11(2)	-3(2)
O(26)	86(2)	57(2)	95(2)	15(2)	23(2)	4(2)
O(27A)	53(3)	20(2)	80(3)	9(2)	20(2)	-6(2)
O(28A)	53(3)	25(2)	72(3)	12(2)	17(2)	-9(2)
O(27B)	400(30)	300(20)	109(9)	84(12)	132(13)	220(20)
O(28B)	231(14)	169(12)	91(7)	-16(7)	94(8)	-55(11)
C(101)	21(1)	19(1)	18(1)	1(1)	8(1)	1(1)
C(102)	20(1)	17(1)	20(1)	-1(1)	5(1)	3(1)
C(103)	23(1)	21(1)	21(1)	-1(1)	8(1)	2(1)
C(104)	20(1)	21(1)	22(1)	-1(1)	6(1)	2(1)
C(105)	25(1)	28(1)	36(2)	-3(1)	8(1)	-5(1)
C(106)	25(1)	22(1)	23(1)	-5(1)	11(1)	1(1)
C(107)	33(1)	23(1)	33(1)	-4(1)	10(1)	5(1)
C(108)	21(1)	22(1)	27(1)	6(1)	8(1)	5(1)
C(109)	24(1)	24(1)	47(2)	10(1)	15(1)	7(1)
C(110)	26(1)	18(1)	23(1)	1(1)	10(1)	2(1)
C(111)	40(2)	18(1)	35(2)	-3(1)	8(1)	-7(1)
C(112)	29(1)	33(2)	37(2)	-4(1)	6(1)	0(1)
C(113)	29(1)	43(2)	38(2)	-11(1)	6(1)	-4(1)
C(114)	48(2)	35(2)	50(2)	-7(2)	13(2)	-1(1)
C(115)	55(2)	33(2)	37(2)	-3(1)	14(2)	-3(1)
C(116)	78(3)	49(2)	67(3)	-13(2)	4(2)	-4(2)
C(117)	70(3)	52(2)	83(3)	1(2)	23(2)	-4(2)
C(118)	89(3)	46(2)	59(2)	6(2)	16(2)	7(2)
C(119)	82(3)	70(3)	43(2)	-5(2)	10(2)	-8(2)
C(120)	49(2)	25(2)	74(3)	7(2)	-8(2)	-7(1)
C(121)	75(3)	41(2)	56(2)	5(2)	7(2)	-16(2)
C(122)	55(2)	27(2)	83(3)	-1(2)	15(2)	-7(2)
C(123)	49(2)	44(2)	114(4)	-11(2)	21(2)	-9(2)
C(124)	77(3)	56(3)	111(4)	23(3)	19(3)	12(2)
C(125)	87(4)	45(2)	114(4)	6(3)	30(3)	5(2)
C(126)	78(3)	63(3)	66(3)	13(2)	16(2)	14(2)

C(127)	85(3)	46(2)	46(2)	10(2)	4(2)	6(2)
C(128)	68(3)	58(3)	151(6)	11(3)	6(3)	-2(2)
C(129)	95(4)	77(4)	125(5)	-34(4)	-3(4)	23(3)
C(130)	69(3)	55(3)	151(5)	0(3)	42(3)	-2(2)
C(131)	217(9)	67(4)	78(4)	-26(3)	1(5)	48(5)

sh2159

Tabelle x. Kristalldaten und Strukturverfeinerung für **18**.

Identifizierungscode	sh2159	
Summenformel	C66 H67 Al2 O10 Si4 Zn	
Molmasse	1251.89	
Temperatur	103(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem	Triclinic	
Raumgruppe	P-1	
Gitterkonstanten	a = 13.909(3) Å	a= 64.33(3)°.
	b = 15.666(3) Å	b= 73.92(3)°.
	c = 17.529(4) Å	g = 80.74(3)°.
Zellvolumen	3304.2(12) $Å^3$	
Anzahl der Formeleinheiten	2	
Röntgenographische Dichte	1.258 Mg/m^3	
Absorptionskoeffizient	0.526 mm^{-1}	
F(000)	1310	
Kristallgröße	0.8 x 0.3 x 0.2 mm^3	
Gemessener Theta-Bereich	2.64 to 31.89°.	
Indexbereich	-19<=h<=20, -23<=k<=23, -25<=l<=26	
Anzahl gemessener Reflexe	88906	
Unabhängige Reflexe	21994 [R(int) = 0.0286]	
Datenvollständigkeit bis Theta = 31.89°	96.7 %	
Absorptionskorrektur	None	
Verfeinerung	Full-matrix least-squares on F^2	
Daten/ Restraints / Parameter	21994 / 0 / 672	
Goodness-of-fit on F^2	2.599	
Endgültige R-Werte [I>2sigma(I)]	R1 = 0.0872, wR2 = 0.2708	
R-Werte (all Daten)	R1 = 0.1061, wR2 = 0.2952	
Restelektronendichte	4.840 and -1.068 e.$Å^{-3}$	

Tabelle x Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$x 10^3) für **18**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalisierten U_{ij}-Tensors.

	x	y	z	U(eq)
Zn	942(1)	5938(1)	9518(1)	22(1)
Si(1)	772(1)	3736(1)	7388(1)	20(1)
Si(2)	2292(1)	2550(1)	8538(1)	21(1)
Al(1)	96(1)	5150(1)	8425(1)	19(1)
Al(2)	1459(1)	3808(1)	9689(1)	21(1)
Si(3)	-2713(1)	6814(1)	8891(1)	26(1)
Si(4)	-689(1)	7390(1)	7468(1)	25(1)
O(1)	957(1)	4959(1)	9093(1)	21(1)
O(2)	1037(1)	5337(1)	10749(1)	23(1)
O(3)	295(2)	3258(1)	10412(1)	24(1)
O(4)	481(2)	4520(1)	7791(1)	25(1)
O(5)	1536(2)	2865(1)	7879(1)	25(1)
O(6)	2081(2)	3199(1)	9077(1)	27(1)
O(8)	2242(2)	3893(1)	10283(1)	25(1)
O(9)	-127(2)	6360(1)	7852(1)	27(1)
O(10)	-1848(2)	7411(2)	8044(1)	36(1)
C(1)	1437(2)	4276(2)	6203(2)	23(1)
C(2)	2400(2)	3943(2)	5886(2)	35(1)
C(3)	2871(3)	4337(3)	4991(2)	44(1)
C(4)	2387(3)	5059(3)	4398(2)	40(1)
C(5)	1425(3)	5407(2)	4696(2)	38(1)
C(6)	956(2)	5009(2)	5587(2)	33(1)
C(7)	-387(2)	3162(2)	7483(2)	25(1)
C(8)	-1378(2)	3470(2)	7773(2)	33(1)
C(9)	-2212(3)	3063(3)	7759(2)	43(1)
C(10)	-2056(3)	2350(3)	7456(2)	47(1)
C(11)	-1078(3)	2024(2)	7179(2)	42(1)
C(12)	-252(3)	2427(2)	7192(2)	32(1)
C(13)	2081(2)	1256(2)	9279(2)	25(1)

C(14)	1444(3)	732(2)	9162(2)	42(1)
C(15)	1278(4)	-238(3)	9717(2)	52(1)
C(16)	1742(3)	-689(2)	10417(2)	45(1)
C(17)	2355(3)	-178(2)	10562(2)	41(1)
C(18)	2528(3)	788(2)	9997(2)	33(1)
C(19)	3615(2)	2743(2)	7853(2)	30(1)
C(20)	3959(3)	3668(3)	7359(2)	44(1)
C(21)	4913(3)	3866(3)	6782(3)	54(1)
C(22)	5550(3)	3115(4)	6712(3)	69(1)
C(23)	5275(4)	2197(4)	7221(5)	92(2)
C(24)	4318(3)	2014(3)	7793(3)	62(1)
C(25)	-3637(2)	7726(2)	9141(2)	34(1)
C(26)	-4242(2)	7526(3)	9987(2)	38(1)
C(27)	-4956(3)	8201(3)	10161(3)	54(1)
C(28)	-5068(4)	9086(4)	9496(4)	70(1)
C(29)	-4467(5)	9321(4)	8668(4)	77(2)
C(30)	-3761(4)	8641(3)	8482(3)	57(1)
C(31)	-3295(3)	6039(3)	8582(2)	41(1)
C(32)	-3313(4)	6287(5)	7709(3)	72(2)
C(33A)	-3721(7)	5881(9)	7364(7)	54(1)
C(34A)	-4126(8)	5029(9)	7951(8)	54(1)
C(33B)	-3776(7)	5474(9)	7630(7)	54(1)
C(34B)	-4211(7)	4686(8)	8314(7)	54(1)
C(35)	-4174(6)	4590(5)	8987(6)	100(2)
C(36)	-3730(4)	5184(4)	9214(4)	66(1)
C(37)	-47(3)	8323(2)	7530(2)	34(1)
C(38)	970(3)	8516(2)	7073(2)	41(1)
C(39)	1462(4)	9203(3)	7124(3)	59(1)
C(40)	931(5)	9682(3)	7655(3)	65(2)
C(41)	-43(4)	9511(3)	8094(3)	54(1)
C(42)	-536(4)	8849(2)	8024(2)	47(1)
C(43)	-747(2)	7746(2)	6316(2)	30(1)
C(44)	-816(3)	7049(2)	6014(2)	41(1)
C(45)	-903(4)	7329(3)	5158(2)	49(1)
C(46)	-916(4)	8301(3)	4594(2)	50(1)
C(47)	-850(4)	8986(3)	4877(2)	55(1)
C(48)	-774(3)	8709(2)	5737(2)	43(1)
O(11)	2149(2)	6725(2)	8780(2)	54(1)
C(49A)	2672(6)	6614(6)	7953(5)	67(1)
C(49B)	3150(16)	6268(16)	8383(13)	67(1)
C(50A)	3499(6)	5861(5)	8097(5)	67(1)
C(50B)	3012(16)	6392(15)	7580(14)	67(1)
C(51A)	2657(6)	7336(5)	8875(5)	50(1)
C(51B)	2242(10)	7567(9)	9063(8)	50(1)
C(52A)	2069(8)	7508(7)	9626(7)	68(2)
C(52B)	3034(10)	7372(9)	9553(8)	68(2)
C(53)	6763(7)	8922(7)	3211(6)	119(3)
C(54)	6781(9)	8570(9)	4105(7)	137(3)
C(55)	6441(7)	9139(7)	4504(6)	111(3)
C(56)	6009(7)	9981(6)	4104(6)	108(2)
C(57)	5855(10)	10352(10)	3230(9)	155(4)
C(58)	6361(8)	9790(8)	2771(7)	128(3)
C(59)	6431(14)	8676(13)	5501(11)	218(7)
C(60)	7513(10)	2914(9)	4649(8)	147(4)
C(61)	8050(7)	2261(7)	5018(6)	113(3)
C(62)	8007(11)	1262(11)	5531(10)	167(5)
C(63)	7212(16)	801(13)	5760(12)	211(7)
C(64)	6429(15)	1549(15)	5344(13)	203(6)
C(65)	6319(16)	2324(16)	4911(13)	211(7)
C(66A)	6899(17)	3557(16)	4214(14)	129(6)
C(66B)	5640(20)	2940(20)	4695(17)	151(8)

Tabelle x. Bindungslängen [Å] und Winkel [°] für **18**.

Zn-O(3)#1	1.969(2)	Al(2)-O(1)-Al(1)	122.64(11)
Zn-O(1)	1.9693(18)	Al(2)-O(1)-Zn	116.58(10)
Zn-O(2)	1.9799(19)	Al(1)-O(1)-Zn	116.90(9)
Zn-O(11)	2.024(3)	Al(1)#1-O(2)-Zn	117.41(10)
Si(1)-O(4)	1.6150(19)	Al(2)-O(3)-Zn#1	119.19(10)
Si(1)-O(5)	1.659(2)	Si(1)-O(4)-Al(1)	167.81(13)
Si(1)-C(1)	1.884(3)	Si(2)-O(5)-Si(1)	143.58(13)
Si(1)-C(7)	1.903(3)		
Si(2)-O(6)	1.610(2)		
Si(2)-O(5)	1.643(2)		
Si(2)-C(19)	1.887(3)		
Si(2)-C(13)	1.892(3)		

Al(1)-O(4)	1.7163(19)	Si(2)-O(6)-Al(2)	160.96(15)
Al(1)-O(9)	1.740(2)	Si(3)#1-O(8)-Al(2)	137.31(13)
Al(1)-O(1)	1.803(2)	Si(4)-O(9)-Al(1)	162.15(15)
Al(1)-O(2)#1	1.825(2)	Si(3)-O(10)-Si(4)	146.32(14)
Al(2)-O(6)	1.707(2)	C(2)-C(1)-C(6)	117.5(2)
Al(2)-O(8)	1.756(2)	C(2)-C(1)-Si(1)	121.99(19)
Al(2)-O(1)	1.7881(19)	C(51A)-O(11)-C(49A)	108.9(5)
Al(2)-O(3)	1.827(2)	C(51A)-O(11)-C(49B)	92.6(9)
Si(3)-O(8)#1	1.630(2)	C(49A)-O(11)-C(49B)	39.8(8)
Si(3)-O(10)	1.642(3)	C(51A)-O(11)-C(51B)	25.5(4)
Si(3)-C(25)	1.877(3)	C(49A)-O(11)-C(51B)	128.4(6)
Si(3)-C(31)	1.884(4)	C(49B)-O(11)-C(51B)	118.1(10)
Si(4)-O(9)	1.618(2)	C(51A)-O(11)-Zn	134.2(4)
Si(4)-O(10)	1.651(2)	C(49A)-O(11)-Zn	116.7(4)
Si(4)-C(43)	1.871(3)	C(49B)-O(11)-Zn	120.9(8)
Si(4)-C(37)	1.885(3)	C(51B)-O(11)-Zn	113.1(5)
O(2)-Al(1)#1	1.825(2)	C(50A)-C(49A)-O(11)	111.3(6)
O(3)-Zn#1	1.969(2)	C(50B)-C(49B)-O(11)	103.4(16)
O(8)-Si(3)#1	1.631(2)	O(11)-C(51A)-C(52A)	107.2(7)
C(1)-C(2)	1.410(4)	C(52B)-C(51B)-O(11)	114.3(10)
C(1)-C(6)	1.417(4)	C(65)-C(66B)-C(66A)	72.2(17)
C(2)-C(3)	1.412(4)	O(3)#1-Zn-O(1)	117.00(8)
C(3)-C(4)	1.391(5)	O(3)#1-Zn-O(2)	101.23(8)
O(4)-Al(1)-O(9)	114.61(10)	O(1)-Zn-O(2)	110.10(8)
O(4)-Al(1)-O(1)	111.51(9)	O(3)#1-Zn-O(11)	111.54(10)
O(9)-Al(1)-O(1)	110.06(10)	O(1)-Zn-O(11)	107.45(11)
O(4)-Al(1)-O(2)#1	109.89(10)	O(2)-Zn-O(11)	109.28(12)
O(9)-Al(1)-O(2)#1	108.69(10)		
O(1)-Al(1)-O(2)#1	101.21(9)	O(6)-Al(2)-O(8)	109.83(10)
		O(6)-Al(2)-O(1)	115.12(9)
		O(8)-Al(2)-O(1)	109.88(10)
		O(6)-Al(2)-O(3)	111.65(11)
		O(8)-Al(2)-O(3)	110.88(10)
		O(1)-Al(2)-O(3)	99.08(10)

Symmetrieoperationen zur Erzeugung äquivalenter Atome: #1 -x,-y+1,-z+2

Tabelle x U_{ij}-Werte ($Å^2 x\ 10^3$) des Temperaturfaktors exp $(-2p^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ])$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn	28(1)	19(1)	19(1)	-8(1)	-3(1)	-3(1)
Si(1)	26(1)	18(1)	15(1)	-7(1)	-5(1)	1(1)

Si(2)	26(1)	19(1)	16(1)	-7(1)	-5(1)	3(1)
Al(1)	27(1)	15(1)	15(1)	-6(1)	-6(1)	2(1)
Al(2)	27(1)	18(1)	18(1)	-8(1)	-8(1)	2(1)
Si(3)	29(1)	28(1)	24(1)	-14(1)	-12(1)	8(1)
Si(4)	39(1)	17(1)	17(1)	-5(1)	-9(1)	4(1)
O(1)	28(1)	19(1)	17(1)	-6(1)	-7(1)	1(1)
O(2)	24(1)	25(1)	20(1)	-8(1)	-6(1)	0(1)
O(3)	29(1)	19(1)	21(1)	-5(1)	-5(1)	0(1)
O(4)	34(1)	24(1)	22(1)	-13(1)	-10(1)	5(1)
O(5)	34(1)	21(1)	21(1)	-10(1)	-9(1)	6(1)
O(6)	33(1)	27(1)	25(1)	-15(1)	-9(1)	6(1)
O(8)	29(1)	25(1)	24(1)	-11(1)	-12(1)	3(1)
O(9)	40(1)	16(1)	21(1)	-5(1)	-9(1)	2(1)
O(10)	41(1)	31(1)	25(1)	-7(1)	-7(1)	10(1)
C(1)	29(1)	22(1)	18(1)	-7(1)	-7(1)	-1(1)
C(2)	33(1)	42(2)	20(1)	-9(1)	-4(1)	6(1)
C(3)	36(2)	59(2)	26(1)	-13(1)	0(1)	6(2)
C(4)	48(2)	45(2)	18(1)	-8(1)	0(1)	-8(1)
C(5)	45(2)	39(2)	19(1)	0(1)	-9(1)	-1(1)
C(6)	36(2)	32(1)	22(1)	-6(1)	-5(1)	3(1)
C(7)	29(1)	23(1)	19(1)	-4(1)	-7(1)	-2(1)
C(8)	31(1)	32(1)	30(1)	-7(1)	-6(1)	-3(1)
C(9)	32(2)	43(2)	37(2)	2(1)	-8(1)	-9(1)
C(10)	54(2)	37(2)	39(2)	8(1)	-24(2)	-21(2)
C(11)	58(2)	31(1)	37(2)	-7(1)	-18(2)	-13(1)
C(12)	42(2)	25(1)	30(1)	-10(1)	-12(1)	-5(1)
C(13)	32(1)	21(1)	20(1)	-8(1)	-5(1)	1(1)
C(14)	64(2)	30(1)	35(2)	-4(1)	-26(2)	-8(1)
C(15)	87(3)	33(2)	40(2)	-5(1)	-31(2)	-16(2)
C(16)	74(3)	25(1)	31(1)	-4(1)	-16(2)	-9(1)
C(17)	62(2)	26(1)	30(1)	-1(1)	-20(1)	0(1)
C(18)	46(2)	23(1)	26(1)	-4(1)	-14(1)	-2(1)
C(19)	28(1)	30(1)	26(1)	-7(1)	-6(1)	1(1)
C(20)	39(2)	45(2)	47(2)	-22(2)	4(1)	-12(1)
C(21)	45(2)	64(2)	43(2)	-16(2)	3(2)	-19(2)
C(22)	36(2)	76(3)	66(3)	-14(2)	6(2)	-4(2)
C(23)	45(2)	54(3)	125(5)	-20(3)	22(3)	12(2)
C(24)	42(2)	37(2)	76(3)	-12(2)	11(2)	6(2)
C(25)	33(1)	36(1)	40(2)	-21(1)	-19(1)	12(1)
C(26)	30(1)	44(2)	48(2)	-28(2)	-7(1)	1(1)
C(27)	30(2)	67(3)	83(3)	-56(2)	-4(2)	7(2)
C(28)	51(2)	69(3)	103(4)	-56(3)	-23(3)	31(2)
C(29)	89(4)	50(2)	81(3)	-22(2)	-32(3)	36(3)
C(30)	67(3)	49(2)	46(2)	-18(2)	-22(2)	30(2)
C(31)	35(2)	59(2)	49(2)	-41(2)	-17(1)	11(1)
C(32)	57(3)	132(5)	63(3)	-70(3)	-26(2)	8(3)
C(35)	99(5)	98(5)	146(7)	-71(5)	-50(5)	-23(4)
C(36)	69(3)	63(3)	91(4)	-45(3)	-33(3)	-7(2)
C(37)	60(2)	19(1)	22(1)	-4(1)	-17(1)	-1(1)
C(38)	63(2)	30(1)	32(1)	-7(1)	-22(1)	-8(1)
C(39)	90(3)	39(2)	50(2)	-2(2)	-33(2)	-22(2)
C(40)	123(5)	30(2)	63(2)	-16(2)	-60(3)	-3(2)
C(41)	90(3)	33(2)	55(2)	-23(2)	-37(2)	8(2)
C(42)	83(3)	26(1)	37(2)	-17(1)	-25(2)	15(2)
C(43)	46(2)	23(1)	21(1)	-9(1)	-11(1)	5(1)
C(44)	73(2)	26(1)	28(1)	-14(1)	-18(1)	8(1)
C(45)	83(3)	44(2)	34(2)	-24(1)	-28(2)	11(2)
C(46)	76(3)	51(2)	28(1)	-17(1)	-24(2)	8(2)
C(47)	95(3)	36(2)	29(2)	-1(1)	-29(2)	-2(2)
C(48)	77(3)	26(1)	27(1)	-6(1)	-23(2)	2(1)
O(11)	41(1)	44(1)	59(2)	-14(1)	9(1)	-17(1)

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sh2212

Tabelle x. Kristalldaten und Strukturverfeinerung für **20**.

Identifizierungscode	sh2212	
Summenformel	C_{111} H_{106} Al_4 SnO_{20} Si_8	
Molmasse	2211.29	
Temperatur	293(2) K	
Wellenlänge	0.71073 Å	
Kristallsystem	triklin	
Raumgruppe	P-1	
Gitterkonstanten	a = 14.6637(12) Å	α= 89, 008(6)°.
	b = 15.1005(13) Å	β= 88.012(6)°.

	c = 24.463(2) Å	γ = 81,251(6)°.
Zellvolumen	5350.2(8) $Å^3$	
Anzahl der Formeleinheiten	2	
Density (calculated)	1.373 Mg/m^3	
Röntgenographische Dichte	0.430 mm^{-1}	
F(000)	2292	
Kristallgröße	0.20 x 0.13 x 0.08 mm^3	
Gemessener Theta-Bereich	1.36 to 29.91°.	
Indexbereich	-20<=h<=20, -20<=k<=21, -34<=l<=32	
Anzahl gemessener Reflexe	127671	
Unabhängige Reflexe	30154 [R(int) = 0.1677]	
Datenvollständigkeit bis Theta = 29.57°	97,5 %	
Absorptionskorrektur	N/A	
Verfeinerung	Full-matrix-block least-squares on F^2	
Daten / Restraints / Parameters	30154 / 0 / 1298	
Goodness-of-fit on F^2	1.128	
Endgültige R-Werte [I>2sigma(I)]	R1 = 0.0692, wR2 = 0.1440	
R-Werte (alle Daten)	R1 = 0.1742, wR2 = 0.1732	
Absolute structure parameter	0.02(5)	
Restelektronendichte	1.791 and -1.515 e.$Å^{-3}$	

Tabelle x Atomkoordinaten (x 10^4) und äquivalente isotrope Auslenkungsparameter ($Å^2$x 10^3) für **21**. U(eq) wird berechnet als ein Drittel der Spur des orthogonalisierten U_{ij}-Tensors.

	x	y	z	U(eq)
Sn	1270(1)	1278(1)	2548(1)	21(1)
Al(1)	1686(1)	2791(1)	3257(1)	19(1)
Al(2)	3499(1)	1422(1)	2953(1)	17(1)
Al(3)	2853(1)	1657(1)	1755(1)	17(1)
Al(4)	1468(1)	3405(1)	2038(1)	18(1)
Si(1)	2511(1)	3192(1)	4412(1)	21(1)
Si(2)	4443(1)	2344(1)	3921(1)	20(1)
Si(3)	3321(1)	-608(1)	3108(1)	21(1)
Si(4)	2970(1)	-495(1)	1905(1)	19(1)
Si(5)	3363(1)	2465(1)	566(1)	18(1)
Si(6)	2544(1)	4327(1)	1041(1)	19(1)
Si(7)	-656(1)	3322(1)	1952(1)	21(1)
Si(8)	-531(1)	2915(1)	3164(1)	19(1)
O(1)	2288(2)	1743(2)	3041(1)	19(1)
O(2)	3683(2)	1782(2)	2258(1)	19(1)
O(3)	1767(2)	2234(2)	1988(1)	17(1)
O(4)	1824(2)	3590(2)	2723(1)	18(1)
O(5)	1902(2)	3180(2)	3877(1)	26(1)
O(6)	3559(2)	2672(2)	4331(1)	25(1)
O(7)	4089(2)	2029(2)	3352(1)	21(1)
O(8)	3792(2)	283(2)	3012(1)	21(1)
O(9)	2942(2)	-903(2)	2525(1)	23(1)
O(10)	2595(2)	583(2)	1906(1)	20(1)
O(11)	3282(2)	1907(2)	1130(1)	21(1)
O(12)	2988(2)	3525(2)	630(1)	23(1)
O(13)	2112(2)	3924(2)	1583(1)	21(1)
O(14)	298(2)	3724(2)	1987(1)	20(1)
O(15)	-951(2)	2936(2)	2556(1)	22(1)
O(16)	577(2)	2530(2)	3120(1)	21(1)
C(1)	1976(3)	2611(3)	4990(2)	23(1)
C(2)	2518(3)	2209(3)	5412(2)	29(1)
C(3)	2128(3)	1816(4)	5866(2)	39(1)
C(4)	1193(4)	1807(4)	5912(3)	44(2)
C(5)	639(4)	2185(4)	5496(2)	42(1)
C(6)	1019(3)	2583(3)	5043(2)	32(1)
C(7)	2609(3)	4348(3)	4606(2)	25(1)
C(8)	1956(4)	5076(4)	4495(2)	43(1)
C(9)	2032(4)	5936(4)	4668(3)	56(2)
C(10)	2778(4)	6076(4)	4951(2)	43(1)
C(11)	3469(4)	5375(4)	5058(2)	41(1)
C(12)	3376(3)	4528(4)	4882(2)	37(1)
C(13)	5176(3)	1404(3)	4269(2)	22(1)
C(14)	5345(3)	549(3)	4047(2)	23(1)
C(15)	5839(3)	-164(3)	4331(2)	27(1)
C(16)	6190(3)	-25(3)	4834(2)	27(1)
C(17)	6043(3)	809(3)	5059(2)	29(1)
C(18)	5540(3)	1524(3)	4782(2)	27(1)

C(19)	5095(3)	3287(3)	3771(2)	25(1)
C(20)	6057(3)	3190(3)	3785(2)	26(1)
C(21)	6539(3)	3869(3)	3610(2)	33(1)
C(22)	6063(4)	4668(4)	3412(2)	37(1)
C(23)	5112(4)	4796(3)	3404(2)	35(1)
C(24)	4633(3)	4110(3)	3576(2)	29(1)
C(25)	4174(3)	-1532(3)	3375(2)	26(1)
C(26)	3904(4)	-2193(3)	3736(2)	34(1)
C(27)	4529(4)	-2888(3)	3926(2)	42(1)
C(28)	5447(4)	-2941(4)	3780(2)	47(2)
C(29)	5750(4)	-2313(4)	3430(2)	46(2)
C(30)	5114(3)	-1611(3)	3237(2)	34(1)
C(31)	2287(3)	-370(3)	3573(2)	26(1)
C(32)	2294(3)	195(3)	4018(2)	27(1)
C(33)	1523(4)	430(4)	4353(2)	42(1)
C(34)	720(4)	133(4)	4249(3)	55(2)
C(35)	683(4)	-433(5)	3824(3)	68(2)
C(36)	1469(4)	-692(4)	3483(2)	45(2)
C(37)	2187(3)	-1065(3)	1493(2)	22(1)
C(38)	1702(4)	-622(4)	1069(2)	43(1)
C(39)	1162(4)	-1065(5)	744(2)	55(2)
C(40)	1083(4)	-1941(4)	834(3)	47(2)
C(41)	1555(4)	-2380(4)	1261(3)	57(2)
C(42)	2095(4)	-1947(4)	1588(3)	50(2)
C(43)	4184(3)	-747(3)	1634(2)	21(1)
C(44)	4583(3)	-210(3)	1253(2)	27(1)
C(45)	5488(3)	-457(3)	1056(2)	30(1)
C(46)	6001(3)	-1235(3)	1228(2)	29(1)
C(47)	5617(3)	-1768(3)	1602(2)	32(1)
C(48)	4725(3)	-1538(3)	1807(2)	26(1)
C(49)	2651(3)	1987(3)	61(2)	20(1)
C(50)	2092(3)	2519(3)	-310(2)	25(1)
C(51)	1566(3)	2140(3)	-677(2)	31(1)
C(52)	1587(3)	1220(3)	-681(2)	33(1)
C(53)	2125(3)	675(3)	-320(2)	29(1)
C(54)	2650(3)	1062(3)	51(2)	25(1)
C(55)	4600(3)	2376(3)	329(2)	21(1)
C(56)	5102(3)	3077(3)	390(2)	33(1)
C(57)	6026(4)	3005(4)	229(2)	42(1)
C(58)	6475(3)	2235(4)	-8(2)	36(1)
C(59)	5994(3)	1531(3)	-72(2)	34(1)
C(60)	5071(3)	1602(3)	93(2)	28(1)
C(61)	3468(3)	4951(3)	1266(2)	22(1)
C(62)	3520(3)	5829(3)	1112(2)	33(1)
C(63)	4141(4)	6313(3)	1328(2)	40(1)
C(64)	4735(3)	5926(4)	1729(2)	38(1)
C(65)	4711(3)	5046(4)	1884(2)	34(1)
C(66)	4090(3)	4568(3)	1660(2)	31(1)
C(67)	1645(3)	5059(3)	661(2)	22(1)
C(68)	1817(3)	5428(3)	146(2)	27(1)
C(69)	1146(3)	5970(3)	-132(2)	32(1)
C(70)	245(3)	6154(3)	92(2)	29(1)
C(71)	54(3)	5794(3)	595(2)	30(1)
C(72)	737(3)	5254(3)	880(2)	25(1)
C(73)	-1585(3)	4215(3)	1705(2)	25(1)
C(74)	-1487(3)	5102(4)	1705(2)	34(1)
C(75)	-2166(4)	5764(4)	1491(2)	45(2)
C(76)	-2941(4)	5512(5)	1286(2)	47(2)
C(77)	-3067(4)	4644(5)	1279(2)	49(2)
C(78)	-2394(3)	3985(4)	1488(2)	36(1)
C(79)	-551(3)	2359(3)	1482(2)	22(1)
C(80)	-1160(3)	1730(4)	1545(2)	37(1)
C(81)	-1149(4)	1050(4)	1180(2)	47(2)
C(82)	-505(4)	956(4)	748(2)	49(2)
C(83)	112(4)	1567(4)	677(2)	36(1)
C(84)	88(3)	2250(3)	1045(2)	26(1)
C(85)	-1112(3)	2116(3)	3580(2)	24(1)
C(86)	-1406(3)	1381(3)	3339(2)	35(1)
C(87)	-1802(4)	746(4)	3645(3)	45(1)
C(88)	-1905(4)	837(4)	4202(3)	44(1)
C(89)	-1634(4)	1546(4)	4453(2)	44(1)
C(90)	-1241(3)	2178(3)	4149(2)	35(1)
C(91)	-753(3)	4061(3)	3445(2)	23(1)
C(92)	-1409(3)	4711(3)	3200(2)	27(1)
C(93)	-1642(3)	5556(3)	3415(2)	32(1)
C(94)	-1240(3)	5775(4)	3893(2)	37(1)
C(95)	-603(4)	5134(4)	4144(2)	41(1)

C(96)	-356(3)	4303(3)	3923(2)	33(1)
O(17)	5248(2)	2322(2)	1966(1)	31(1)
C(97)	5816(3)	1734(4)	1595(2)	35(1)
C(98)	6347(4)	966(4)	1902(2)	43(1)
C(99)	6379(4)	1873(4)	2652(2)	43(1)
C(100)	5829(3)	2632(4)	2367(2)	36(1)
O(18)	6938(2)	1291(3)	2281(2)	52(1)
O(19)	1835(3)	5267(2)	2894(2)	51(1)
C(101)	2465(4)	5790(4)	2656(3)	52(2)
C(102)	2456(6)	6613(5)	2977(3)	79(2)
C(103)	874(5)	6596(5)	3228(3)	71(2)
C(104)	890(4)	5779(4)	2899(3)	59(2)
O(20)	1539(4)	7128(3)	3002(2)	80(2)
C(105)	8742(5)	7377(6)	2331(3)	77(2)
C(106)	9403(5)	7930(5)	2273(3)	76(2)
C(107)	9164(5)	8855(5)	2301(3)	69(2)
C(108)	8215(4)	9190(5)	2376(3)	67(2)
C(109)	7575(6)	8656(5)	2411(3)	75(2)
C(110)	7831(6)	7731(6)	2406(4)	87(3)
C(111)	9816(5)	9426(6)	2260(4)	91(3)

Sn-O(1)	2.155(3)	C(17)-C(18)	1.391(7)
Sn-O(3)	2.163(3)	C(19)-C(20)	1.398(6)
Sn-O(16)	2.442(3)	C(19)-C(24)	1.405(7)
Sn-Al(1)	3.0378(13)	C(20)-C(21)	1.385(6)
Sn-Al(3)	3.0888(12)	C(21)-C(22)	1.387(7)
Al(1)-O(5)	1.694(3)	C(22)-C(23)	1.379(7)
Al(1)-O(1)	1.771(3)	C(23)-C(24)	1.390(6)
Al(1)-O(16)	1.774(3)	C(25)-C(30)	1.395(6)
Al(1)-O(4)	1.790(3)	C(25)-C(26)	1.415(7)
Al(2)-O(7)	1.695(3)	C(26)-C(27)	1.371(7)
Al(2)-O(8)	1.712(3)	C(27)-C(28)	1.372(8)
Al(2)-O(1)	1.774(3)	C(28)-C(29)	1.378(8)
Al(2)-O(2)	1.801(3)	C(29)-C(30)	1.389(7)
Al(3)-O(11)	1.690(3)	C(31)-C(36)	1.387(6)
Al(3)-O(10)	1.751(3)	C(31)-C(32)	1.395(6)
Al(3)-O(3)	1.776(3)	C(32)-C(33)	1.379(6)
Al(3)-O(2)	1.793(3)	C(33)-C(34)	1.355(8)
Al(4)-O(13)	1.692(3)	C(34)-C(35)	1.365(8)
Al(4)-O(14)	1.718(3)	C(35)-C(36)	1.408(8)
Al(4)-O(3)	1.760(3)	C(37)-C(42)	1.374(7)
Al(4)-O(4)	1.812(3)	C(37)-C(38)	1.381(7)
Si(1)-O(5)	1.612(3)	C(38)-C(39)	1.390(7)
Si(1)-O(6)	1.623(3)	C(39)-C(40)	1.358(8)
Si(1)-C(7)	1.845(5)	C(40)-C(41)	1.377(9)
Si(1)-C(1)	1.864(5)	C(41)-C(42)	1.383(8)
Si(2)-O(7)	1.607(3)	C(43)-C(44)	1.397(6)
Si(2)-O(6)	1.631(3)	C(43)-C(48)	1.397(6)
Si(2)-C(19)	1.858(5)	C(44)-C(45)	1.393(6)
Si(2)-C(13)	1.859(5)	C(45)-C(46)	1.365(7)
Si(3)-O(8)	1.613(3)	C(46)-C(47)	1.370(7)
Si(3)-O(9)	1.642(3)	C(47)-C(48)	1.380(6)
Si(3)-C(25)	1.852(5)	C(49)-C(54)	1.398(6)
Si(3)-C(31)	1.858(4)	C(49)-C(50)	1.402(6)
Si(4)-O(9)	1.630(3)	C(50)-C(51)	1.389(6)
Si(4)-O(10)	1.636(3)	C(51)-C(52)	1.385(7)
Si(4)-C(43)	1.864(4)	C(52)-C(53)	1.379(7)
Si(4)-C(37)	1.867(4)	C(53)-C(54)	1.402(6)
Si(5)-O(11)	1.615(3)	C(55)-C(60)	1.388(6)
Si(5)-O(12)	1.620(3)	C(55)-C(56)	1.390(6)
Si(5)-C(49)	1.868(4)	C(56)-C(57)	1.386(6)
Si(5)-C(55)	1.872(4)	C(57)-C(58)	1.373(7)
Si(6)-O(13)	1.600(3)	C(58)-C(59)	1.376(7)
Si(6)-O(12)	1.630(3)	C(59)-C(60)	1.388(6)
Si(6)-C(67)	1.853(5)	C(61)-C(62)	1.384(6)
Si(6)-C(61)	1.867(4)	C(61)-C(66)	1.406(7)
Si(7)-O(14)	1.612(3)	C(62)-C(63)	1.376(7)
Si(7)-O(15)	1.646(3)	C(63)-C(64)	1.396(8)
Si(7)-C(79)	1.855(4)	C(64)-C(65)	1.380(7)
Si(7)-C(73)	1.874(5)	C(65)-C(66)	1.379(6)
Si(8)-O(15)	1.626(3)	C(67)-C(68)	1.399(6)
Si(8)-O(16)	1.642(3)	C(67)-C(72)	1.407(6)
Si(8)-C(85)	1.852(5)	C(68)-C(69)	1.372(7)
Si(8)-C(91)	1.852(4)	C(69)-C(70)	1.400(6)
C(1)-C(2)	1.398(7)	C(70)-C(71)	1.376(7)
C(1)-C(6)	1.411(6)	C(71)-C(72)	1.391(7)

C(2)-C(3)	1.396(7)	C(73)-C(74)	1.368(7)
C(3)-C(4)	1.373(7)	C(73)-C(78)	1.409(6)
C(4)-C(5)	1.384(8)	C(74)-C(75)	1.408(7)
C(5)-C(6)	1.391(7)	C(75)-C(76)	1.365(8)
C(7)-C(8)	1.373(7)	C(76)-C(77)	1.352(8)
C(7)-C(12)	1.396(6)	C(77)-C(78)	1.394(8)
C(8)-C(9)	1.396(7)	C(79)-C(84)	1.392(6)
C(9)-C(10)	1.359(8)	C(79)-C(80)	1.402(6)
C(10)-C(11)	1.379(8)	C(80)-C(81)	1.370(7)
C(11)-C(12)	1.384(7)	C(81)-C(82)	1.387(7)
C(13)-C(14)	1.392(6)	C(82)-C(83)	1.391(7)
C(13)-C(18)	1.406(6)	C(83)-C(84)	1.376(6)
C(14)-C(15)	1.392(7)	C(85)-C(86)	1.397(6)
C(15)-C(16)	1.382(6)	C(85)-C(90)	1.400(6)
C(16)-C(17)	1.367(6)	C(86)-C(87)	1.389(7)

C(87)-C(88)	1.372(8)	O(3)-Al(4)-O(4)	101.19(14)
C(88)-C(89)	1.362(8)	O(5)-Si(1)-O(6)	113.42(15)
C(89)-C(90)	1.381(7)	O(5)-Si(1)-C(7)	111.2(2)
C(91)-C(96)	1.402(6)	O(6)-Si(1)-C(7)	106.32(18)
C(91)-C(92)	1.408(7)	O(5)-Si(1)-C(1)	109.49(18)
C(92)-C(93)	1.377(6)	O(6)-Si(1)-C(1)	106.26(19)
C(93)-C(94)	1.393(7)	C(7)-Si(1)-C(1)	109.96(19)
C(94)-C(95)	1.391(8)	O(7)-Si(2)-O(6)	109.61(16)
C(95)-C(96)	1.367(7)	O(7)-Si(2)-C(19)	107.85(18)
O(17)-C(97)	1.434(5)	O(6)-Si(2)-C(19)	110.07(18)
O(17)-C(100)	1.450(6)	O(7)-Si(2)-C(13)	111.07(18)
C(97)-C(98)	1.499(8)	O(6)-Si(2)-C(13)	107.30(18)
C(98)-O(18)	1.432(6)	C(19)-Si(2)-C(13)	111.0(2)
C(99)-O(18)	1.423(6)	O(8)-Si(3)-O(9)	109.19(16)
C(99)-C(100)	1.476(8)	O(8)-Si(3)-C(25)	110.16(18)
O(19)-C(101)	1.410(6)	O(9)-Si(3)-C(25)	109.51(18)
O(19)-C(104)	1.480(7)	O(8)-Si(3)-C(31)	110.28(18)
C(101)-C(102)	1.480(8)	O(9)-Si(3)-C(31)	105.85(19)
C(102)-O(20)	1.447(9)	C(25)-Si(3)-C(31)	111.8(2)
C(103)-O(20)	1.446(8)	O(9)-Si(4)-O(10)	110.23(15)
C(103)-C(104)	1.483(8)	O(9)-Si(4)-C(43)	107.55(19)
C(105)-C(110)	1.369(10)	O(10)-Si(4)-C(43)	111.86(17)
C(105)-C(106)	1.375(9)	O(9)-Si(4)-C(37)	107.36(18)
C(106)-C(107)	1.391(10)	O(10)-Si(4)-C(37)	108.99(19)
C(107)-C(111)	1.382(9)	C(43)-Si(4)-C(37)	110.74(18)
C(107)-C(108)	1.413(9)	O(11)-Si(5)-O(12)	112.89(15)
C(108)-C(109)	1.327(9)	O(11)-Si(5)-C(49)	106.76(17)
C(109)-C(110)	1.390(10)	O(12)-Si(5)-C(49)	109.01(18)
		O(11)-Si(5)-C(55)	110.15(19)
O(1)-Sn-O(3)	79.73(10)	O(12)-Si(5)-C(55)	
O(1)-Sn-O(16)	68.84(10)		
O(3)-Sn-O(16)	88.55(10)		
O(1)-Sn-Al(1)	34.92(8)		
O(3)-Sn-Al(1)	74.45(7)		
O(16)-Sn-Al(1)	35.73(7)		
O(1)-Sn-Al(3)	73.49(7)		
O(3)-Sn-Al(3)	34.09(8)		
O(16)-Sn-Al(3)	115.77(7)		
Al(1)-Sn-Al(3)	88.43(3)		
O(5)-Al(1)-O(1)	119.01(16)		
O(5)-Al(1)-O(16)	120.43(15)		
O(1)-Al(1)-O(16)	94.78(14)		
O(5)-Al(1)-O(4)	111.68(15)		
O(1)-Al(1)-O(4)	107.35(14)		
O(16)-Al(1)-O(4)			

101.01(14)
O(5)-Al(1)-Sn 150.00(13)
O(1)-Al(1)-Sn 44.15(9)
O(16)-Al(1)-Sn 53.49(9)
O(4)-Al(1)-Sn 98.12(10)
O(7)-Al(2)-O(8) 115.24(16)
O(7)-Al(2)-O(1) 111.62(14)
O(8)-Al(2)-O(1) 110.86(14)
O(7)-Al(2)-O(2) 106.67(14)
O(8)-Al(2)-O(2) 110.37(14)
O(1)-Al(2)-O(2) 101.06(14)
O(11)-Al(3)-O(10) 120.87(14)
O(11)-Al(3)-O(3) 119.47(15)
O(10)-Al(3)-O(3) 95.47(14)
O(11)-Al(3)-O(2) 109.03(14)
O(10)-Al(3)-O(2) 102.10(15)
O(3)-Al(3)-O(2) 107.87(13)
O(11)-Al(3)-Sn 152.68(12)
O(10)-Al(3)-Sn 56.12(9)
O(3)-Al(3)-Sn 43.04(9)
O(2)-Al(3)-Sn 97.67(10)
O(13)-Al(4)-O(14) 114.15(15)
O(13)-Al(4)-O(3) 110.21(14)
O(14)-Al(4)-O(3) 111.05(14)
O(13)-Al(4)-O(4) 108.94(14)
O(14)-Al(4)-O(4) 110.51(14)

106.19(18)
C(49)-Si(5)-C(55) 111.92(18)
O(13)-Si(6)-O(12) 110.62(16)
O(13)-Si(6)-C(67) 110.94(18)
O(12)-Si(6)-C(67) 107.05(18)
O(13)-Si(6)-C(61) 106.57(18)
O(12)-Si(6)-C(61) 109.80(17)
C(67)-Si(6)-C(61) 111.9(2)
O(14)-Si(7)-O(15) 110.08(16)
O(14)-Si(7)-C(79) 112.21(17)
O(15)-Si(7)-C(79) 105.87(18)
O(14)-Si(7)-C(73) 109.67(19)
O(15)-Si(7)-C(73) 110.49(17)
C(79)-Si(7)-C(73) 108.5(2)
O(15)-Si(8)-O(16) 108.82(15)
O(15)-Si(8)-C(85) 106.76(18)
O(16)-Si(8)-C(85) 108.44(18)
O(15)-Si(8)-C(91) 108.87(19)
O(16)-Si(8)-C(91) 111.67(17)
C(85)-Si(8)-C(91) 112.12(19)
Al(1)-O(1)-Al(2) 127.83(16)
Al(1)-O(1)-Sn 100.93(13)
Al(2)-O(1)-Sn 124.80(14)
Al(3)-O(2)-Al(2) 119.85(15)
Al(4)-O(3)-Al(3) 125.72(16)
Al(4)-O(3)-Sn 124.43(14)
Al(3)-O(3)-Sn 102.87(14)
Al(1)-O(4)-Al(4) 120.06(16)
Si(1)-O(5)-Al(1) 153.2(2)
Si(1)-O(6)-Si(2) 148.7(2)
Si(2)-O(7)-Al(2) 154.9(2)
Si(3)-O(8)-Al(2) 140.50(18)
Si(4)-O(9)-Si(3) 133.31(18)
Si(4)-O(10)-Al(3) 146.32(19)
Si(5)-O(11)-Al(3) 157.4(2)
Si(5)-O(12)-Si(6) 146.5(2)
Si(6)-O(13)-Al(4) 164.9(2)
Si(7)-O(14)-Al(4) 142.1(2)
Si(8)-O(15)-Si(7) 134.88(18)
Si(8)-O(16)-Al(1) 143.40(19)
Si(8)-O(16)-Sn 124.64(15)

Al(1)-O(16)-Sn 90.78(12)	C(53)-C(52)-C(51) 120.5(4)
C(2)-C(1)-C(6) 116.6(4)	C(52)-C(53)-C(54) 119.2(4)
C(2)-C(1)-Si(1) 120.3(3)	C(49)-C(54)-C(53) 121.7(5)
C(6)-C(1)-Si(1) 123.1(4)	C(60)-C(55)-C(56) 116.5(4)
C(1)-C(2)-C(3) 121.5(4)	C(60)-C(55)-Si(5) 121.8(3)
C(4)-C(3)-C(2) 120.9(5)	C(56)-C(55)-Si(5) 121.7(3)
C(3)-C(4)-C(5) 119.0(5)	C(57)-C(56)-C(55) 121.9(4)
C(4)-C(5)-C(6) 120.7(5)	C(58)-C(57)-C(56) 120.6(5)
C(5)-C(6)-C(1) 121.4(5)	C(57)-C(58)-C(59) 118.5(4)
C(8)-C(7)-C(12) 115.8(4)	C(58)-C(59)-C(60) 120.7(5)
C(8)-C(7)-Si(1) 123.7(4)	C(59)-C(60)-C(55) 121.7(4)
C(12)-C(7)-Si(1) 120.4(4)	C(62)-C(61)-C(66) 116.6(4)
C(7)-C(8)-C(9) 122.2(5)	C(62)-C(61)-Si(6) 123.3(4)
C(10)-C(9)-C(8) 119.9(6)	C(66)-C(61)-Si(6) 119.8(3)
C(9)-C(10)-C(11) 120.3(5)	C(63)-C(62)-C(61) 122.6(5)
C(10)-C(11)-C(12) 118.6(5)	C(62)-C(63)-C(64) 119.8(5)
C(11)-C(12)-C(7) 123.1(5)	C(65)-C(64)-C(63) 118.8(5)
C(14)-C(13)-C(18) 117.7(4)	C(66)-C(65)-C(64) 120.6(5)
C(14)-C(13)-Si(2) 121.5(3)	C(65)-C(66)-C(61) 121.5(5)
C(18)-C(13)-Si(2) 120.7(3)	C(68)-C(67)-C(72) 116.8(4)
C(15)-C(14)-C(13) 121.0(4)	C(68)-C(67)-Si(6) 122.7(3)
C(16)-C(15)-C(14) 120.0(4)	C(72)-C(67)-Si(6) 120.5(3)
C(17)-C(16)-C(15) 120.3(5)	C(69)-C(68)-C(67) 122.2(4)
C(16)-C(17)-C(18) 120.2(4)	C(68)-C(69)-C(70) 120.2(5)
C(17)-C(18)-C(13) 120.9(4)	C(71)-C(70)-C(69) 118.8(5)
C(20)-C(19)-C(24) 117.2(4)	C(70)-C(71)-C(72) 121.0(4)
C(20)-C(19)-Si(2) 122.6(4)	C(71)-C(72)-C(67) 121.0(4)
C(24)-C(19)-Si(2) 119.9(3)	C(74)-C(73)-C(78) 117.8(5)
C(21)-C(20)-C(19) 121.7(5)	C(74)-C(73)-Si(7) 121.6(4)
C(20)-C(21)-C(22) 119.8(4)	C(78)-C(73)-Si(7) 120.5(4)
C(23)-C(22)-C(21) 120.2(5)	C(73)-C(74)-C(75) 121.2(5)
C(22)-C(23)-C(24) 119.8(5)	C(76)-C(75)-C(74) 119.0(6)
C(23)-C(24)-C(19) 121.4(4)	C(77)-C(76)-C(75) 121.7(6)
C(30)-C(25)-C(26) 116.4(5)	C(76)-C(77)-C(78) 119.5(5)
C(30)-C(25)-Si(3) 122.3(4)	C(77)-C(78)-C(73) 120.7(5)
C(26)-C(25)-Si(3) 121.3(4)	C(84)-C(79)-C(80) 117.5(4)

C(27)-C(26)-C(25) 121.6(5)	C(84)-C(79)-Si(7) 122.5(3)
C(28)-C(27)-C(26) 120.0(5)	C(80)-C(79)-Si(7) 119.8(3)
C(27)-C(28)-C(29) 120.8(6)	C(81)-C(80)-C(79) 121.4(4)
C(28)-C(29)-C(30) 119.0(5)	C(80)-C(81)-C(82) 119.9(5)
C(29)-C(30)-C(25) 122.2(5)	C(81)-C(82)-C(83) 120.1(5)
C(36)-C(31)-C(32) 117.1(4)	C(84)-C(83)-C(82) 119.4(4)
C(36)-C(31)-Si(3) 122.7(4)	C(83)-C(84)-C(79) 121.8(4)
C(32)-C(31)-Si(3) 120.1(3)	C(86)-C(85)-C(90) 116.1(4)
C(33)-C(32)-C(31) 121.8(5)	C(86)-C(85)-Si(8) 120.8(4)
C(34)-C(33)-C(32) 120.3(5)	C(90)-C(85)-Si(8) 123.1(4)
C(33)-C(34)-C(35) 119.9(5)	C(87)-C(86)-C(85) 122.1(5)
C(34)-C(35)-C(36) 120.4(5)	C(88)-C(87)-C(86) 119.3(5)
C(31)-C(36)-C(35) 120.4(5)	C(89)-C(88)-C(87) 120.6(5)
C(42)-C(37)-C(38) 117.6(4)	C(88)-C(89)-C(90) 120.1(5)
C(42)-C(37)-Si(4) 121.3(4)	C(89)-C(90)-C(85) 121.9(5)
C(38)-C(37)-Si(4) 121.0(3)	C(96)-C(91)-C(92) 117.2(4)
C(37)-C(38)-C(39) 120.8(5)	C(96)-C(91)-Si(8) 123.2(4)
C(40)-C(39)-C(38) 121.5(6)	C(92)-C(91)-Si(8) 119.3(3)
C(39)-C(40)-C(41) 117.8(5)	C(93)-C(92)-C(91) 121.5(4)
C(40)-C(41)-C(42) 121.3(6)	C(92)-C(93)-C(94) 120.0(5)
C(37)-C(42)-C(41) 121.0(6)	C(95)-C(94)-C(93) 119.1(5)
C(44)-C(43)-C(48) 117.4(4)	C(96)-C(95)-C(94) 120.8(5)
C(44)-C(43)-Si(4) 124.2(4)	C(95)-C(96)-C(91) 121.3(5)
C(48)-C(43)-Si(4) 118.4(3)	C(97)-O(17)-C(100) 108.9(3)
C(45)-C(44)-C(43) 120.9(5)	O(17)-C(97)-C(98) 110.4(4)
C(46)-C(45)-C(44) 120.6(5)	O(18)-C(98)-C(97) 110.3(5)
C(45)-C(46)-C(47) 119.1(4)	O(18)-C(99)-C(100) 112.1(4)
C(46)-C(47)-C(48) 121.6(5)	O(17)-C(100)-C(99) 111.3(4)
C(47)-C(48)-C(43) 120.4(5)	C(99)-O(18)-C(98) 108.2(4)
C(54)-C(49)-C(50) 117.4(4)	C(101)-O(19)-C(104) 110.0(4)
C(54)-C(49)-Si(5) 119.7(4)	O(19)-C(101)-C(102) 109.8(5)
C(50)-C(49)-Si(5) 122.9(3)	O(20)-C(102)-C(101) 110.6(5)
C(51)-C(50)-C(49) 121.3(4)	O(20)-C(103)-C(104) 109.9(5)
C(52)-C(51)-C(50) 119.9(5)	O(19)-C(104)-C(103) 108.7(5)

C(103)-O(20)-C(102)	110.9(5)	C(111)-C(107)-C(108)
C(110)-C(105)-C(106)	120.4(8)	121.1(8)
C(105)-C(106)-C(107)	120.8(7)	C(109)-C(108)-C(107)
C(106)-C(107)-C(111)	122.1(7)	122.2(8)

C(106)-C(107)-C(108) 116.8(7) C(108)-C(109)-C(110) 120.2(8)
C(105)-C(110)-C(109) 119.6(8)

Symmetrieoperationen zur Erzeugung äquivalenter Atome: #1 -x,-y+1,-z+2

Tabelle x U_{ij}-Werte ($Å^2 x\ 10^3$) des Temperaturfaktors exp $(-2p^2[\ h^2\ a^{*2}U_{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U_{12}\ ])$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sn	20(1)	21(1)	23(1)	0(1)	-1(1)	-2(1)
Al(1)	15(1)	22(1)	17(1)	-2(1)	-2(1)	2(1)
Al(2)	17(1)	18(1)	16(1)	-1(1)	-2(1)	1(1)
Al(3)	18(1)	16(1)	16(1)	-1(1)	0(1)	0(1)
Al(4)	17(1)	18(1)	18(1)	-1(1)	-1(1)	1(1)
Si(1)	19(1)	26(1)	18(1)	-6(1)	-1(1)	0(1)
Si(2)	17(1)	24(1)	18(1)	-3(1)	-1(1)	-1(1)
Si(3)	25(1)	18(1)	20(1)	0(1)	-2(1)	1(1)
Si(4)	22(1)	15(1)	18(1)	0(1)	-1(1)	-1(1)
Si(5)	20(1)	16(1)	16(1)	-1(1)	0(1)	1(1)
Si(6)	21(1)	18(1)	19(1)	-1(1)	0(1)	-1(1)
Si(7)	16(1)	25(1)	19(1)	-1(1)	-1(1)	1(1)
Si(8)	14(1)	23(1)	18(1)	-1(1)	1(1)	-1(1)
O(1)	17(1)	19(2)	19(2)	-3(1)	-1(1)	1(1)
O(2)	17(1)	22(2)	17(2)	-3(1)	1(1)	-3(1)
O(3)	17(1)	16(2)	17(2)	2(1)	-3(1)	1(1)
O(4)	16(1)	18(2)	20(2)	-3(1)	-3(1)	-2(1)
O(5)	20(2)	31(2)	24(2)	-7(1)	-4(1)	4(1)
O(6)	21(2)	34(2)	17(2)	-4(1)	-3(1)	3(1)
O(7)	20(2)	23(2)	20(2)	1(1)	-4(1)	0(1)
O(8)	18(1)	23(2)	21(2)	0(1)	-4(1)	4(1)
O(9)	30(2)	18(2)	21(2)	2(1)	-4(1)	-5(1)
O(10)	24(2)	16(2)	20(2)	0(1)	-3(1)	-1(1)
O(11)	25(2)	17(2)	21(2)	1(1)	2(1)	2(1)
O(12)	29(2)	19(2)	20(2)	-1(1)	1(1)	-2(1)
O(13)	20(2)	22(2)	20(2)	2(1)	1(1)	0(1)
O(14)	18(2)	20(2)	20(2)	4(1)	0(1)	2(1)
O(15)	18(2)	27(2)	21(2)	1(1)	-1(1)	-1(1)
O(16)	17(1)	24(2)	18(2)	1(1)	-3(1)	3(1)
C(1)	21(2)	23(2)	23(2)	-8(2)	1(2)	0(2)
C(2)	19(2)	31(3)	33(3)	5(2)	-2(2)	3(2)
C(3)	30(3)	38(3)	47(3)	21(3)	1(2)	-1(2)
C(4)	34(3)	32(3)	62(4)	18(3)	10(3)	2(2)
C(5)	25(3)	39(3)	61(4)	0(3)	7(3)	-8(2)
C(6)	20(2)	37(3)	37(3)	-3(2)	-6(2)	-2(2)
C(7)	26(2)	31(3)	17(2)	-4(2)	0(2)	-2(2)
C(8)	41(3)	34(3)	52(4)	-12(3)	-16(3)	2(3)
C(9)	62(4)	40(4)	60(4)	-8(3)	-15(3)	14(3)
C(10)	60(4)	30(3)	41(3)	-10(3)	-5(3)	-11(3)
C(11)	42(3)	47(4)	35(3)	-14(3)	-7(2)	-12(3)
C(12)	30(3)	44(3)	36(3)	-14(3)	-1(2)	0(2)
C(13)	19(2)	27(3)	20(2)	0(2)	-2(2)	0(2)
C(14)	23(2)	26(3)	20(2)	0(2)	-2(2)	-1(2)
C(15)	24(2)	27(3)	28(3)	0(2)	-1(2)	1(2)
C(16)	25(2)	27(3)	27(3)	6(2)	0(2)	4(2)
C(17)	28(2)	38(3)	20(2)	1(2)	-8(2)	5(2)
C(18)	27(2)	28(3)	25(2)	-5(2)	0(2)	1(2)
C(19)	26(2)	26(3)	21(2)	-9(2)	2(2)	-2(2)
C(20)	27(2)	28(3)	24(2)	-1(2)	-7(2)	-4(2)
C(21)	26(2)	37(3)	37(3)	-3(2)	1(2)	-12(2)
C(22)	43(3)	35(3)	36(3)	1(2)	3(2)	-18(3)
C(23)	44(3)	25(3)	36(3)	0(2)	-5(2)	-1(2)
C(24)	26(2)	29(3)	31(3)	-2(2)	-4(2)	-5(2)
C(25)	37(3)	21(2)	19(2)	-5(2)	-5(2)	1(2)
C(26)	45(3)	28(3)	25(3)	-3(2)	-7(2)	6(2)
C(27)	68(4)	23(3)	30(3)	5(2)	-11(3)	9(3)
C(28)	64(4)	29(3)	42(3)	-4(3)	-25(3)	14(3)
C(29)	38(3)	43(4)	52(4)	-11(3)	-18(3)	13(3)
C(30)	37(3)	31(3)	32(3)	-3(2)	-8(2)	4(2)
C(31)	28(2)	26(3)	21(2)	6(2)	0(2)	0(2)
C(32)	32(3)	26(3)	21(2)	8(2)	-1(2)	6(2)

C(33)	49(3)	44(3)	28(3)	5(2)	9(2)	2(3)
C(34)	49(4)	58(4)	54(4)	4(3)	26(3)	3(3)
C(35)	36(3)	80(5)	91(5)	-10(4)	22(4)	-28(3)
C(36)	42(3)	48(4)	48(3)	-5(3)	2(3)	-23(3)
C(37)	20(2)	22(2)	22(2)	-4(2)	0(2)	-1(2)
C(38)	50(3)	41(3)	41(3)	5(3)	-20(3)	-18(3)
C(39)	54(4)	68(5)	47(4)	0(3)	-28(3)	-19(3)
C(40)	27(3)	59(4)	59(4)	-30(3)	-4(3)	-11(3)
C(41)	51(4)	32(3)	91(5)	-15(3)	-16(4)	-13(3)
C(42)	49(3)	31(3)	72(4)	-5(3)	-22(3)	-7(3)
C(43)	23(2)	18(2)	22(2)	-5(2)	-5(2)	-2(2)
C(44)	25(2)	23(3)	30(3)	-4(2)	-1(2)	2(2)
C(45)	30(3)	28(3)	32(3)	-4(2)	4(2)	-2(2)
C(46)	26(2)	29(3)	30(3)	-7(2)	4(2)	1(2)
C(47)	30(3)	27(3)	37(3)	-5(2)	-5(2)	2(2)
C(48)	26(2)	19(2)	31(3)	1(2)	-2(2)	3(2)
C(49)	20(2)	18(2)	18(2)	1(2)	4(2)	2(2)
C(50)	27(2)	17(2)	28(2)	-4(2)	-1(2)	2(2)
C(51)	26(2)	27(3)	38(3)	-5(2)	-9(2)	1(2)
C(52)	23(2)	39(3)	36(3)	-9(2)	-5(2)	-1(2)
C(53)	26(2)	21(3)	41(3)	-6(2)	-1(2)	-3(2)
C(54)	26(2)	18(2)	30(3)	0(2)	-1(2)	2(2)
C(55)	23(2)	24(2)	16(2)	2(2)	-1(2)	-4(2)
C(56)	34(3)	29(3)	35(3)	-1(2)	9(2)	0(2)
C(57)	36(3)	47(4)	45(3)	-8(3)	9(3)	-18(3)
C(58)	22(2)	50(3)	36(3)	2(3)	5(2)	-3(2)
C(59)	30(3)	35(3)	35(3)	-2(2)	3(2)	5(2)
C(60)	26(2)	26(3)	32(3)	-2(2)	-2(2)	-3(2)
C(61)	22(2)	19(2)	22(2)	-3(2)	1(2)	1(2)
C(62)	39(3)	29(3)	33(3)	0(2)	-14(2)	-6(2)
C(63)	48(3)	21(3)	54(4)	8(3)	-12(3)	-9(2)
C(64)	32(3)	41(3)	45(3)	-16(3)	-2(2)	-10(2)
C(65)	24(2)	38(3)	37(3)	-2(2)	-7(2)	0(2)
C(66)	30(3)	26(3)	37(3)	5(2)	-6(2)	-1(2)
C(67)	28(2)	15(2)	22(2)	-3(2)	-3(2)	-1(2)
C(68)	26(2)	28(3)	24(2)	3(2)	-1(2)	2(2)
C(69)	42(3)	33(3)	19(2)	5(2)	0(2)	0(2)
C(70)	28(2)	28(3)	29(3)	2(2)	-10(2)	5(2)
C(71)	23(2)	30(3)	34(3)	0(2)	-3(2)	7(2)
C(72)	28(2)	24(3)	22(2)	3(2)	0(2)	0(2)
C(73)	19(2)	34(3)	18(2)	2(2)	3(2)	5(2)
C(74)	20(2)	40(3)	39(3)	11(2)	1(2)	5(2)
C(75)	38(3)	46(4)	44(3)	19(3)	13(3)	12(3)
C(76)	26(3)	73(5)	34(3)	19(3)	1(2)	22(3)
C(77)	25(3)	75(5)	40(3)	1(3)	-6(2)	13(3)
C(78)	24(2)	50(3)	31(3)	-2(3)	-2(2)	7(2)
C(79)	24(2)	25(2)	16(2)	0(2)	-6(2)	1(2)
C(80)	38(3)	48(3)	27(3)	-10(2)	4(2)	-14(3)
C(81)	58(4)	51(4)	39(3)	-12(3)	8(3)	-27(3)
C(82)	60(4)	57(4)	32(3)	-16(3)	-1(3)	-15(3)
C(83)	41(3)	46(3)	17(2)	-7(2)	0(2)	3(3)
C(84)	23(2)	32(3)	21(2)	-1(2)	-3(2)	-2(2)
C(85)	18(2)	28(3)	25(2)	2(2)	-2(2)	4(2)
C(86)	35(3)	36(3)	35(3)	0(2)	-2(2)	-9(2)
C(87)	44(3)	34(3)	60(4)	0(3)	-4(3)	-14(3)
C(88)	34(3)	40(3)	59(4)	14(3)	4(3)	-7(3)
C(89)	51(3)	49(4)	30(3)	8(3)	12(3)	-2(3)
C(90)	36(3)	35(3)	33(3)	-3(2)	4(2)	-7(2)
C(91)	22(2)	27(3)	19(2)	-5(2)	3(2)	-1(2)
C(92)	24(2)	31(3)	27(3)	1(2)	1(2)	-4(2)
C(93)	26(2)	29(3)	40(3)	5(2)	1(2)	0(2)
C(94)	39(3)	29(3)	42(3)	-16(2)	7(3)	0(2)
C(95)	43(3)	45(3)	34(3)	-13(3)	-7(3)	0(3)
C(96)	32(3)	34(3)	30(3)	-9(2)	-5(2)	7(2)
O(17)	24(2)	42(2)	27(2)	-3(2)	0(1)	-7(2)
C(97)	31(3)	46(3)	26(3)	-4(2)	1(2)	0(2)
C(98)	37(3)	53(4)	37(3)	-13(3)	-4(3)	0(3)
C(99)	31(3)	57(4)	35(3)	-12(3)	-5(2)	11(3)
C(100)	33(3)	42(3)	33(3)	-8(2)	4(2)	-6(2)
O(18)	30(2)	76(3)	43(2)	-22(2)	-9(2)	17(2)
O(19)	66(3)	24(2)	63(3)	-10(2)	19(2)	-8(2)
C(101)	42(3)	48(4)	69(4)	-12(3)	6(3)	-15(3)
C(102)	100(6)	60(5)	86(6)	2(4)	-38(5)	-37(5)
C(103)	103(6)	48(4)	56(4)	-5(4)	11(4)	5(4)
C(104)	53(4)	46(4)	74(5)	-9(3)	18(3)	1(3)
O(20)	143(5)	35(3)	64(3)	-6(2)	5(3)	-19(3)
C(105)	64(5)	72(5)	95(6)	-15(5)	7(4)	-4(4)

C(106)	57(4)	49(5)	120(7)	-18(4)	0(4)	-3(4)
C(107)	66(5)	71(5)	72(5)	-5(4)	-2(4)	-17(4)
C(108)	45(4)	72(5)	74(5)	-10(4)	-7(4)	20(4)
C(109)	71(5)	70(6)	79(6)	-4(4)	-13(4)	3(4)
C(110)	75(6)	81(6)	103(7)	0(5)	3(5)	-9(5)
C(111)	75(6)	86(6)	111(7)	4(5)	1(5)	-9(5)

sh2084a

Table 1. Crystal data and structure refinement for sh2084a.

Identification code	sh2084a	
Empirical formula	C130 H162 Al4 N5 O17 Si8	
Formula weight	2399.29	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.808(3) Å	a= 87.48(3)°.
	b = 18.765(4) Å	b= 74.88(3)°.
	c = 22.445(4) Å	g = 79.44(3)°.
Volume	6718(2) $Å^3$	
Z	2	
Density (calculated)	1.186 Mg/m^3	
Absorption coefficient	0.168 mm^{-1}	
F(000)	2554	
Crystal size	0.32 x 0.25 x 0.18 mm^3	
Theta range for data collection	2.16 to 24.04°.	
Index ranges	-18<=h<=18, -21<=k<=21, -25<=l<=25	
Reflections collected	51806	
Independent reflections	19591 [R(int) = 0.0958]	
Completeness to theta = 24.04°	92.4 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	19591 / 0 / 1452	
Goodness-of-fit on F^2	0.785	
Final R indices [I>2sigma(I)]	R1 = 0.0583, wR2 = 0.1350	
R indices (all data)	R1 = 0.1612, wR2 = 0.1747	
Largest diff. peak and hole	0.489 and -0.282 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2084a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	7276(1)	7253(1)	1384(1)	66(1)
Al(2)	5372(1)	6980(1)	1722(1)	64(1)
Al(3)	5324(1)	7021(1)	3147(1)	68(1)
Al(4)	6982(1)	7735(1)	2804(1)	69(1)
Si(1)	6952(1)	7819(1)	131(1)	69(1)
Si(2)	5037(1)	8263(1)	758(1)	70(1)
Si(3)	4613(1)	5492(1)	1890(1)	68(1)
Si(4)	4740(1)	5451(1)	3271(1)	72(1)
Si(5)	4819(1)	8013(1)	4358(1)	74(1)
Si(6)	5981(1)	9073(1)	3754(1)	74(1)
Si(7)	8950(1)	7164(1)	2698(1)	73(1)
Si(8)	9125(1)	6397(1)	1420(1)	70(1)
O(1)	6458(2)	6765(2)	1481(1)	66(1)
O(2)	5030(2)	7325(2)	2479(1)	65(1)
O(3)	6405(2)	7030(2)	3054(1)	68(1)
O(4)	7079(2)	7886(2)	2004(1)	66(1)
O(5)	7310(2)	7794(2)	730(1)	67(1)
O(6)	5955(3)	8179(2)	276(2)	75(1)
O(7)	4955(3)	7632(2)	1261(1)	71(1)
O(8)	5051(3)	6167(2)	1646(2)	71(1)
O(9)	4684(3)	5240(2)	2583(1)	72(1)
O(10)	5188(3)	6131(2)	3291(2)	77(1)
O(11)	4738(3)	7586(2)	3769(1)	74(1)
O(12)	5159(3)	8781(2)	4170(2)	76(1)
O(13)	6485(3)	8544(2)	3178(2)	76(1)
O(14)	7965(3)	7450(2)	2919(2)	82(1)
O(15)	9245(3)	6622(2)	2090(1)	76(1)
O(16)	8191(2)	6645(2)	1356(2)	70(1)
C(1)	7097(5)	6878(3)	-187(2)	72(2)
C(2)	6454(5)	6620(4)	-351(3)	88(2)
C(3)	6577(6)	5907(4)	-573(3)	94(2)
C(4)	7344(6)	5447(4)	-633(3)	97(2)
C(5)	7988(5)	5683(4)	-481(3)	92(2)
C(6)	7861(5)	6395(4)	-256(2)	79(2)
C(7)	7533(4)	8415(4)	-434(2)	76(2)
C(8)	8159(5)	8166(4)	-944(3)	104(2)
C(9)	8611(7)	8633(7)	-1344(4)	145(4)
C(10)	8425(7)	9364(7)	-1217(5)	134(4)
C(11)	7813(8)	9628(5)	-718(5)	132(3)
C(12)	7356(6)	9168(5)	-336(3)	107(3)
C(13)	4251(5)	8293(3)	298(2)	72(2)
C(14)	3452(5)	8156(3)	569(3)	82(2)
C(15)	2841(5)	8218(4)	248(4)	95(2)
C(16)	3033(6)	8426(4)	-357(4)	99(2)
C(17)	3799(6)	8559(4)	-647(3)	103(2)
C(18)	4413(5)	8498(4)	-323(3)	90(2)
C(19)	4800(4)	9156(3)	1171(2)	72(2)
C(20)	5092(5)	9239(4)	1690(3)	87(2)
C(21)	4900(5)	9905(4)	2007(3)	100(2)
C(22)	4412(6)	10499(4)	1811(3)	104(2)
C(23)	4115(5)	10431(4)	1309(3)	97(2)
C(24)	4305(5)	9767(4)	988(3)	89(2)
C(25)	3492(4)	5724(3)	1876(2)	66(2)
C(26)	2898(5)	5317(4)	2191(3)	85(2)
C(27)	2060(5)	5481(4)	2177(3)	95(2)
C(28)	1805(5)	6058(5)	1840(3)	100(2)
C(29)	2376(6)	6470(4)	1508(3)	96(2)
C(30)	3207(5)	6300(4)	1527(3)	83(2)
C(31)	5107(4)	4698(3)	1363(2)	71(2)
C(32)	5130(5)	3980(4)	1563(3)	89(2)
C(33)	5466(5)	3392(4)	1155(4)	102(2)
C(34)	5794(5)	3505(5)	540(4)	104(2)
C(35)	5806(5)	4195(5)	322(3)	94(2)
C(36)	5451(4)	4790(4)	729(3)	85(2)
C(37)	5340(4)	4641(3)	3564(3)	72(2)
C(38)	5675(5)	4723(4)	4063(3)	93(2)
C(39)	6138(5)	4153(5)	4310(3)	99(2)
C(40)	6266(5)	3481(5)	4071(4)	108(3)
C(41)	5959(6)	3362(4)	3578(4)	118(3)
C(42)	5496(5)	3939(4)	3330(3)	100(2)
C(43)	3648(5)	5620(4)	3779(2)	80(2)

C(44)	3085(5)	5147(4)	3784(3)	92(2)
C(45)	2299(5)	5252(5)	4167(3)	108(3)
C(46)	2011(6)	5838(5)	4568(3)	109(3)
C(47)	2533(6)	6317(5)	4586(3)	104(2)
C(48)	3327(5)	6213(4)	4199(3)	91(2)
C(49)	3773(5)	8230(3)	4912(2)	76(2)
C(50)	3027(5)	8160(4)	4763(3)	89(2)
C(51)	2256(5)	8308(4)	5184(3)	112(3)
C(52)	2171(6)	8531(4)	5774(3)	111(3)
C(53)	2875(6)	8601(4)	5952(3)	105(3)
C(54)	3671(5)	8455(3)	5531(3)	85(2)
C(55)	5535(4)	7441(4)	4774(2)	79(2)
C(56)	5582(4)	6681(4)	4818(3)	85(2)
C(57)	6079(5)	6246(4)	5132(3)	91(2)
C(58)	6545(5)	6556(5)	5426(3)	106(3)
C(59)	6517(6)	7306(5)	5417(4)	122(3)
C(60)	5999(6)	7741(4)	5098(3)	111(3)
C(61)	5624(5)	9996(3)	3466(3)	74(2)
C(62)	4804(6)	10366(4)	3643(3)	99(2)
C(63)	4574(7)	11064(5)	3429(4)	121(3)
C(64)	5143(9)	11382(5)	3038(5)	123(3)
C(65)	5972(8)	11054(6)	2846(4)	124(3)
C(66)	6209(5)	10342(4)	3072(3)	94(2)
C(67)	6692(5)	9179(4)	4247(2)	80(2)
C(68)	7420(6)	8697(5)	4214(4)	135(3)
C(69)	7939(6)	8753(6)	4591(4)	152(4)
C(70)	7740(6)	9308(5)	5015(3)	115(3)
C(71)	7021(5)	9783(4)	5070(3)	92(2)
C(72)	6495(5)	9718(4)	4702(3)	85(2)
C(73)	9264(4)	6635(3)	3350(2)	70(2)
C(74)	9954(5)	6081(4)	3265(3)	101(2)
C(75)	10196(5)	5697(4)	3756(4)	107(2)
C(76)	9716(6)	5853(5)	4355(4)	115(3)
C(77)	9045(6)	6387(5)	4455(3)	115(3)
C(78)	8797(5)	6767(4)	3964(3)	98(2)
C(79)	9548(5)	7924(4)	2512(3)	81(2)
C(80)	10251(6)	7901(5)	2051(4)	110(3)
C(81)	10754(7)	8432(6)	1946(5)	144(4)
C(82)	10514(9)	9033(7)	2315(5)	153(4)
C(83)	9768(9)	9130(6)	2772(5)	151(4)
C(84)	9270(7)	8578(5)	2868(3)	135(3)
C(85)	9857(5)	6817(4)	797(2)	74(2)
C(86)	9574(5)	7407(4)	470(3)	93(2)
C(87)	10137(7)	7731(5)	16(4)	113(3)
C(88)	10967(7)	7481(6)	-116(3)	111(3)
C(89)	11285(5)	6875(5)	185(3)	103(2)
C(90)	10719(5)	6544(4)	641(3)	89(2)
C(91)	9453(4)	5392(3)	1356(2)	72(2)
C(92)	9405(4)	5018(4)	835(3)	86(2)
C(93)	9658(5)	4267(4)	773(3)	97(2)
C(94)	9967(5)	3878(4)	1217(4)	104(2)
C(95)	10030(5)	4217(4)	1728(4)	103(2)
C(96)	9771(4)	4969(4)	1796(3)	84(2)
N(1)	3666(4)	8253(3)	2549(2)	93(2)
C(97)	3402(5)	8888(4)	2977(3)	90(2)
C(98)	2695(5)	9432(4)	2810(3)	92(2)
C(99)	2398(5)	10092(4)	3229(3)	94(2)
C(100)	1679(5)	10607(4)	3056(3)	114(3)
C(101)	1352(5)	11304(4)	3437(3)	112(3)
C(102)	614(6)	11783(4)	3260(4)	126(3)
C(103)	241(5)	12479(4)	3615(3)	112(3)
C(104)	-413(6)	12950(4)	3373(3)	127(3)
C(105)	9192(5)	3682(4)	3683(3)	110(3)
C(106)	8574(5)	4147(4)	3387(3)	112(3)
C(107)	8157(5)	4871(4)	3678(3)	91(2)
C(108)	7666(5)	5349(4)	3294(3)	92(2)
N(2)	7216(4)	6034(3)	3605(2)	96(2)
N(3)	2629(6)	7168(4)	2956(3)	136(3)
C(109)	1737(7)	7231(5)	3223(4)	133(3)
C(110)	1435(6)	7794(5)	3743(4)	124(3)
C(111)	539(7)	7827(6)	4066(5)	146(3)
C(112)	234(6)	8387(8)	4627(4)	165(5)
C(113)	292(8)	9160(7)	4459(5)	172(5)
C(114)	9(8)	9627(5)	5082(6)	180(5)
N(4)	7013(4)	5452(3)	1129(2)	94(2)
C(115)	7124(5)	5009(4)	1661(3)	101(2)
C(116)	7369(5)	4185(4)	1487(3)	104(2)

C(117)	7573(7)	3768(5)	2001(4)	146(4)
C(118)	7805(7)	2952(4)	1884(4)	142(4)
C(119)	8193(10)	2542(6)	2311(5)	219(7)
C(120)	8437(8)	1753(6)	2295(4)	172(5)
C(121)	8858(7)	11399(5)	1687(4)	138(3)
C(122)	9101(6)	10580(5)	1725(4)	138(3)
C(123)	9426(9)	10133(9)	1125(5)	213(7)
C(124)	8928(9)	10165(8)	751(6)	200(6)
C(125)	7993(8)	9992(7)	1051(5)	179(5)
C(126)	7992(8)	9271(5)	1327(5)	167(5)
N(5)	7116(5)	9183(3)	1605(3)	116(2)
O(17)	2315(11)	3211(9)	2183(7)	240(6)
C(127)	2048(12)	3567(9)	2763(8)	175(6)
C(128)	2760(13)	3208(10)	2962(8)	174(6)
C(129)	3132(14)	2644(11)	2019(9)	197(7)
C(130)	3349(16)	2727(13)	2584(11)	229(8)

Table 3. Bond lengths [Å] and angles [°] for sh2084a.

Al(1)-O(16)	1.728(4)
Al(1)-O(5)	1.741(4)
Al(1)-O(1)	1.751(4)
Al(1)-O(4)	1.794(4)
Al(2)-O(7)	1.734(4)
Al(2)-O(8)	1.738(4)
Al(2)-O(1)	1.738(4)
Al(2)-O(2)	1.756(3)
Al(3)-O(10)	1.731(4)
Al(3)-O(2)	1.739(4)
Al(3)-O(11)	1.754(4)
Al(3)-O(3)	1.777(4)
Al(4)-O(14)	1.724(5)
Al(4)-O(13)	1.728(4)
Al(4)-O(3)	1.768(4)
Al(4)-O(4)	1.775(3)
Si(1)-O(5)	1.607(4)
Si(1)-O(6)	1.641(4)
Si(1)-C(7)	1.854(6)
Si(1)-C(1)	1.884(6)
Si(2)-O(7)	1.601(4)
Si(2)-O(6)	1.623(4)
Si(2)-C(13)	1.867(7)
Si(2)-C(19)	1.879(6)
Si(3)-O(8)	1.585(4)
Si(3)-O(9)	1.636(3)
Si(3)-C(25)	1.863(6)
Si(3)-C(31)	1.870(6)
Si(4)-O(10)	1.604(4)
Si(4)-O(9)	1.641(4)
Si(4)-C(37)	1.859(6)
Si(4)-C(43)	1.869(7)
Si(5)-O(11)	1.622(4)
Si(5)-O(12)	1.644(4)
Si(5)-C(49)	1.857(7)
Si(5)-C(55)	1.869(7)
Si(6)-O(13)	1.614(4)
Si(6)-O(12)	1.624(4)
Si(6)-C(67)	1.870(7)
Si(6)-C(61)	1.871(7)
Si(7)-O(14)	1.595(4)
Si(7)-O(15)	1.651(4)
Si(7)-C(79)	1.864(7)
Si(7)-C(73)	1.869(6)
Si(8)-O(16)	1.595(4)
Si(8)-O(15)	1.652(4)
Si(8)-C(85)	1.857(7)
Si(8)-C(91)	1.866(6)
C(1)-C(2)	1.397(9)
C(1)-C(6)	1.405(9)
C(2)-C(3)	1.408(9)
C(3)-C(4)	1.393(10)
C(4)-C(5)	1.365(10)
C(5)-C(6)	1.408(9)
C(7)-C(8)	1.371(9)
C(7)-C(12)	1.404(9)
C(8)-C(9)	1.403(11)
C(9)-C(10)	1.376(13)
C(10)-C(11)	1.348(13)
C(11)-C(12)	1.381(11)
C(13)-C(14)	1.388(9)
C(13)-C(18)	1.400(8)
C(14)-C(15)	1.386(9)
C(15)-C(16)	1.369(9)
C(16)-C(17)	1.346(10)
C(17)-C(18)	1.396(10)
C(19)-C(24)	1.400(8)
C(19)-C(20)	1.401(8)
C(20)-C(21)	1.407(9)
C(21)-C(22)	1.385(10)
C(22)-C(23)	1.365(9)
C(23)-C(24)	1.408(9)
C(25)-C(26)	1.393(9)
C(25)-C(30)	1.394(8)
C(26)-C(27)	1.395(9)

C(27)-C(28)	1.361(9)
C(28)-C(29)	1.386(10)
C(29)-C(30)	1.385(9)
C(31)-C(32)	1.398(8)
C(31)-C(36)	1.406(7)
C(32)-C(33)	1.403(9)
C(33)-C(34)	1.369(9)
C(34)-C(35)	1.367(9)
C(35)-C(36)	1.412(9)
C(37)-C(42)	1.393(9)
C(37)-C(38)	1.404(8)
C(38)-C(39)	1.388(9)
C(39)-C(40)	1.350(10)
C(40)-C(41)	1.379(11)
C(41)-C(42)	1.398(10)
C(43)-C(44)	1.410(9)
C(43)-C(48)	1.422(9)
C(44)-C(45)	1.361(10)
C(45)-C(46)	1.385(10)
C(46)-C(47)	1.373(11)
C(47)-C(48)	1.375(10)
C(49)-C(50)	1.410(9)
C(49)-C(54)	1.427(7)
C(50)-C(51)	1.379(9)
C(51)-C(52)	1.370(9)
C(52)-C(53)	1.374(10)
C(53)-C(54)	1.410(10)
C(55)-C(60)	1.397(9)
C(55)-C(56)	1.414(9)
C(56)-C(57)	1.367(9)
C(57)-C(58)	1.363(10)
C(58)-C(59)	1.398(11)
C(59)-C(60)	1.397(10)
C(61)-C(66)	1.379(9)
C(61)-C(62)	1.388(9)
C(62)-C(63)	1.397(10)
C(63)-C(64)	1.328(12)
C(64)-C(65)	1.380(13)
C(65)-C(66)	1.433(11)
C(67)-C(68)	1.368(10)
C(67)-C(72)	1.402(8)
C(68)-C(69)	1.383(11)
C(69)-C(70)	1.378(10)
C(70)-C(71)	1.345(10)
C(71)-C(72)	1.380(9)
C(73)-C(74)	1.387(9)
C(73)-C(78)	1.404(8)
C(74)-C(75)	1.399(9)
C(75)-C(76)	1.387(10)
C(76)-C(77)	1.342(11)
C(77)-C(78)	1.397(9)
C(79)-C(80)	1.346(9)
C(79)-C(84)	1.431(10)
C(80)-C(81)	1.397(11)
C(81)-C(82)	1.363(13)
C(82)-C(83)	1.386(15)
C(83)-C(84)	1.422(13)
C(85)-C(86)	1.383(9)
C(85)-C(90)	1.400(9)
C(86)-C(87)	1.398(10)
C(87)-C(88)	1.346(11)
C(88)-C(89)	1.391(11)
C(89)-C(90)	1.411(9)
C(91)-C(96)	1.394(8)
C(91)-C(92)	1.418(8)
C(92)-C(93)	1.396(9)
C(93)-C(94)	1.367(10)
C(94)-C(95)	1.371(10)
C(95)-C(96)	1.401(9)
N(1)-C(97)	1.492(7)
C(97)-C(98)	1.532(8)
C(98)-C(99)	1.516(8)
C(99)-C(100)	1.525(9)
C(100)-C(101)	1.528(10)
C(101)-C(102)	1.524(10)
C(102)-C(103)	1.505(10)
C(103)-C(104)	1.482(10)

C(104)-C(105)#1	1.522(9)
C(105)-C(106)	1.503(10)
C(105)-C(104)#2	1.522(9)
C(106)-C(107)	1.500(9)
C(107)-C(108)	1.503(8)
C(108)-N(2)	1.470(8)
N(3)-C(109)	1.446(11)
C(109)-C(110)	1.529(11)
C(110)-C(111)	1.482(12)
C(111)-C(112)	1.591(13)
C(112)-C(113)	1.497(14)
C(113)-C(114)	1.599(14)
C(114)-C(114)#3	1.428(19)
N(4)-C(115)	1.458(8)
C(115)-C(116)	1.565(9)
C(116)-C(117)	1.446(10)
C(117)-C(118)	1.525(11)
C(118)-C(119)	1.419(13)
C(119)-C(120)	1.462(13)
C(120)-C(121)#4	1.487(11)
C(121)-C(120)#5	1.487(11)
C(121)-C(122)	1.519(11)
C(122)-C(123)	1.537(14)
C(123)-C(124)	1.325(15)
C(124)-C(125)	1.627(16)
C(125)-C(126)	1.464(13)
C(126)-N(5)	1.477(12)
O(17)-C(127)	1.415(18)
O(17)-C(129)	1.55(2)
C(127)-C(128)	1.43(2)
C(128)-C(130)	1.35(2)
C(129)-C(130)	1.43(2)

O(16)-Al(1)-O(5)	113.97(19)
O(16)-Al(1)-O(1)	108.3(2)
O(5)-Al(1)-O(1)	109.11(19)
O(16)-Al(1)-O(4)	109.87(19)
O(5)-Al(1)-O(4)	104.30(18)
O(1)-Al(1)-O(4)	111.23(18)
O(7)-Al(2)-O(8)	109.4(2)
O(7)-Al(2)-O(1)	112.5(2)
O(8)-Al(2)-O(1)	103.6(2)
O(7)-Al(2)-O(2)	106.57(19)
O(8)-Al(2)-O(2)	113.20(19)
O(1)-Al(2)-O(2)	111.64(19)
O(10)-Al(3)-O(2)	110.0(2)
O(10)-Al(3)-O(11)	111.0(2)
O(2)-Al(3)-O(11)	109.8(2)
O(10)-Al(3)-O(3)	106.8(2)
O(2)-Al(3)-O(3)	110.36(19)
O(11)-Al(3)-O(3)	108.8(2)
O(14)-Al(4)-O(13)	112.3(2)
O(14)-Al(4)-O(3)	107.3(2)
O(13)-Al(4)-O(3)	112.0(2)
O(14)-Al(4)-O(4)	108.91(19)
O(13)-Al(4)-O(4)	106.99(19)
O(3)-Al(4)-O(4)	109.34(19)
O(5)-Si(1)-O(6)	112.5(2)
O(5)-Si(1)-C(7)	106.4(3)
O(6)-Si(1)-C(7)	107.2(3)
O(5)-Si(1)-C(1)	110.4(3)
O(6)-Si(1)-C(1)	108.4(3)
C(7)-Si(1)-C(1)	111.9(3)
O(7)-Si(2)-O(6)	113.5(2)
O(7)-Si(2)-C(13)	110.8(3)
O(6)-Si(2)-C(13)	107.6(3)
O(7)-Si(2)-C(19)	108.5(2)
O(6)-Si(2)-C(19)	109.1(3)
C(13)-Si(2)-C(19)	107.1(3)
O(8)-Si(3)-O(9)	113.1(2)
O(8)-Si(3)-C(25)	108.8(3)
O(9)-Si(3)-C(25)	110.0(2)
O(8)-Si(3)-C(31)	110.0(2)
O(9)-Si(3)-C(31)	107.4(2)
C(25)-Si(3)-C(31)	107.4(3)
O(10)-Si(4)-O(9)	115.0(2)
O(10)-Si(4)-C(37)	108.6(3)

O(9)-Si(4)-C(37)	106.8(2)
O(10)-Si(4)-C(43)	110.4(3)
O(9)-Si(4)-C(43)	107.4(3)
C(37)-Si(4)-C(43)	108.4(3)
O(11)-Si(5)-O(12)	113.0(2)
O(11)-Si(5)-C(49)	109.2(3)
O(12)-Si(5)-C(49)	107.4(2)
O(11)-Si(5)-C(55)	111.4(3)
O(12)-Si(5)-C(55)	108.3(3)
C(49)-Si(5)-C(55)	107.3(3)
O(13)-Si(6)-O(12)	112.5(2)
O(13)-Si(6)-C(67)	109.7(3)
O(12)-Si(6)-C(67)	109.7(2)
O(13)-Si(6)-C(61)	109.9(2)
O(12)-Si(6)-C(61)	107.8(3)
C(67)-Si(6)-C(61)	107.0(3)
O(14)-Si(7)-O(15)	114.4(2)
O(14)-Si(7)-C(79)	111.9(3)
O(15)-Si(7)-C(79)	107.4(3)
O(14)-Si(7)-C(73)	107.1(3)
O(15)-Si(7)-C(73)	107.3(2)
C(79)-Si(7)-C(73)	108.5(3)
O(16)-Si(8)-O(15)	113.1(2)
O(16)-Si(8)-C(85)	109.7(3)
O(15)-Si(8)-C(85)	108.3(3)
O(16)-Si(8)-C(91)	111.4(3)
O(15)-Si(8)-C(91)	105.9(2)
C(85)-Si(8)-C(91)	108.3(3)
Al(2)-O(1)-Al(1)	134.9(2)
Al(3)-O(2)-Al(2)	131.1(2)
Al(4)-O(3)-Al(3)	129.9(2)
Al(4)-O(4)-Al(1)	130.4(2)
Si(1)-O(5)-Al(1)	136.3(2)
Si(2)-O(6)-Si(1)	147.2(2)
Si(2)-O(7)-Al(2)	152.2(3)
Si(3)-O(8)-Al(2)	154.9(2)
Si(3)-O(9)-Si(4)	149.4(3)
Si(4)-O(10)-Al(3)	154.0(3)
Si(5)-O(11)-Al(3)	142.7(3)
Si(6)-O(12)-Si(5)	139.6(3)
Si(6)-O(13)-Al(4)	156.9(3)
Si(7)-O(14)-Al(4)	154.1(2)
Si(7)-O(15)-Si(8)	149.5(3)
Si(8)-O(16)-Al(1)	155.3(3)
C(2)-C(1)-C(6)	116.9(6)
C(2)-C(1)-Si(1)	122.2(6)
C(6)-C(1)-Si(1)	120.9(5)
C(1)-C(2)-C(3)	120.8(7)
C(4)-C(3)-C(2)	120.4(7)
C(5)-C(4)-C(3)	120.4(8)
C(4)-C(5)-C(6)	119.0(7)
C(1)-C(6)-C(5)	122.6(7)
C(8)-C(7)-C(12)	116.3(6)
C(8)-C(7)-Si(1)	123.9(6)
C(12)-C(7)-Si(1)	119.7(5)
C(7)-C(8)-C(9)	122.1(8)
C(10)-C(9)-C(8)	119.0(9)
C(11)-C(10)-C(9)	120.5(9)
C(10)-C(11)-C(12)	120.2(9)
C(11)-C(12)-C(7)	121.8(8)
C(14)-C(13)-C(18)	116.3(6)
C(14)-C(13)-Si(2)	121.3(5)
C(18)-C(13)-Si(2)	122.3(6)
C(15)-C(14)-C(13)	122.5(6)
C(16)-C(15)-C(14)	118.7(7)
C(17)-C(16)-C(15)	121.6(7)
C(16)-C(17)-C(18)	119.6(7)
C(17)-C(18)-C(13)	121.3(7)
C(24)-C(19)-C(20)	116.6(6)
C(24)-C(19)-Si(2)	121.9(5)
C(20)-C(19)-Si(2)	121.5(5)
C(19)-C(20)-C(21)	121.5(6)
C(22)-C(21)-C(20)	120.4(7)
C(23)-C(22)-C(21)	119.3(7)
C(22)-C(23)-C(24)	120.7(7)
C(19)-C(24)-C(23)	121.6(6)
C(26)-C(25)-C(30)	116.2(6)

C(26)-C(25)-Si(3)	122.3(5)
C(30)-C(25)-Si(3)	121.5(5)
C(25)-C(26)-C(27)	122.6(7)
C(28)-C(27)-C(26)	119.2(7)
C(27)-C(28)-C(29)	120.3(8)
C(30)-C(29)-C(28)	119.8(7)
C(29)-C(30)-C(25)	121.9(7)
C(32)-C(31)-C(36)	115.6(5)
C(32)-C(31)-Si(3)	122.9(4)
C(36)-C(31)-Si(3)	121.5(5)
C(31)-C(32)-C(33)	122.0(6)
C(34)-C(33)-C(32)	120.6(7)
C(35)-C(34)-C(33)	119.8(7)
C(34)-C(35)-C(36)	119.8(6)
C(31)-C(36)-C(35)	122.2(6)
C(42)-C(37)-C(38)	115.5(6)
C(42)-C(37)-Si(4)	125.7(5)
C(38)-C(37)-Si(4)	118.8(5)
C(39)-C(38)-C(37)	123.1(7)
C(40)-C(39)-C(38)	119.2(7)
C(39)-C(40)-C(41)	120.7(7)
C(40)-C(41)-C(42)	119.8(8)
C(37)-C(42)-C(41)	121.6(7)
C(44)-C(43)-C(48)	114.9(7)
C(44)-C(43)-Si(4)	121.6(5)
C(48)-C(43)-Si(4)	123.5(6)
C(45)-C(44)-C(43)	121.9(7)
C(44)-C(45)-C(46)	121.2(8)
C(47)-C(46)-C(45)	119.5(8)
C(46)-C(47)-C(48)	119.5(8)
C(47)-C(48)-C(43)	123.0(8)
C(50)-C(49)-C(54)	115.1(6)
C(50)-C(49)-Si(5)	122.8(4)
C(54)-C(49)-Si(5)	122.1(6)
C(51)-C(50)-C(49)	122.1(6)
C(52)-C(51)-C(50)	121.9(8)
C(51)-C(52)-C(53)	119.0(8)
C(52)-C(53)-C(54)	120.4(7)
C(53)-C(54)-C(49)	121.6(7)
C(60)-C(55)-C(56)	116.2(6)
C(60)-C(55)-Si(5)	122.2(6)
C(56)-C(55)-Si(5)	121.4(5)
C(57)-C(56)-C(55)	123.2(7)
C(58)-C(57)-C(56)	118.9(7)
C(57)-C(58)-C(59)	121.4(7)
C(60)-C(59)-C(58)	118.8(8)
C(59)-C(60)-C(55)	121.4(7)
C(66)-C(61)-C(62)	117.7(7)
C(66)-C(61)-Si(6)	118.6(6)
C(62)-C(61)-Si(6)	123.7(6)
C(61)-C(62)-C(63)	121.5(8)
C(64)-C(63)-C(62)	119.9(10)
C(63)-C(64)-C(65)	122.1(10)
C(64)-C(65)-C(66)	117.9(9)
C(61)-C(66)-C(65)	120.8(8)
C(68)-C(67)-C(72)	115.5(6)
C(68)-C(67)-Si(6)	121.4(5)
C(72)-C(67)-Si(6)	123.0(6)
C(67)-C(68)-C(69)	122.2(7)
C(70)-C(69)-C(68)	120.5(8)
C(71)-C(70)-C(69)	118.9(7)
C(70)-C(71)-C(72)	120.5(7)
C(71)-C(72)-C(67)	122.3(7)
C(74)-C(73)-C(78)	115.5(6)
C(74)-C(73)-Si(7)	122.9(4)
C(78)-C(73)-Si(7)	121.5(5)
C(73)-C(74)-C(75)	122.6(7)
C(76)-C(75)-C(74)	119.5(8)
C(77)-C(76)-C(75)	119.4(7)
C(76)-C(77)-C(78)	121.2(7)
C(77)-C(78)-C(73)	121.6(7)
C(80)-C(79)-C(84)	116.2(7)
C(80)-C(79)-Si(7)	123.7(6)
C(84)-C(79)-Si(7)	120.1(7)
C(79)-C(80)-C(81)	124.3(8)
C(82)-C(81)-C(80)	118.9(10)
C(81)-C(82)-C(83)	120.8(11)

C(82)-C(83)-C(84)	118.9(10)
C(83)-C(84)-C(79)	120.4(9)
C(86)-C(85)-C(90)	117.5(6)
C(86)-C(85)-Si(8)	121.4(6)
C(90)-C(85)-Si(8)	121.1(5)
C(85)-C(86)-C(87)	120.7(8)
C(88)-C(87)-C(86)	121.3(8)
C(87)-C(88)-C(89)	120.5(8)
C(88)-C(89)-C(90)	118.3(8)
C(85)-C(90)-C(89)	121.6(7)
C(96)-C(91)-C(92)	116.2(6)
C(96)-C(91)-Si(8)	123.4(5)
C(92)-C(91)-Si(8)	120.4(5)
C(93)-C(92)-C(91)	121.5(6)
C(94)-C(93)-C(92)	120.0(7)
C(93)-C(94)-C(95)	120.5(7)
C(94)-C(95)-C(96)	119.8(7)
C(91)-C(96)-C(95)	122.0(6)
N(1)-C(97)-C(98)	110.8(5)
C(99)-C(98)-C(97)	113.4(6)
C(98)-C(99)-C(100)	111.4(6)
C(99)-C(100)-C(101)	115.7(7)
C(102)-C(101)-C(100)	113.3(7)
C(103)-C(102)-C(101)	117.3(7)
C(104)-C(103)-C(102)	114.0(7)
C(103)-C(104)-C(105)#1	118.4(7)
C(106)-C(105)-C(104)#2	115.2(7)
C(107)-C(106)-C(105)	117.4(6)
C(106)-C(107)-C(108)	113.7(6)
N(2)-C(108)-C(107)	112.8(5)
N(3)-C(109)-C(110)	110.7(8)
C(111)-C(110)-C(109)	112.3(9)
C(110)-C(111)-C(112)	112.5(8)
C(113)-C(112)-C(111)	115.5(9)
C(112)-C(113)-C(114)	108.1(9)
C(114)#3-C(114)-C(113)	108.1(13)
N(4)-C(115)-C(116)	111.1(6)
C(117)-C(116)-C(115)	109.9(7)
C(116)-C(117)-C(118)	114.2(8)
C(119)-C(118)-C(117)	115.8(9)
C(118)-C(119)-C(120)	124.5(11)
C(119)-C(120)-C(121)#4	117.9(9)
C(120)#5-C(121)-C(122)	113.5(8)
C(121)-C(122)-C(123)	119.1(9)
C(124)-C(123)-C(122)	118.1(13)
C(123)-C(124)-C(125)	116.9(12)
C(126)-C(125)-C(124)	113.4(11)
C(125)-C(126)-N(5)	108.7(10)
C(127)-O(17)-C(129)	120.6(15)
O(17)-C(127)-C(128)	93.5(15)
C(130)-C(128)-C(127)	119.5(19)
C(130)-C(129)-O(17)	95.0(17)
C(128)-C(130)-C(129)	111(2)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y+1,z #2 x+1,y-1,z #3 -x,-y+2,-z+1
#4 x,y-1,z #5 x,y+1,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2084a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	71(1)	70(1)	55(1)	-5(1)	-17(1)	-8(1)
Al(2)	69(1)	65(1)	57(1)	-3(1)	-17(1)	-7(1)
Al(3)	78(2)	69(1)	56(1)	-7(1)	-17(1)	-5(1)
Al(4)	66(1)	78(1)	63(1)	-11(1)	-20(1)	-4(1)
Si(1)	73(1)	76(1)	59(1)	-1(1)	-16(1)	-14(1)
Si(2)	77(1)	70(1)	62(1)	0(1)	-20(1)	-7(1)
Si(3)	76(1)	68(1)	60(1)	-5(1)	-16(1)	-10(1)
Si(4)	83(1)	71(1)	60(1)	-2(1)	-19(1)	-7(1)
Si(5)	84(2)	75(1)	60(1)	-9(1)	-18(1)	-6(1)
Si(6)	83(2)	71(1)	65(1)	-13(1)	-21(1)	-3(1)
Si(7)	76(2)	81(1)	61(1)	-9(1)	-19(1)	-9(1)
Si(8)	72(1)	78(1)	59(1)	-8(1)	-15(1)	-7(1)
O(1)	68(3)	69(2)	60(2)	-7(2)	-14(2)	-12(2)
O(2)	77(3)	68(2)	48(2)	-8(2)	-16(2)	-6(2)
O(3)	72(3)	68(2)	60(2)	-7(2)	-17(2)	-7(2)
O(4)	74(3)	72(2)	52(2)	-10(2)	-16(2)	-10(2)
O(5)	83(3)	68(2)	53(2)	1(2)	-25(2)	-12(2)
O(6)	65(3)	82(3)	70(2)	1(2)	-9(2)	-7(2)
O(7)	81(3)	66(2)	63(2)	3(2)	-23(2)	-4(2)
O(8)	81(3)	67(3)	70(2)	-3(2)	-20(2)	-21(2)
O(9)	90(3)	75(3)	51(2)	-2(2)	-22(2)	-8(2)
O(10)	101(4)	64(3)	67(2)	1(2)	-23(2)	-17(2)
O(11)	79(3)	83(3)	56(2)	-19(2)	-14(2)	-2(2)
O(12)	86(3)	74(3)	66(2)	-4(2)	-13(2)	-18(2)
O(13)	85(3)	70(3)	62(2)	-26(2)	-8(2)	3(2)
O(14)	69(3)	101(3)	72(2)	-22(2)	-20(2)	3(2)
O(15)	88(3)	84(3)	55(2)	-17(2)	-24(2)	-5(2)
O(16)	62(3)	78(3)	68(2)	-6(2)	-18(2)	0(2)
C(1)	80(6)	77(4)	54(3)	-3(3)	-8(3)	-14(4)
C(2)	79(6)	103(6)	84(4)	-16(4)	-24(4)	-16(4)
C(3)	96(7)	102(6)	93(5)	-19(4)	-28(4)	-28(5)
C(4)	118(8)	91(6)	77(4)	-15(4)	-12(4)	-24(6)
C(5)	98(7)	86(6)	84(4)	-7(4)	-11(4)	-14(5)
C(6)	83(6)	79(5)	75(4)	-7(3)	-18(3)	-15(4)
C(7)	85(5)	83(5)	58(3)	5(3)	-16(3)	-15(4)
C(8)	99(6)	115(6)	87(4)	21(4)	-3(4)	-26(5)
C(9)	136(9)	164(10)	114(6)	30(7)	6(6)	-37(8)
C(10)	135(10)	158(10)	129(8)	61(8)	-44(7)	-74(8)
C(11)	182(11)	110(7)	124(7)	42(6)	-57(7)	-65(7)
C(12)	137(8)	96(6)	92(5)	14(4)	-34(5)	-30(5)
C(13)	89(6)	65(4)	63(3)	-5(3)	-24(3)	-9(4)
C(14)	89(6)	84(5)	73(4)	-6(3)	-21(4)	-11(4)
C(15)	85(6)	94(5)	111(6)	-12(4)	-38(5)	-10(4)
C(16)	99(7)	94(6)	116(6)	-2(4)	-57(5)	-8(5)
C(17)	121(8)	114(6)	80(4)	12(4)	-37(5)	-22(6)
C(18)	105(6)	92(5)	79(4)	7(3)	-36(4)	-18(4)
C(19)	87(5)	67(4)	62(3)	2(3)	-19(3)	-11(4)
C(20)	97(6)	85(5)	81(4)	-8(4)	-34(4)	-5(4)
C(21)	120(7)	102(6)	86(4)	-14(4)	-33(4)	-24(5)
C(22)	137(8)	77(5)	97(5)	-13(4)	-34(5)	-10(5)
C(23)	118(7)	74(5)	101(5)	-8(4)	-39(4)	-3(4)
C(24)	107(6)	83(5)	79(4)	0(4)	-35(4)	-9(4)
C(25)	45(4)	86(4)	66(3)	-12(3)	-13(3)	-6(3)
C(26)	75(6)	97(5)	79(4)	-3(4)	-16(4)	-11(4)
C(27)	76(7)	116(6)	85(4)	4(4)	-10(4)	-14(5)
C(28)	76(6)	118(6)	100(5)	0(5)	-26(4)	-1(5)
C(29)	85(7)	105(6)	94(5)	13(4)	-34(4)	4(5)
C(30)	87(6)	85(5)	76(4)	-1(3)	-26(4)	-3(4)
C(31)	77(5)	72(4)	63(3)	-9(3)	-17(3)	-12(3)
C(32)	118(6)	68(5)	76(4)	-16(3)	-18(4)	-9(4)
C(33)	125(7)	74(5)	106(5)	-9(4)	-30(5)	-12(5)
C(34)	116(7)	86(6)	110(6)	-32(5)	-34(5)	-3(5)
C(35)	94(6)	111(6)	71(4)	-25(4)	-11(3)	-12(5)
C(36)	91(6)	91(5)	68(4)	-12(3)	-9(3)	-24(4)
C(37)	69(5)	76(5)	69(4)	5(3)	-16(3)	-11(3)
C(38)	108(7)	80(5)	106(5)	13(4)	-49(4)	-22(4)
C(39)	97(7)	97(6)	114(5)	24(5)	-45(4)	-23(5)
C(40)	88(6)	110(7)	116(6)	34(5)	-25(5)	-2(5)
C(41)	142(8)	79(5)	115(6)	3(5)	-27(6)	15(5)
C(42)	127(7)	80(5)	89(4)	1(4)	-34(4)	3(5)
C(43)	95(6)	81(5)	61(3)	-2(3)	-24(3)	1(4)

C(44)	107(7)	84(5)	80(4)	2(4)	-16(4)	-17(5)
C(45)	97(7)	132(7)	89(5)	2(5)	-9(5)	-27(5)
C(46)	99(7)	134(8)	83(5)	-10(5)	-17(4)	-1(6)
C(47)	90(7)	123(7)	85(5)	-24(4)	-10(4)	4(5)
C(48)	87(6)	104(6)	80(4)	-7(4)	-22(4)	-7(4)
C(49)	99(6)	70(4)	55(3)	-5(3)	-17(3)	-6(4)
C(50)	85(6)	104(5)	71(4)	-17(3)	-20(4)	1(4)
C(51)	87(7)	148(7)	95(5)	-39(5)	-16(4)	-11(5)
C(52)	106(8)	122(7)	96(5)	-35(4)	-14(5)	-1(5)
C(53)	121(8)	113(6)	64(4)	-22(4)	4(5)	-10(5)
C(54)	105(6)	83(5)	71(4)	-13(3)	-25(4)	-21(4)
C(55)	78(5)	94(5)	61(3)	-4(3)	-15(3)	-9(4)
C(56)	80(5)	96(6)	76(4)	-2(4)	-22(3)	-7(4)
C(57)	98(6)	91(5)	79(4)	6(4)	-27(4)	-1(5)
C(58)	108(7)	106(7)	97(5)	24(5)	-38(5)	9(5)
C(59)	134(8)	131(8)	129(6)	25(6)	-81(6)	-31(6)
C(60)	149(8)	98(6)	110(5)	19(4)	-76(5)	-28(5)
C(61)	83(6)	75(4)	65(3)	-16(3)	-20(3)	-8(4)
C(62)	125(8)	83(5)	86(4)	-12(4)	-36(4)	6(5)
C(63)	142(10)	95(7)	119(6)	-24(5)	-47(6)	22(6)
C(64)	143(11)	100(7)	150(8)	2(6)	-79(8)	-20(7)
C(65)	159(11)	120(8)	132(7)	23(6)	-78(7)	-68(7)
C(66)	91(6)	92(6)	107(5)	2(4)	-37(4)	-21(5)
C(67)	100(6)	77(4)	61(3)	-16(3)	-17(3)	-9(4)
C(68)	108(8)	167(9)	130(6)	-80(6)	-56(5)	33(7)
C(69)	105(8)	203(10)	149(7)	-96(7)	-71(6)	46(7)
C(70)	92(7)	158(8)	103(5)	-39(5)	-51(4)	3(6)
C(71)	98(7)	103(6)	84(4)	-18(4)	-40(4)	-15(5)
C(72)	97(6)	88(5)	74(4)	-6(3)	-29(4)	-13(4)
C(73)	67(5)	82(4)	64(3)	-8(3)	-20(3)	-14(4)
C(74)	98(7)	116(6)	85(4)	7(4)	-27(4)	-8(5)
C(75)	92(7)	105(6)	121(6)	13(5)	-36(5)	-2(5)
C(76)	126(8)	128(8)	94(6)	27(5)	-39(5)	-20(6)
C(77)	129(8)	143(8)	70(4)	11(5)	-28(5)	-13(6)
C(78)	121(7)	105(5)	64(4)	-9(4)	-27(4)	-2(5)
C(79)	103(6)	76(5)	70(4)	2(3)	-35(4)	-15(4)
C(80)	108(7)	100(6)	121(6)	-6(5)	-17(5)	-33(5)
C(81)	139(10)	120(8)	173(9)	11(7)	-21(7)	-56(8)
C(82)	226(14)	142(10)	130(8)	52(8)	-78(9)	-98(10)
C(83)	258(15)	107(8)	113(7)	10(6)	-61(8)	-83(9)
C(84)	209(11)	112(7)	87(5)	-2(5)	-44(6)	-28(8)
C(85)	78(6)	84(5)	56(3)	-13(3)	-10(3)	-12(4)
C(86)	99(6)	100(6)	81(4)	5(4)	-15(4)	-34(5)
C(87)	113(8)	119(7)	110(6)	22(5)	-28(5)	-36(6)
C(88)	115(9)	139(8)	91(5)	5(5)	-21(5)	-61(7)
C(89)	75(6)	153(8)	83(5)	-23(5)	-9(4)	-35(6)
C(90)	95(7)	107(6)	66(4)	-12(4)	-11(4)	-31(5)
C(91)	72(5)	77(4)	64(3)	-6(3)	-14(3)	-8(3)
C(92)	87(6)	82(5)	84(4)	-16(4)	-20(3)	-4(4)
C(93)	89(6)	97(6)	99(5)	-25(4)	-15(4)	-11(5)
C(94)	101(7)	75(5)	120(6)	-18(5)	-3(5)	-7(4)
C(95)	108(7)	86(6)	103(5)	8(4)	-18(4)	-2(5)
C(96)	80(5)	91(5)	76(4)	-9(4)	-15(3)	-6(4)
N(1)	92(5)	96(4)	77(3)	-13(3)	-20(3)	20(3)
C(97)	85(6)	90(5)	83(4)	-8(4)	-20(3)	15(4)
C(98)	87(6)	87(5)	88(4)	-4(4)	-18(4)	11(4)
C(99)	82(6)	91(5)	98(4)	-12(4)	-23(4)	18(4)
C(100)	116(7)	94(6)	119(5)	-12(5)	-25(5)	15(5)
C(101)	107(7)	96(6)	118(5)	2(5)	-28(5)	17(5)
C(102)	141(8)	90(6)	128(6)	-10(5)	-34(5)	31(5)
C(103)	106(7)	98(6)	110(5)	2(4)	-19(4)	26(5)
C(104)	140(8)	96(6)	117(6)	3(5)	-24(5)	36(6)
C(105)	114(7)	88(5)	107(5)	5(4)	-20(4)	20(5)
C(106)	125(7)	90(5)	103(5)	-4(4)	-24(5)	17(5)
C(107)	84(6)	89(5)	88(4)	5(4)	-15(4)	4(4)
C(108)	95(6)	80(5)	88(4)	0(4)	-17(4)	8(4)
N(2)	93(5)	92(4)	91(3)	11(3)	-20(3)	9(3)
N(3)	159(8)	124(6)	120(5)	-30(4)	-31(5)	-13(5)
C(109)	168(11)	125(7)	107(6)	-12(5)	-38(6)	-23(7)
C(110)	129(9)	141(8)	106(6)	-18(5)	-38(5)	-18(6)
C(111)	109(9)	193(11)	149(8)	6(7)	-46(7)	-40(7)
C(112)	99(8)	267(15)	122(7)	-42(9)	-25(5)	-9(9)
C(113)	192(13)	150(10)	170(10)	-9(9)	-38(8)	-34(9)
C(114)	173(12)	173(12)	169(10)	-15(10)	-2(8)	-22(11)
N(4)	94(5)	71(4)	103(4)	-21(3)	-3(3)	-9(3)
C(115)	107(7)	76(5)	119(5)	-5(4)	-35(4)	-8(4)
C(116)	99(7)	93(6)	113(5)	3(4)	-24(4)	-2(4)

C(117)	188(11)	119(8)	120(6)	-1(6)	-32(6)	-12(7)
C(118)	208(11)	76(6)	135(7)	11(5)	-43(7)	-7(6)
C(119)	330(20)	121(9)	165(10)	-29(8)	-56(11)	55(11)
C(120)	245(14)	120(9)	133(8)	-18(7)	-38(8)	1(8)
C(121)	163(10)	93(7)	149(8)	14(6)	-41(6)	0(6)
C(122)	134(9)	125(8)	143(8)	3(6)	-28(6)	-7(6)
C(123)	135(12)	370(20)	123(9)	-3(11)	-44(8)	10(12)
C(124)	148(14)	234(14)	176(12)	24(10)	13(10)	-16(11)
C(125)	175(14)	219(14)	147(8)	-9(9)	-54(8)	-25(10)
C(126)	233(14)	78(6)	157(8)	6(6)	34(8)	-64(7)
N(5)	153(7)	75(4)	124(5)	14(3)	-38(5)	-30(4)

sh 2049

Table 1. Crystal data and structure refinement for sh2049.

Identification code	sh2049	
Empirical formula	$C_{126}\ H_{146}\ Al_4\ N_4\ O_{20}\ Si_8$	
Formula weight	2369.11	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 17.067(3) Å	a= 90°.
	b = 17.267(3) Å	b= 90°.
	c = 47.357(9) Å	g = 90°.
Volume	13956(4) $Å^3$	
Z	4	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.162 mm^{-1}	
F(000)	5016	
Crystal size	0.32 x 0.25 x 0.15 mm^3	
Theta range for data collection	1.68 to 20.97°.	
Index ranges	-16<=h<=16, -17<=k<=17, -47<=l<=46	
Reflections collected	60713	
Independent reflections	14542 [R(int) = 0.1180]	
Completeness to theta = 20.97°	97.5 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14542 / 0 / 1403	
Goodness-of-fit on F^2	1.817	
Final R indices [I>2sigma(I)]	R1 = 0.0838, wR2 = 0.1961	
R indices (all data)	R1 = 0.1155, wR2 = 0.2118	
Absolute structure parameter	-0.11(18)	
Largest diff. peak and hole	0.863 and -0.409 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2049. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	7044(2)	4922(1)	8926(1)	39(1)
Al(2)	5275(2)	4466(2)	9121(1)	42(1)
Al(3)	5481(2)	2892(1)	8768(1)	43(1)
Al(4)	7126(2)	3489(1)	8476(1)	40(1)
Si(1)	7420(2)	4719(1)	9586(1)	45(1)
Si(2)	5687(2)	5167(1)	9715(1)	47(1)
Si(3)	3473(2)	4591(2)	8897(1)	50(1)
Si(4)	3619(2)	2944(2)	8631(1)	57(1)
Si(5)	6201(2)	1201(1)	8797(1)	51(1)
Si(6)	7692(2)	1776(1)	8450(1)	46(1)
Si(7)	7205(2)	4781(1)	8004(1)	46(1)
Si(8)	7833(2)	5968(1)	8467(1)	46(1)
O(1)	6017(3)	5030(3)	8956(1)	42(1)
O(2)	5480(3)	3492(3)	9065(1)	45(1)
O(3)	6129(3)	3181(3)	8494(1)	45(1)
O(4)	7388(3)	4112(3)	8747(1)	43(1)
O(5)	7468(3)	4910(3)	9262(1)	50(2)
O(6)	6647(4)	5063(4)	9741(1)	58(2)
O(7)	5295(3)	4599(3)	9487(1)	49(2)
O(8)	4363(3)	4725(3)	8986(1)	51(2)
O(9)	3331(4)	3823(4)	8704(1)	65(2)
O(10)	4564(4)	2866(3)	8614(1)	54(2)
O(11)	5752(4)	1981(3)	8884(1)	53(2)
O(12)	7054(4)	1352(3)	8659(1)	55(2)
O(13)	7748(4)	2688(3)	8499(1)	48(2)
O(14)	7267(3)	3955(3)	8154(1)	45(1)
O(15)	7623(4)	5484(3)	8183(1)	56(2)
O(16)	7311(4)	5748(3)	8738(1)	53(2)
C(1)	8259(6)	5180(5)	9768(2)	52(2)
C(2)	8982(6)	5260(6)	9638(2)	63(3)
C(3)	9604(7)	5684(7)	9760(3)	84(4)
C(4)	9536(7)	6003(7)	10016(3)	76(3)
C(5)	8839(9)	5921(8)	10157(3)	102(4)
C(6)	8196(7)	5503(7)	10039(2)	77(3)
C(7)	7399(5)	3643(5)	9639(2)	48(2)
C(8)	7407(6)	3137(5)	9410(2)	55(3)
C(9)	7418(7)	2333(6)	9445(3)	70(3)
C(10)	7394(7)	2029(6)	9706(3)	77(3)
C(11)	7372(7)	2503(7)	9939(2)	76(3)
C(12)	7368(7)	3288(7)	9905(2)	69(3)
C(13)	5293(6)	4929(6)	10074(2)	57(3)
C(14)	4551(8)	4658(9)	10112(2)	89(4)
C(15)	4231(9)	4444(10)	10379(3)	109(5)
C(16)	4689(9)	4543(9)	10613(3)	94(4)
C(17)	5430(9)	4798(11)	10580(3)	118(6)
C(18)	5725(7)	4986(10)	10315(2)	102(5)
C(19)	5506(6)	6203(6)	9609(2)	60(3)
C(20)	6126(8)	6737(6)	9583(3)	91(4)
C(21)	5985(12)	7490(8)	9489(4)	117(5)
C(22)	5255(11)	7712(8)	9418(3)	94(4)
C(23)	4646(9)	7218(8)	9436(3)	85(4)
C(24)	4772(7)	6455(6)	9532(2)	75(3)
C(25)	2831(6)	4523(5)	9216(2)	51(2)
C(26)	3130(7)	4550(8)	9490(2)	88(4)
C(27)	2655(9)	4531(11)	9723(3)	119(6)
C(28)	1873(8)	4479(8)	9700(3)	89(4)
C(29)	1549(7)	4482(8)	9430(3)	92(4)
C(30)	2024(7)	4480(8)	9201(3)	85(4)
C(31)	3085(6)	5415(7)	8681(2)	58(3)
C(32)	3215(7)	6148(8)	8774(3)	90(4)
C(33)	2949(11)	6817(8)	8624(4)	118(6)
C(34)	2507(11)	6747(16)	8413(6)	167(12)
C(35)	2358(9)	5961(14)	8287(3)	122(6)
C(36)	2651(7)	5313(9)	8435(3)	87(4)
C(37)	3195(6)	2722(7)	8279(3)	75(3)
C(38)	3032(9)	1955(9)	8204(3)	110(5)
C(39)	2792(11)	1761(11)	7929(4)	138(7)
C(40)	2730(12)	2376(18)	7729(4)	151(8)
C(41)	2874(11)	3098(12)	7800(4)	122(6)
C(42)	3117(8)	3260(8)	8070(3)	87(4)
C(43)	3221(7)	2257(7)	8909(3)	80(4)

C(44)	3674(9)	1645(9)	9015(3)	98(4)
C(45)	3393(11)	1100(11)	9206(4)	118(5)
C(46)	2681(18)	1187(9)	9308(4)	142(9)
C(47)	2167(14)	1708(13)	9194(6)	204(14)
C(48)	2452(12)	2283(10)	8987(5)	168(9)
C(49)	5615(6)	623(5)	8538(2)	50(2)
C(50)	5067(7)	951(7)	8358(3)	77(3)
C(51)	4702(8)	550(8)	8141(3)	95(4)
C(52)	4861(9)	-208(8)	8109(3)	89(4)
C(53)	5413(10)	-576(7)	8282(3)	105(5)
C(54)	5770(7)	-158(6)	8492(3)	82(3)
C(55)	6350(7)	607(5)	9118(2)	64(3)
C(56)	5768(9)	539(7)	9320(3)	88(4)
C(57)	5885(14)	42(11)	9558(3)	123(6)
C(58)	6557(15)	-330(9)	9596(4)	116(6)
C(59)	7120(12)	-290(7)	9408(3)	105(5)
C(60)	7089(8)	195(7)	9178(3)	91(4)
C(61)	7416(5)	1586(5)	8075(2)	49(2)
C(62)	7052(6)	889(6)	7985(2)	67(3)
C(63)	6910(7)	737(7)	7706(3)	78(3)
C(64)	7131(7)	1256(7)	7504(2)	74(3)
C(65)	7470(7)	1946(7)	7579(2)	73(3)
C(66)	7598(7)	2077(6)	7860(2)	66(3)
C(67)	8648(6)	1295(5)	8517(2)	52(3)
C(68)	9377(7)	1667(6)	8520(2)	67(3)
C(69)	10067(8)	1291(8)	8559(3)	95(4)
C(70)	10081(10)	509(10)	8600(3)	103(5)
C(71)	9362(10)	94(8)	8596(3)	93(4)
C(72)	8677(7)	496(6)	8553(2)	71(3)
C(73)	7682(6)	4762(6)	7653(2)	59(3)
C(74)	8223(6)	5342(7)	7561(2)	75(3)
C(75)	8553(8)	5303(11)	7291(3)	100(5)
C(76)	8361(11)	4719(12)	7119(3)	115(6)
C(77)	7855(11)	4098(10)	7196(3)	127(6)
C(78)	7567(9)	4171(7)	7464(2)	95(4)
C(79)	6125(5)	4986(5)	7960(2)	47(2)
C(80)	5637(6)	4920(6)	8187(2)	65(3)
C(81)	4817(6)	5011(7)	8158(2)	73(3)
C(82)	4498(7)	5175(7)	7907(3)	83(3)
C(83)	4965(7)	5272(8)	7678(3)	89(4)
C(84)	5785(6)	5169(7)	7703(2)	71(3)
C(85)	8890(6)	5799(5)	8553(2)	52(2)
C(86)	9149(7)	5911(6)	8826(2)	67(3)
C(87)	9972(8)	5818(8)	8897(3)	88(4)
C(88)	10485(7)	5588(7)	8686(4)	90(4)
C(89)	10236(7)	5490(8)	8414(3)	80(3)
C(90)	9439(6)	5582(6)	8352(2)	65(3)
C(91)	7676(6)	7009(5)	8386(2)	54(3)
C(92)	7669(7)	7545(6)	8603(3)	77(3)
C(93)	7541(9)	8327(6)	8552(3)	107(5)
C(94)	7461(8)	8580(7)	8277(4)	98(4)
C(95)	7443(10)	8076(6)	8057(3)	101(5)
C(96)	7559(8)	7288(6)	8113(2)	82(4)
N(1)	5756(7)	6462(5)	8864(2)	91(3)
C(97)	5302(11)	6624(10)	8610(5)	177(10)
C(98)	5214(15)	7323(11)	8485(4)	174(10)
C(99)	4757(10)	7384(10)	8229(3)	125(6)
C(100)	5149(8)	7393(8)	7963(3)	92(4)
C(101)	4627(9)	7559(9)	7716(3)	110(5)
C(102)	4990(9)	7690(10)	7449(3)	109(5)
C(103)	4448(12)	7771(12)	7201(3)	147(8)
N(2)	4655(8)	8092(7)	6974(3)	114(4)
N(3)	8927(4)	3965(4)	8770(2)	55(2)
C(104)	9081(6)	3438(6)	9013(2)	65(3)
C(105)	9965(7)	3350(8)	9070(3)	84(4)
C(106)	10117(8)	2815(8)	9329(3)	90(4)
C(107)	9762(7)	3111(7)	9605(2)	71(3)
C(108)	10008(8)	2626(8)	9856(2)	80(3)
C(109)	9635(8)	2881(8)	10125(3)	92(4)
C(110)	9713(7)	2355(8)	10379(3)	87(4)
N(4)	10523(5)	2256(5)	10477(2)	66(2)
O(17)	-183(5)	3534(5)	8268(2)	96(3)
C(111)	-583(10)	3613(10)	8013(3)	118(5)
C(112)	-229(12)	2999(13)	7819(5)	159(7)
C(113)	531(11)	2814(11)	7955(4)	138(6)
C(114)	613(10)	3297(10)	8201(4)	129(5)
O(18)	9279(10)	10550(12)	7747(4)	209(7)

C(115)	9374(13)	10672(13)	7399(5)	158(7)
C(116)	8938(12)	10032(12)	7299(4)	140(6)
C(117)	8731(15)	9534(15)	7517(6)	186(9)
C(118)	9120(13)	9748(14)	7783(5)	161(7)
O(19B)	3305(19)	8827(17)	9024(7)	171(10)
C(1B9)	2390(20)	9460(20)	8738(9)	148(13)
C(1B0)	2600(20)	9076(19)	9012(7)	116(10)
C(1B1)	3730(20)	9190(20)	8804(9)	142(12)
C(1B2)	3210(20)	9500(20)	8620(8)	137(12)
O(19A)	6009(14)	6841(13)	11713(5)	127(7)
C(1A9)	4746(17)	7105(18)	11685(7)	101(8)
C(1A0)	5610(30)	6870(20)	11485(10)	156(14)
C(1A1)	5760(20)	7370(20)	11900(9)	144(13)
C(1A2)	4790(20)	7380(20)	11906(10)	146(13)
O(20A)	3010(16)	7093(16)	10344(6)	155(9)
C(1A3)	4300(20)	6894(19)	10380(7)	115(10)
C(1A4)	3210(20)	7250(20)	10643(8)	125(11)
C(1A5)	3690(20)	6840(20)	10215(8)	134(11)
C(1A6)	3880(30)	6880(30)	10741(11)	189(19)
O(20B)	6140(20)	8071(19)	10533(7)	184(11)
C(1B3)	6890(30)	8210(30)	10647(11)	173(16)
C(1B4)	7430(40)	7900(30)	10505(13)	200(20)
C(1B5)	6950(30)	7350(30)	10329(10)	167(15)
C(1B6)	6430(30)	7890(30)	10241(10)	170(15)

Table 3. Bond lengths [Å] and angles [°] for sh2049.

Al(1)-O(4)	1.736(6)
Al(1)-O(16)	1.740(6)
Al(1)-O(5)	1.752(6)
Al(1)-O(1)	1.768(6)
Al(2)-O(2)	1.738(6)
Al(2)-O(8)	1.740(7)
Al(2)-O(7)	1.750(6)
Al(2)-O(1)	1.781(6)
Al(3)-O(10)	1.727(7)
Al(3)-O(11)	1.731(6)
Al(3)-O(2)	1.748(6)
Al(3)-O(3)	1.774(6)
Al(4)-O(4)	1.736(6)
Al(4)-O(14)	1.742(6)
Al(4)-O(13)	1.747(6)
Al(4)-O(3)	1.786(7)
Si(1)-O(5)	1.568(6)
Si(1)-O(6)	1.624(7)
Si(1)-C(1)	1.853(10)
Si(1)-C(7)	1.875(9)
Si(2)-O(7)	1.603(6)
Si(2)-O(6)	1.652(7)
Si(2)-C(13)	1.873(10)
Si(2)-C(19)	1.884(11)
Si(3)-O(8)	1.594(7)
Si(3)-O(9)	1.629(7)
Si(3)-C(25)	1.869(10)
Si(3)-C(31)	1.874(11)
Si(4)-O(10)	1.620(7)
Si(4)-O(9)	1.633(7)
Si(4)-C(37)	1.855(12)
Si(4)-C(43)	1.898(13)
Si(5)-O(11)	1.602(6)
Si(5)-O(12)	1.617(7)
Si(5)-C(55)	1.852(11)
Si(5)-C(49)	1.872(10)
Si(6)-O(13)	1.595(6)
Si(6)-O(12)	1.645(7)
Si(6)-C(67)	1.859(10)
Si(6)-C(61)	1.863(10)
Si(7)-O(14)	1.595(6)
Si(7)-O(15)	1.645(6)
Si(7)-C(73)	1.852(10)
Si(7)-C(79)	1.889(10)
Si(8)-O(16)	1.607(7)
Si(8)-O(15)	1.622(6)
Si(8)-C(91)	1.858(9)
Si(8)-C(85)	1.872(11)
C(1)-C(2)	1.386(13)
C(1)-C(6)	1.404(14)
C(2)-C(3)	1.411(15)
C(3)-C(4)	1.337(16)
C(4)-C(5)	1.372(18)
C(5)-C(6)	1.426(16)
C(7)-C(8)	1.390(13)
C(7)-C(12)	1.404(14)
C(8)-C(9)	1.400(14)
C(9)-C(10)	1.340(16)
C(10)-C(11)	1.375(16)
C(11)-C(12)	1.366(15)
C(13)-C(14)	1.362(15)
C(13)-C(18)	1.362(15)
C(14)-C(15)	1.426(18)
C(15)-C(16)	1.366(19)
C(16)-C(17)	1.348(19)
C(17)-C(18)	1.393(18)
C(19)-C(24)	1.375(15)
C(19)-C(20)	1.408(16)
C(20)-C(21)	1.397(19)
C(21)-C(22)	1.35(2)
C(22)-C(23)	1.347(19)
C(23)-C(24)	1.411(16)
C(25)-C(30)	1.382(15)
C(25)-C(26)	1.394(15)
C(26)-C(27)	1.370(17)

C(27)-C(28)	1.342(17)
C(28)-C(29)	1.391(17)
C(29)-C(30)	1.357(16)
C(31)-C(32)	1.356(17)
C(31)-C(36)	1.393(16)
C(32)-C(33)	1.429(19)
C(33)-C(34)	1.26(3)
C(34)-C(35)	1.50(3)
C(35)-C(36)	1.41(2)
C(37)-C(42)	1.365(17)
C(37)-C(38)	1.401(18)
C(38)-C(39)	1.40(2)
C(39)-C(40)	1.43(3)
C(40)-C(41)	1.32(3)
C(41)-C(42)	1.37(2)
C(43)-C(48)	1.364(19)
C(43)-C(44)	1.402(19)
C(44)-C(45)	1.390(19)
C(45)-C(46)	1.32(3)
C(46)-C(47)	1.37(3)
C(47)-C(48)	1.48(3)
C(49)-C(50)	1.386(15)
C(49)-C(54)	1.392(14)
C(50)-C(51)	1.387(17)
C(51)-C(52)	1.346(17)
C(52)-C(53)	1.400(19)
C(53)-C(54)	1.372(17)
C(55)-C(56)	1.383(16)
C(55)-C(60)	1.474(17)
C(56)-C(57)	1.43(2)
C(57)-C(58)	1.33(2)
C(58)-C(59)	1.31(2)
C(59)-C(60)	1.376(18)
C(61)-C(66)	1.361(14)
C(61)-C(62)	1.421(13)
C(62)-C(63)	1.368(14)
C(63)-C(64)	1.362(16)
C(64)-C(65)	1.371(16)
C(65)-C(66)	1.367(15)
C(67)-C(72)	1.390(14)
C(67)-C(68)	1.400(15)
C(68)-C(69)	1.357(16)
C(69)-C(70)	1.37(2)
C(70)-C(71)	1.42(2)
C(71)-C(72)	1.376(16)
C(73)-C(78)	1.370(15)
C(73)-C(74)	1.429(15)
C(74)-C(75)	1.400(17)
C(75)-C(76)	1.34(2)
C(76)-C(77)	1.42(2)
C(77)-C(78)	1.366(17)
C(79)-C(80)	1.366(13)
C(79)-C(84)	1.386(13)
C(80)-C(81)	1.415(15)
C(81)-C(82)	1.337(16)
C(82)-C(83)	1.356(16)
C(83)-C(84)	1.415(15)
C(85)-C(86)	1.383(14)
C(85)-C(90)	1.387(14)
C(86)-C(87)	1.453(16)
C(87)-C(88)	1.385(18)
C(88)-C(89)	1.368(18)
C(89)-C(90)	1.400(16)
C(91)-C(92)	1.386(14)
C(91)-C(96)	1.394(15)
C(92)-C(93)	1.390(16)
C(93)-C(94)	1.378(19)
C(94)-C(95)	1.359(18)
C(95)-C(96)	1.399(15)
N(1)-C(97)	1.46(2)
C(97)-C(98)	1.35(2)
C(98)-C(99)	1.44(2)
C(99)-C(100)	1.42(2)
C(100)-C(101)	1.498(17)
C(101)-C(102)	1.43(2)
C(102)-C(103)	1.50(2)
C(103)-N(2)	1.260(17)

N(3)-C(104)	1.490(12)
C(104)-C(105)	1.541(15)
C(105)-C(106)	1.556(16)
C(106)-C(107)	1.528(17)
C(107)-C(108)	1.513(15)
C(108)-C(109)	1.494(17)
C(109)-C(110)	1.513(17)
C(110)-N(4)	1.467(14)
O(17)-C(111)	1.394(17)
O(17)-C(114)	1.454(18)
C(111)-C(112)	1.53(2)
C(112)-C(113)	1.48(2)
C(113)-C(114)	1.44(2)
O(18)-C(118)	1.42(3)
O(18)-C(115)	1.67(3)
C(115)-C(116)	1.41(3)
C(116)-C(117)	1.39(3)
C(117)-C(118)	1.47(3)
O(19B)-C(1B0)	1.28(4)
O(19B)-C(1B1)	1.41(4)
C(1B9)-C(1B2)	1.50(5)
C(1B9)-C(1B0)	1.50(5)
C(1B1)-C(1B2)	1.36(5)
O(19A)-C(1A0)	1.28(4)
O(19A)-C(1A1)	1.34(4)
C(1A9)-C(1A2)	1.15(4)
C(1A9)-C(1A0)	1.80(5)
C(1A1)-C(1A2)	1.66(5)
O(20A)-C(1A5)	1.37(4)
O(20A)-C(1A4)	1.48(4)
C(1A3)-C(1A5)	1.31(4)
C(1A3)-C(1A6)	1.85(6)
C(1A4)-C(1A6)	1.40(6)
O(20B)-C(1B3)	1.42(5)
O(20B)-C(1B6)	1.51(5)
C(1B3)-C(1B4)	1.26(6)
C(1B4)-C(1B5)	1.50(6)
C(1B5)-C(1B6)	1.34(6)

O(4)-Al(1)-O(16)	108.8(3)
O(4)-Al(1)-O(5)	107.0(3)
O(16)-Al(1)-O(5)	111.5(3)
O(4)-Al(1)-O(1)	117.4(3)
O(16)-Al(1)-O(1)	102.4(3)
O(5)-Al(1)-O(1)	109.7(3)
O(2)-Al(2)-O(8)	111.9(3)
O(2)-Al(2)-O(7)	106.0(3)
O(8)-Al(2)-O(7)	110.4(3)
O(2)-Al(2)-O(1)	108.6(3)
O(8)-Al(2)-O(1)	109.5(3)
O(7)-Al(2)-O(1)	110.5(3)
O(10)-Al(3)-O(11)	110.7(3)
O(10)-Al(3)-O(2)	110.8(3)
O(11)-Al(3)-O(2)	106.3(3)
O(10)-Al(3)-O(3)	105.4(3)
O(11)-Al(3)-O(3)	108.7(3)
O(2)-Al(3)-O(3)	114.9(3)
O(4)-Al(4)-O(14)	109.1(3)
O(4)-Al(4)-O(13)	106.7(3)
O(14)-Al(4)-O(13)	109.8(3)
O(4)-Al(4)-O(3)	113.2(3)
O(14)-Al(4)-O(3)	108.2(3)
O(13)-Al(4)-O(3)	109.9(3)
O(5)-Si(1)-O(6)	114.1(3)
O(5)-Si(1)-C(1)	109.0(4)
O(6)-Si(1)-C(1)	105.0(4)
O(5)-Si(1)-C(7)	109.9(4)
O(6)-Si(1)-C(7)	106.6(4)
C(1)-Si(1)-C(7)	112.2(4)
O(7)-Si(2)-O(6)	113.4(3)
O(7)-Si(2)-C(13)	109.0(4)
O(6)-Si(2)-C(13)	105.3(4)
O(7)-Si(2)-C(19)	109.5(4)
O(6)-Si(2)-C(19)	106.6(4)
C(13)-Si(2)-C(19)	113.0(4)
O(8)-Si(3)-O(9)	114.1(3)
O(8)-Si(3)-C(25)	110.8(4)

O(9)-Si(3)-C(25)	108.4(4)
O(8)-Si(3)-C(31)	111.7(4)
O(9)-Si(3)-C(31)	105.0(4)
C(25)-Si(3)-C(31)	106.4(4)
O(10)-Si(4)-O(9)	112.8(3)
O(10)-Si(4)-C(37)	109.0(4)
O(9)-Si(4)-C(37)	105.3(5)
O(10)-Si(4)-C(43)	109.8(5)
O(9)-Si(4)-C(43)	109.1(5)
C(37)-Si(4)-C(43)	110.8(6)
O(11)-Si(5)-O(12)	113.5(3)
O(11)-Si(5)-C(55)	108.7(4)
O(12)-Si(5)-C(55)	107.3(5)
O(11)-Si(5)-C(49)	111.2(4)
O(12)-Si(5)-C(49)	107.5(4)
C(55)-Si(5)-C(49)	108.4(4)
O(13)-Si(6)-O(12)	113.0(3)
O(13)-Si(6)-C(67)	111.2(4)
O(12)-Si(6)-C(67)	106.2(4)
O(13)-Si(6)-C(61)	109.2(4)
O(12)-Si(6)-C(61)	109.2(4)
C(67)-Si(6)-C(61)	107.9(4)
O(14)-Si(7)-O(15)	113.7(3)
O(14)-Si(7)-C(73)	110.8(4)
O(15)-Si(7)-C(73)	106.7(4)
O(14)-Si(7)-C(79)	106.3(4)
O(15)-Si(7)-C(79)	109.9(4)
C(73)-Si(7)-C(79)	109.5(4)
O(16)-Si(8)-O(15)	114.7(3)
O(16)-Si(8)-C(91)	108.3(4)
O(15)-Si(8)-C(91)	107.1(4)
O(16)-Si(8)-C(85)	108.9(4)
O(15)-Si(8)-C(85)	108.2(4)
C(91)-Si(8)-C(85)	109.6(4)
Al(1)-O(1)-Al(2)	133.1(3)
Al(2)-O(2)-Al(3)	134.1(3)
Al(3)-O(3)-Al(4)	135.6(3)
Al(4)-O(4)-Al(1)	140.6(4)
Si(1)-O(5)-Al(1)	150.5(4)
Si(1)-O(6)-Si(2)	144.2(4)
Si(2)-O(7)-Al(2)	139.1(4)
Si(3)-O(8)-Al(2)	155.7(4)
Si(3)-O(9)-Si(4)	146.1(4)
Si(4)-O(10)-Al(3)	151.5(4)
Si(5)-O(11)-Al(3)	144.1(4)
Si(5)-O(12)-Si(6)	155.7(4)
Si(6)-O(13)-Al(4)	137.3(4)
Si(7)-O(14)-Al(4)	142.5(4)
Si(8)-O(15)-Si(7)	154.7(4)
Si(8)-O(16)-Al(1)	138.3(4)
C(2)-C(1)-C(6)	115.8(9)
C(2)-C(1)-Si(1)	121.6(7)
C(6)-C(1)-Si(1)	122.5(8)
C(1)-C(2)-C(3)	122.7(10)
C(4)-C(3)-C(2)	121.2(12)
C(3)-C(4)-C(5)	118.2(11)
C(4)-C(5)-C(6)	122.1(12)
C(1)-C(6)-C(5)	119.8(11)
C(8)-C(7)-C(12)	115.3(9)
C(8)-C(7)-Si(1)	121.2(7)
C(12)-C(7)-Si(1)	123.6(7)
C(7)-C(8)-C(9)	122.0(10)
C(10)-C(9)-C(8)	119.8(11)
C(9)-C(10)-C(11)	120.5(10)
C(12)-C(11)-C(10)	119.8(10)
C(11)-C(12)-C(7)	122.5(10)
C(14)-C(13)-C(18)	114.7(10)
C(14)-C(13)-Si(2)	122.0(8)
C(18)-C(13)-Si(2)	123.3(9)
C(13)-C(14)-C(15)	124.2(11)
C(16)-C(15)-C(14)	117.9(13)
C(17)-C(16)-C(15)	119.0(12)
C(16)-C(17)-C(18)	121.2(12)
C(13)-C(18)-C(17)	122.9(13)
C(24)-C(19)-C(20)	117.0(10)
C(24)-C(19)-Si(2)	121.4(8)
C(20)-C(19)-Si(2)	121.4(8)

C(21)-C(20)-C(19)	120.5(13)
C(22)-C(21)-C(20)	120.3(14)
C(21)-C(22)-C(23)	121.2(14)
C(22)-C(23)-C(24)	119.6(13)
C(19)-C(24)-C(23)	121.3(12)
C(30)-C(25)-C(26)	114.6(10)
C(30)-C(25)-Si(3)	123.0(8)
C(26)-C(25)-Si(3)	122.3(8)
C(27)-C(26)-C(25)	122.2(12)
C(28)-C(27)-C(26)	121.5(13)
C(27)-C(28)-C(29)	118.1(12)
C(30)-C(29)-C(28)	119.9(12)
C(29)-C(30)-C(25)	123.6(11)
C(32)-C(31)-C(36)	118.4(11)
C(32)-C(31)-Si(3)	118.3(9)
C(36)-C(31)-Si(3)	123.3(10)
C(31)-C(32)-C(33)	122.8(15)
C(34)-C(33)-C(32)	120.4(19)
C(33)-C(34)-C(35)	120.2(17)
C(36)-C(35)-C(34)	117.2(15)
C(31)-C(36)-C(35)	120.3(15)
C(42)-C(37)-C(38)	116.0(12)
C(42)-C(37)-Si(4)	123.3(9)
C(38)-C(37)-Si(4)	120.2(11)
C(37)-C(38)-C(39)	121.4(16)
C(38)-C(39)-C(40)	117.4(15)
C(41)-C(40)-C(39)	121.3(15)
C(40)-C(41)-C(42)	119.3(17)
C(37)-C(42)-C(41)	124.6(14)
C(48)-C(43)-C(44)	117.3(14)
C(48)-C(43)-Si(4)	120.7(13)
C(44)-C(43)-Si(4)	121.5(9)
C(45)-C(44)-C(43)	123.6(15)
C(46)-C(45)-C(44)	118.6(19)
C(45)-C(46)-C(47)	121.5(19)
C(46)-C(47)-C(48)	119.4(18)
C(43)-C(48)-C(47)	118(2)
C(50)-C(49)-C(54)	115.3(10)
C(50)-C(49)-Si(5)	123.0(7)
C(54)-C(49)-Si(5)	121.3(9)
C(49)-C(50)-C(51)	123.7(11)
C(52)-C(51)-C(50)	118.6(13)
C(51)-C(52)-C(53)	120.7(12)
C(54)-C(53)-C(52)	119.0(12)
C(53)-C(54)-C(49)	122.7(12)
C(56)-C(55)-C(60)	116.1(11)
C(56)-C(55)-Si(5)	121.1(9)
C(60)-C(55)-Si(5)	122.8(9)
C(55)-C(56)-C(57)	119.7(15)
C(58)-C(57)-C(56)	121.2(16)
C(59)-C(58)-C(57)	121.0(16)
C(58)-C(59)-C(60)	122.7(16)
C(59)-C(60)-C(55)	118.6(13)
C(66)-C(61)-C(62)	113.6(9)
C(66)-C(61)-Si(6)	123.0(7)
C(62)-C(61)-Si(6)	123.2(8)
C(63)-C(62)-C(61)	122.1(11)
C(64)-C(63)-C(62)	120.1(11)
C(63)-C(64)-C(65)	120.5(10)
C(66)-C(65)-C(64)	117.6(11)
C(61)-C(66)-C(65)	126.1(10)
C(72)-C(67)-C(68)	115.0(9)
C(72)-C(67)-Si(6)	119.7(8)
C(68)-C(67)-Si(6)	125.2(7)
C(69)-C(68)-C(67)	123.5(11)
C(68)-C(69)-C(70)	120.6(14)
C(69)-C(70)-C(71)	118.8(12)
C(72)-C(71)-C(70)	118.8(12)
C(71)-C(72)-C(67)	123.3(12)
C(78)-C(73)-C(74)	114.6(10)
C(78)-C(73)-Si(7)	122.4(9)
C(74)-C(73)-Si(7)	123.0(8)
C(75)-C(74)-C(73)	120.3(13)
C(76)-C(75)-C(74)	119.5(14)
C(75)-C(76)-C(77)	124.2(13)
C(78)-C(77)-C(76)	112.7(14)
C(77)-C(78)-C(73)	128.6(13)

C(80)-C(79)-C(84)	117.2(9)
C(80)-C(79)-Si(7)	119.5(7)
C(84)-C(79)-Si(7)	123.2(7)
C(79)-C(80)-C(81)	121.0(10)
C(82)-C(81)-C(80)	121.0(11)
C(81)-C(82)-C(83)	119.8(12)
C(82)-C(83)-C(84)	119.9(11)
C(79)-C(84)-C(83)	121.1(10)
C(86)-C(85)-C(90)	117.7(10)
C(86)-C(85)-Si(8)	119.3(8)
C(90)-C(85)-Si(8)	123.0(8)
C(85)-C(86)-C(87)	120.6(11)
C(88)-C(87)-C(86)	118.5(12)
C(89)-C(88)-C(87)	121.1(12)
C(88)-C(89)-C(90)	119.1(11)
C(85)-C(90)-C(89)	122.8(10)
C(92)-C(91)-C(96)	117.2(9)
C(92)-C(91)-Si(8)	119.5(8)
C(96)-C(91)-Si(8)	123.3(8)
C(91)-C(92)-C(93)	121.3(11)
C(94)-C(93)-C(92)	119.3(12)
C(95)-C(94)-C(93)	121.6(11)
C(94)-C(95)-C(96)	118.3(12)
C(91)-C(96)-C(95)	122.1(11)
C(98)-C(97)-N(1)	126.3(17)
C(97)-C(98)-C(99)	119.5(17)
C(100)-C(99)-C(98)	119.3(17)
C(99)-C(100)-C(101)	114.4(14)
C(102)-C(101)-C(100)	117.7(14)
C(101)-C(102)-C(103)	116.1(14)
N(2)-C(103)-C(102)	122.3(16)
N(3)-C(104)-C(105)	111.6(8)
C(104)-C(105)-C(106)	111.1(10)
C(107)-C(106)-C(105)	114.1(10)
C(108)-C(107)-C(106)	112.1(10)
C(109)-C(108)-C(107)	112.9(10)
C(108)-C(109)-C(110)	117.7(11)
N(4)-C(110)-C(109)	113.8(10)
C(111)-O(17)-C(114)	107.2(12)
O(17)-C(111)-C(112)	105.0(14)
C(113)-C(112)-C(111)	103.5(17)
C(114)-C(113)-C(112)	108.3(17)
C(113)-C(114)-O(17)	104.4(14)
C(118)-O(18)-C(115)	105.0(18)
C(116)-C(115)-O(18)	100.3(18)
C(117)-C(116)-C(115)	112(2)
C(116)-C(117)-C(118)	111(2)
O(18)-C(118)-C(117)	103(2)
C(1B0)-O(19B)-C(1B1)	107(3)
C(1B2)-C(1B9)-C(1B0)	97(3)
O(19B)-C(1B0)-C(1B9)	114(3)
C(1B2)-C(1B1)-O(19B)	108(4)
C(1B1)-C(1B2)-C(1B9)	110(4)
C(1A0)-O(19A)-C(1A1)	111(3)
C(1A2)-C(1A9)-C(1A0)	122(4)
O(19A)-C(1A0)-C(1A9)	90(3)
O(19A)-C(1A1)-C(1A2)	110(3)
C(1A9)-C(1A2)-C(1A1)	92(3)
C(1A5)-O(20A)-C(1A4)	107(3)
C(1A5)-C(1A3)-C(1A6)	104(3)
C(1A6)-C(1A4)-O(20A)	115(4)
C(1A3)-C(1A5)-O(20A)	113(3)
C(1A4)-C(1A6)-C(1A3)	90(3)
C(1B3)-O(20B)-C(1B6)	95(4)
C(1B4)-C(1B3)-O(20B)	112(5)
C(1B3)-C(1B4)-C(1B5)	100(5)
C(1B6)-C(1B5)-C(1B4)	95(4)
C(1B5)-C(1B6)-O(20B)	94(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2049. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	51(2)	35(1)	32(1)	-2(1)	-1(1)	2(1)
Al(2)	50(2)	42(2)	36(2)	-4(1)	3(1)	0(1)
Al(3)	54(2)	36(1)	40(2)	-3(1)	2(1)	-1(1)
Al(4)	52(2)	35(1)	32(1)	-2(1)	1(1)	1(1)
Si(1)	52(2)	50(1)	35(1)	-5(1)	0(1)	1(1)
Si(2)	57(2)	47(1)	38(1)	-6(1)	1(1)	3(1)
Si(3)	49(2)	54(2)	46(2)	-4(1)	-2(1)	5(1)
Si(4)	54(2)	61(2)	56(2)	-18(1)	-2(1)	-4(1)
Si(5)	65(2)	35(1)	53(2)	-1(1)	2(1)	2(1)
Si(6)	54(2)	37(1)	46(2)	-3(1)	-1(1)	4(1)
Si(7)	61(2)	42(1)	36(1)	2(1)	-1(1)	1(1)
Si(8)	58(2)	36(1)	44(2)	3(1)	1(1)	0(1)
O(1)	47(4)	40(3)	39(3)	-1(3)	1(3)	5(3)
O(2)	53(4)	45(3)	36(3)	5(3)	-1(3)	2(3)
O(3)	53(4)	47(3)	37(3)	0(3)	-4(3)	5(3)
O(4)	54(4)	42(3)	34(3)	-1(3)	-2(3)	0(3)
O(5)	53(4)	49(3)	47(4)	-2(3)	-9(3)	-3(3)
O(6)	55(4)	67(4)	50(4)	-7(3)	-5(3)	4(3)
O(7)	54(4)	55(4)	37(3)	-5(3)	-3(3)	0(3)
O(8)	51(4)	52(4)	49(4)	-2(3)	-4(3)	-2(3)
O(9)	54(4)	75(4)	67(5)	-21(4)	-9(3)	6(3)
O(10)	60(4)	45(3)	57(4)	-11(3)	2(3)	0(3)
O(11)	72(4)	37(3)	49(4)	-2(3)	6(3)	-1(3)
O(12)	68(4)	40(3)	57(4)	3(3)	4(3)	-2(3)
O(13)	57(4)	39(3)	49(4)	-7(3)	1(3)	1(3)
O(14)	60(4)	42(3)	32(3)	-1(3)	-1(3)	-1(3)
O(15)	70(4)	49(3)	50(4)	-3(3)	-8(3)	-6(3)
O(16)	62(4)	46(3)	49(4)	2(3)	2(3)	-9(3)
C(1)	69(7)	40(5)	46(6)	-7(4)	-3(5)	3(5)
C(2)	59(7)	87(8)	43(6)	-19(5)	-6(5)	-7(6)
C(3)	55(8)	104(9)	94(10)	-13(8)	-13(7)	-6(7)
C(4)	68(9)	90(8)	70(8)	-13(7)	-23(7)	-20(7)
C(5)	103(12)	117(11)	85(9)	-46(8)	-20(9)	-21(9)
C(6)	68(8)	108(9)	54(7)	-20(7)	-4(6)	-15(7)
C(7)	48(6)	51(5)	45(6)	-5(5)	-4(4)	-2(4)
C(8)	63(7)	46(6)	56(6)	8(5)	0(5)	-11(5)
C(9)	84(9)	53(7)	74(8)	0(6)	-3(6)	3(6)
C(10)	95(9)	51(6)	86(9)	0(7)	-13(7)	-5(6)
C(11)	96(9)	70(8)	62(8)	30(6)	-21(6)	-25(7)
C(12)	82(8)	77(8)	48(7)	-2(6)	-7(5)	-3(6)
C(13)	55(7)	55(6)	61(7)	-7(5)	5(5)	5(5)
C(14)	91(10)	145(12)	31(6)	-12(7)	-1(6)	-10(9)
C(15)	105(11)	151(13)	71(10)	-16(9)	13(9)	-34(10)
C(16)	105(12)	124(11)	54(9)	13(7)	30(8)	1(9)
C(17)	93(11)	215(18)	46(8)	4(9)	-5(7)	16(12)
C(18)	75(8)	189(15)	41(7)	1(8)	-6(6)	-11(9)
C(19)	67(8)	62(7)	50(6)	-17(5)	-4(5)	12(6)
C(20)	92(10)	45(7)	135(12)	2(7)	-7(8)	-14(7)
C(21)	147(16)	55(8)	150(15)	6(8)	-12(12)	-21(9)
C(22)	132(14)	70(9)	81(9)	-10(7)	-1(9)	34(11)
C(23)	100(10)	73(9)	83(9)	3(7)	6(7)	24(9)
C(24)	84(9)	59(7)	81(8)	10(6)	11(7)	12(6)
C(25)	57(7)	48(5)	47(6)	-2(4)	-16(5)	1(5)
C(26)	65(8)	137(11)	62(8)	3(8)	20(7)	21(7)
C(27)	76(11)	209(18)	71(9)	21(10)	-17(8)	-30(10)
C(28)	95(11)	111(10)	61(9)	5(7)	15(7)	-22(8)
C(29)	57(8)	123(11)	97(11)	-21(8)	20(8)	-20(7)
C(30)	65(9)	128(11)	62(8)	-15(7)	-5(6)	-13(7)
C(31)	47(6)	75(8)	52(7)	2(5)	9(5)	14(5)
C(32)	80(9)	94(10)	96(10)	21(9)	4(7)	9(7)
C(33)	116(13)	73(9)	164(16)	62(11)	15(12)	25(9)
C(34)	72(12)	210(20)	220(30)	170(20)	36(14)	43(14)
C(35)	72(10)	199(19)	94(11)	70(13)	-2(8)	39(12)
C(36)	69(8)	125(10)	65(8)	12(8)	2(6)	14(8)
C(37)	62(8)	84(9)	78(9)	-23(7)	-4(6)	-4(6)
C(38)	129(12)	100(11)	100(11)	-47(9)	-26(9)	9(9)
C(39)	148(16)	125(13)	141(16)	-80(13)	-63(13)	-12(11)
C(40)	147(17)	230(30)	72(11)	-42(15)	-39(11)	39(17)
C(41)	152(16)	130(14)	85(12)	-22(10)	-16(10)	8(12)
C(42)	118(11)	97(9)	47(8)	-25(7)	-12(7)	2(8)
C(43)	73(9)	80(8)	86(9)	-23(7)	30(7)	-19(7)

C(44)	82(10)	119(11)	93(10)	24(9)	10(8)	-30(9)
C(45)	116(14)	134(14)	105(12)	20(11)	12(10)	-41(12)
C(46)	260(30)	61(9)	105(12)	-5(8)	48(15)	24(14)
C(47)	190(20)	130(16)	290(30)	-51(19)	210(20)	-41(16)
C(48)	143(16)	103(12)	260(20)	20(13)	132(17)	14(11)
C(49)	56(6)	43(6)	51(6)	0(4)	4(5)	-6(5)
C(50)	93(9)	63(7)	74(8)	-15(6)	-11(7)	-5(7)
C(51)	107(11)	82(10)	96(10)	-12(8)	-25(8)	7(8)
C(52)	123(11)	71(9)	74(9)	-11(7)	-9(8)	-24(8)
C(53)	159(14)	48(7)	109(11)	-16(8)	-21(10)	-14(8)
C(54)	88(9)	45(6)	112(10)	-8(7)	-15(7)	-8(6)
C(55)	90(9)	38(5)	62(7)	-7(5)	0(6)	-6(6)
C(56)	102(10)	77(8)	87(10)	16(7)	9(8)	-5(7)
C(57)	190(19)	122(13)	59(9)	29(9)	29(10)	-62(13)
C(58)	210(20)	73(9)	64(11)	17(8)	-22(13)	-14(12)
C(59)	187(17)	69(8)	59(8)	19(7)	-25(10)	22(9)
C(60)	104(11)	74(8)	97(10)	9(7)	6(8)	8(8)
C(61)	50(6)	42(5)	55(6)	-7(5)	4(5)	7(4)
C(62)	79(8)	59(7)	62(7)	-14(5)	-1(6)	-12(6)
C(63)	89(9)	87(9)	59(8)	-36(7)	-9(6)	-6(7)
C(64)	86(9)	89(9)	46(7)	-21(7)	-6(6)	6(7)
C(65)	95(9)	77(8)	49(7)	-10(6)	-1(6)	1(7)
C(66)	88(8)	50(6)	60(8)	-10(6)	-1(6)	-4(6)
C(67)	70(8)	38(6)	47(6)	-10(4)	-4(5)	12(5)
C(68)	62(8)	58(6)	82(8)	1(6)	-3(6)	13(6)
C(69)	84(10)	85(10)	118(12)	-3(8)	-4(8)	17(8)
C(70)	104(12)	126(13)	81(9)	2(9)	1(8)	80(11)
C(71)	101(11)	78(8)	100(10)	11(7)	-8(8)	25(9)
C(72)	69(8)	60(7)	84(8)	-3(6)	-2(6)	16(6)
C(73)	68(7)	58(6)	52(6)	19(5)	-3(5)	4(6)
C(74)	61(7)	95(9)	68(8)	13(7)	10(6)	10(7)
C(75)	76(9)	155(14)	69(9)	59(10)	30(7)	14(9)
C(76)	151(15)	151(15)	42(8)	3(10)	29(9)	25(12)
C(77)	200(18)	118(12)	62(10)	-11(8)	62(10)	-12(12)
C(78)	162(13)	67(7)	57(8)	8(6)	9(8)	-7(8)
C(79)	64(6)	44(5)	34(5)	0(4)	0(5)	-1(5)
C(80)	71(8)	67(7)	56(7)	13(5)	5(6)	10(6)
C(81)	54(8)	104(9)	61(8)	6(7)	5(6)	8(6)
C(82)	72(8)	102(9)	75(9)	10(7)	4(7)	-3(7)
C(83)	76(9)	127(11)	66(8)	28(8)	-15(7)	1(8)
C(84)	64(8)	92(8)	57(7)	8(6)	0(6)	2(6)
C(85)	70(7)	41(5)	44(7)	3(4)	2(5)	-7(5)
C(86)	84(9)	64(6)	55(8)	0(5)	2(6)	0(6)
C(87)	75(9)	113(10)	75(9)	-1(8)	-30(8)	1(7)
C(88)	52(8)	92(9)	128(13)	7(8)	12(9)	7(6)
C(89)	67(9)	108(9)	65(9)	13(7)	8(6)	2(7)
C(90)	61(8)	78(7)	56(7)	1(5)	0(6)	-12(6)
C(91)	60(7)	38(5)	65(7)	11(5)	-1(5)	-2(5)
C(92)	112(10)	49(6)	70(7)	-1(6)	-8(7)	-5(6)
C(93)	162(15)	42(7)	116(12)	-19(7)	-37(10)	33(7)
C(94)	107(11)	58(8)	131(13)	32(9)	-19(9)	1(7)
C(95)	181(15)	48(7)	74(9)	19(7)	9(9)	21(8)
C(96)	128(11)	57(7)	60(8)	-2(6)	10(7)	-5(7)
N(1)	137(10)	46(5)	91(8)	17(5)	34(7)	25(6)
C(97)	125(14)	105(12)	300(30)	109(16)	-90(17)	-6(10)
C(98)	280(30)	147(17)	94(12)	62(12)	-69(15)	-89(17)
C(99)	137(14)	147(14)	90(12)	45(10)	-21(10)	-73(11)
C(100)	108(11)	89(9)	79(10)	0(7)	-29(8)	-19(7)
C(101)	126(13)	118(11)	85(11)	8(8)	-52(10)	-18(9)
C(102)	139(13)	139(13)	49(9)	22(8)	-18(8)	-38(10)
C(103)	199(19)	179(17)	63(10)	54(11)	-31(11)	-80(15)
N(2)	130(10)	115(9)	97(10)	-3(8)	-36(8)	-2(8)
N(3)	51(5)	58(5)	55(5)	4(4)	-7(4)	6(4)
C(104)	74(8)	73(7)	48(6)	14(5)	5(5)	9(6)
C(105)	69(8)	112(10)	71(8)	11(7)	-7(6)	15(7)
C(106)	92(9)	98(9)	80(9)	21(7)	-14(7)	26(8)
C(107)	65(7)	97(8)	52(7)	13(6)	2(6)	7(6)
C(108)	87(9)	98(9)	55(8)	19(7)	-11(6)	2(7)
C(109)	98(10)	100(9)	79(9)	25(8)	-25(8)	26(8)
C(110)	70(9)	121(11)	69(8)	18(7)	3(6)	14(7)
N(4)	79(7)	69(6)	49(5)	16(4)	-6(4)	-8(5)

sh 2333

Table 1. Crystal data and structure refinement for sh2333.

Identification code	sh2333	
Empirical formula	C131.50 H146 Al4 N3 O19 Si8	
Formula weight	2405.15	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.0204(8) Å	α= 85.484(2)°.
	b = 16.3844(7) Å	β= 82.799(2)°.
	c = 26.2869(12) Å	γ = 67.510(2)°.
Volume	6321.3(5) $Å^3$	
Z	2	
Density (calculated)	1.264 Mg/m^3	
Absorption coefficient	0.180 mm^{-1}	
F(000)	2544	
Crystal size	0.15 x 0.29 x 0.38 mm^3	
Theta range for data collection	1.38 to 28.20°.	
Index ranges	-21<=h<=21, -21<=k<=18, -34<=l<=34	
Reflections collected	110738	
Independent reflections	30354 [R(int) = 0.0434]	
Completeness to theta = 28.20°	97.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	30354 / 0 / 1433	
Goodness-of-fit on F^2	1.653	
Final R indices [I>2sigma(I)]	R1 = 0.0655, wR2 = 0.1796	
R indices (all data)	R1 = 0.1004, wR2 = 0.1952	
Largest diff. peak and hole	1.809 and -0.829 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2333. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	4180(1)	7677(1)	2712(1)	16(1)
Al(2)	2754(1)	9513(1)	3227(1)	16(1)
Al(3)	2399(1)	10309(1)	2101(1)	17(1)
Al(4)	3274(1)	8392(1)	1655(1)	16(1)
Si(1)	3776(1)	6577(1)	3733(1)	18(1)
Si(2)	2250(1)	8315(1)	4167(1)	19(1)
Si(3)	2110(1)	11466(1)	3497(1)	19(1)
Si(4)	2787(1)	11971(1)	2413(1)	18(1)
Si(5)	701(1)	10803(1)	1419(1)	17(1)
Si(6)	1403(1)	8851(1)	1141(1)	17(1)
Si(7)	5033(1)	7016(1)	1117(1)	19(1)
Si(8)	6062(1)	7256(1)	1996(1)	18(1)
O(1)	3875(1)	8716(1)	3028(1)	18(1)
O(2)	2163(1)	9794(1)	2685(1)	18(1)
O(3)	3219(1)	9484(1)	1707(1)	19(1)
O(4)	3459(1)	7813(1)	2244(1)	18(1)
O(5)	4000(1)	6916(1)	3165(1)	20(1)
O(6)	2862(1)	7283(1)	4043(1)	23(1)
O(7)	2255(1)	8983(1)	3690(1)	21(1)
O(8)	2818(1)	10453(1)	3460(1)	21(1)
O(9)	2268(1)	12073(1)	2995(1)	22(1)
O(10)	2880(1)	11068(1)	2171(1)	20(1)
O(11)	1394(1)	10767(1)	1818(1)	22(1)
O(12)	687(1)	9816(1)	1350(1)	20(1)
O(13)	2251(1)	8438(1)	1476(1)	19(1)
O(14)	4169(1)	7924(1)	1183(1)	20(1)
O(15)	5821(1)	6933(1)	1479(1)	23(1)
O(16)	5316(1)	7366(1)	2480(1)	20(1)
C(1)	3519(2)	5564(2)	3685(1)	20(1)
C(2)	3938(2)	4986(2)	3277(1)	27(1)
C(3)	3734(2)	4244(2)	3228(1)	35(1)
C(4)	3116(2)	4054(2)	3584(1)	36(1)
C(5)	2700(2)	4604(2)	3995(1)	35(1)
C(6)	2900(2)	5344(2)	4041(1)	26(1)
C(7)	4752(2)	6352(2)	4117(1)	26(1)
C(8)	5554(3)	6451(2)	3899(1)	40(1)
C(9)	6265(3)	6301(3)	4198(2)	56(1)
C(10)	6211(3)	6026(3)	4704(2)	57(1)
C(11)	5413(3)	5952(3)	4928(2)	59(1)
C(12)	4705(3)	6111(3)	4637(1)	49(1)
C(13)	1065(2)	8371(2)	4359(1)	23(1)
C(14)	841(2)	7622(2)	4443(1)	32(1)
C(15)	-48(2)	7687(2)	4600(1)	39(1)
C(16)	-736(2)	8514(2)	4675(1)	33(1)
C(17)	-528(2)	9261(2)	4593(1)	30(1)
C(18)	355(2)	9187(2)	4439(1)	25(1)
C(19)	2671(2)	8621(2)	4727(1)	24(1)
C(20)	2733(2)	9442(2)	4752(1)	26(1)
C(21)	3042(2)	9674(2)	5175(1)	32(1)
C(22)	3295(3)	9066(3)	5581(1)	41(1)
C(23)	3220(3)	8257(3)	5570(2)	54(1)
C(24)	2909(3)	8039(2)	5150(1)	43(1)
C(25)	2307(2)	11930(2)	4081(1)	27(1)
C(26)	3123(3)	11551(3)	4293(2)	45(1)
C(27)	3268(4)	11923(4)	4727(2)	73(2)
C(28)	2597(5)	12657(4)	4939(2)	72(2)
C(29)	1800(4)	13034(3)	4732(2)	58(1)
C(30)	1650(3)	12690(2)	4309(1)	37(1)
C(31)	894(2)	11575(2)	3535(1)	22(1)
C(32)	428(2)	11461(2)	4008(1)	29(1)
C(33)	-474(2)	11547(2)	4052(1)	36(1)
C(34)	-944(2)	11742(2)	3623(2)	37(1)
C(35)	-500(2)	11839(2)	3147(1)	40(1)
C(36)	408(2)	11774(2)	3104(1)	30(1)
C(37)	2118(2)	12919(2)	1997(1)	20(1)
C(38)	2008(2)	13797(2)	2066(1)	29(1)
C(39)	1511(3)	14481(2)	1746(1)	36(1)
C(40)	1118(2)	14309(2)	1347(1)	31(1)
C(41)	1219(2)	13455(2)	1270(1)	30(1)
C(42)	1719(2)	12768(2)	1592(1)	26(1)
C(43)	3920(2)	12033(2)	2466(1)	22(1)

C(44)	4322(2)	11807(2)	2929(1)	29(1)
C(45)	5158(2)	11853(2)	2970(1)	38(1)
C(46)	5618(2)	12118(2)	2553(1)	35(1)
C(47)	5249(2)	12343(2)	2093(1)	33(1)
C(48)	4403(2)	12294(2)	2051(1)	27(1)
C(49)	-480(2)	11516(2)	1662(1)	20(1)
C(50)	-1198(2)	11227(2)	1741(1)	28(1)
C(51)	-2079(2)	11794(2)	1908(1)	37(1)
C(52)	-2258(2)	12663(2)	2003(1)	36(1)
C(53)	-1561(2)	12974(2)	1933(2)	40(1)
C(54)	-685(2)	12407(2)	1762(1)	35(1)
C(55)	1003(2)	11255(2)	777(1)	20(1)
C(56)	1891(2)	11157(2)	602(1)	33(1)
C(57)	2119(2)	11448(2)	114(1)	40(1)
C(58)	1466(3)	11842(2)	-215(1)	37(1)
C(59)	583(3)	11936(3)	-57(2)	50(1)
C(60)	359(2)	11649(2)	434(1)	38(1)
C(61)	1783(2)	8962(2)	444(1)	20(1)
C(62)	2687(2)	8765(2)	249(1)	33(1)
C(63)	2926(2)	8861(3)	-275(1)	38(1)
C(64)	2268(2)	9142(2)	-610(1)	30(1)
C(65)	1373(2)	9345(2)	-430(1)	36(1)
C(66)	1133(2)	9251(2)	92(1)	32(1)
C(67)	759(2)	8099(2)	1214(1)	21(1)
C(68)	1200(2)	7253(2)	1020(1)	25(1)
C(69)	789(2)	6641(2)	1077(1)	32(1)
C(70)	-76(2)	6854(2)	1332(1)	34(1)
C(71)	-529(2)	7690(2)	1522(1)	33(1)
C(72)	-120(2)	8308(2)	1465(1)	26(1)
C(73)	5566(2)	6954(2)	438(1)	26(1)
C(74)	6441(3)	6937(3)	316(1)	42(1)
C(75)	6848(3)	6884(3)	-193(1)	50(1)
C(76)	6371(3)	6865(3)	-584(1)	46(1)
C(77)	5504(3)	6898(4)	-480(2)	69(2)
C(78)	5106(3)	6945(3)	27(1)	56(1)
C(79)	4655(2)	6073(2)	1314(1)	22(1)
C(80)	5071(2)	5426(2)	1681(1)	27(1)
C(81)	4765(2)	4739(2)	1839(1)	32(1)
C(82)	4041(2)	4695(2)	1625(1)	34(1)
C(83)	3610(2)	5330(2)	1258(1)	34(1)
C(84)	3919(2)	6008(2)	1109(1)	28(1)
C(85)	6176(2)	8350(2)	1835(1)	21(1)
C(86)	6792(2)	8455(2)	1433(1)	29(1)
C(87)	6869(2)	9265(2)	1308(1)	32(1)
C(88)	6327(2)	9998(2)	1585(1)	29(1)
C(89)	5704(2)	9918(2)	1988(1)	38(1)
C(90)	5636(2)	9105(2)	2111(1)	29(1)
C(91)	7186(2)	6392(2)	2122(1)	24(1)
C(92)	7766(2)	5869(2)	1723(1)	34(1)
C(93)	8623(2)	5244(2)	1809(2)	41(1)
C(94)	8916(2)	5114(2)	2284(2)	42(1)
C(95)	8366(3)	5620(2)	2684(2)	43(1)
C(96)	7508(2)	6248(2)	2602(1)	37(1)
N(1)	2886(2)	6524(2)	2360(1)	29(1)
C(97)	1906(2)	6695(2)	2351(1)	39(1)
C(98)	1346(3)	7069(3)	2843(2)	42(1)
C(99)	1279(2)	7995(2)	2967(1)	34(1)
C(100)	749(2)	8727(2)	2610(1)	35(1)
N(2)	643(2)	9613(2)	2789(1)	37(1)
N(3)	4373(3)	9881(3)	1086(2)	99(2)
C(1A1)	4416(4)	9713(4)	623(2)	42(2)
C(1B1)	4367(7)	10543(7)	767(5)	62(3)
C(102)	4982(3)	10185(5)	236(2)	101(3)
O(17)	5189(2)	8691(2)	3553(1)	41(1)
C(103)	4883(3)	9007(3)	4062(1)	45(1)
C(104)	5453(3)	9528(3)	4146(2)	53(1)
C(105)	6352(3)	9029(3)	3841(2)	55(1)
C(106)	6078(3)	8687(4)	3412(2)	78(2)
O(18)	6123(2)	3995(2)	2853(1)	39(1)
C(107)	6273(3)	3463(2)	3321(1)	42(1)
C(108)	6620(3)	3927(3)	3672(2)	47(1)
C(109)	7141(3)	4346(3)	3287(2)	50(1)
C(110)	6544(3)	4634(2)	2849(2)	41(1)
C(111)	8454(3)	8439(3)	3041(2)	52(1)
C(112)	8734(3)	8868(3)	3399(2)	45(1)
C(113)	8495(3)	9762(3)	3376(2)	46(1)
C(114)	7990(3)	10259(3)	3006(2)	57(1)

C(115)	7707(3)	9869(3)	2653(2)	55(1)
C(116)	7931(3)	8980(3)	2663(2)	47(1)
C(117)	8696(4)	7465(3)	3069(3)	83(2)
C(118)	9235(4)	4399(4)	4080(2)	74(1)
C(119)	9569(5)	5112(5)	4162(3)	107(2)
C(120)	10187(6)	5222(5)	3805(3)	119(2)
C(121)	10564(4)	4766(4)	3372(2)	87(2)
C(122)	10272(4)	4101(4)	3321(2)	79(2)
C(123)	9616(3)	3965(3)	3661(2)	61(1)
C(124)	8579(5)	4221(5)	4441(3)	111(2)
O(19)	3130(8)	6694(7)	-682(4)	273(5)
C(125)	2323(4)	6836(4)	-295(2)	78(2)
C(126)	2692(3)	6153(3)	89(2)	56(1)
C(127)	3421(4)	5422(4)	-149(3)	85(2)
C(128)	3723(10)	5646(10)	-597(6)	229(6)
C(129)	8817(8)	4896(7)	405(4)	166(4)
C(130)	9541(9)	4898(9)	150(5)	80(3)
C(131)	9721(5)	5724(4)	122(2)	87(2)
C(132)	9105(9)	5692(8)	340(5)	82(3)
C(133)	10394(10)	5783(9)	-127(5)	92(4)

Table 3. Bond lengths [Å] and angles [°] for sh2333.

Al(1)-O(16)	1.733(2)
Al(1)-O(4)	1.736(2)
Al(1)-O(5)	1.736(2)
Al(1)-O(1)	1.822(2)
Al(2)-O(7)	1.731(2)
Al(2)-O(8)	1.743(2)
Al(2)-O(2)	1.745(2)
Al(2)-O(1)	1.812(2)
Al(3)-O(10)	1.727(2)
Al(3)-O(11)	1.730(2)
Al(3)-O(2)	1.7618(19)
Al(3)-O(3)	1.774(2)
Al(4)-O(13)	1.736(2)
Al(4)-O(14)	1.745(2)
Al(4)-O(4)	1.747(2)
Al(4)-O(3)	1.772(2)
Si(1)-O(5)	1.5980(19)
Si(1)-O(6)	1.642(2)
Si(1)-C(7)	1.869(3)
Si(1)-C(1)	1.873(3)
Si(2)-O(7)	1.598(2)
Si(2)-O(6)	1.633(2)
Si(2)-C(19)	1.870(3)
Si(2)-C(13)	1.872(3)
Si(3)-O(8)	1.615(2)
Si(3)-O(9)	1.642(2)
Si(3)-C(25)	1.877(3)
Si(3)-C(31)	1.879(3)
Si(4)-O(10)	1.603(2)
Si(4)-O(9)	1.638(2)
Si(4)-C(37)	1.873(3)
Si(4)-C(43)	1.879(3)
Si(5)-O(11)	1.602(2)
Si(5)-O(12)	1.650(2)
Si(5)-C(49)	1.864(3)
Si(5)-C(55)	1.871(3)
Si(6)-O(13)	1.606(2)
Si(6)-O(12)	1.647(2)
Si(6)-C(67)	1.872(3)
Si(6)-C(61)	1.875(3)
Si(7)-O(14)	1.602(2)
Si(7)-O(15)	1.634(2)
Si(7)-C(73)	1.873(3)
Si(7)-C(79)	1.879(3)
Si(8)-O(16)	1.603(2)
Si(8)-O(15)	1.636(2)
Si(8)-C(91)	1.866(3)
Si(8)-C(85)	1.880(3)
C(1)-C(6)	1.406(4)
C(1)-C(2)	1.411(4)
C(2)-C(3)	1.393(4)
C(3)-C(4)	1.383(5)
C(4)-C(5)	1.390(5)
C(5)-C(6)	1.386(4)
C(7)-C(12)	1.393(4)
C(7)-C(8)	1.402(5)
C(8)-C(9)	1.398(5)
C(9)-C(10)	1.373(6)
C(10)-C(11)	1.384(6)
C(11)-C(12)	1.379(5)
C(13)-C(18)	1.395(4)
C(13)-C(14)	1.399(4)
C(14)-C(15)	1.398(5)
C(15)-C(16)	1.391(5)
C(16)-C(17)	1.381(5)
C(17)-C(18)	1.384(4)
C(19)-C(20)	1.394(4)
C(19)-C(24)	1.398(4)
C(20)-C(21)	1.405(4)
C(21)-C(22)	1.388(5)
C(22)-C(23)	1.378(5)
C(23)-C(24)	1.390(5)
C(25)-C(26)	1.382(5)
C(25)-C(30)	1.405(5)
C(26)-C(27)	1.418(6)

C(27)-C(28)	1.371(8)
C(28)-C(29)	1.350(7)
C(29)-C(30)	1.372(5)
C(31)-C(36)	1.402(4)
C(31)-C(32)	1.405(4)
C(32)-C(33)	1.387(5)
C(33)-C(34)	1.383(5)
C(34)-C(35)	1.390(5)
C(35)-C(36)	1.409(5)
C(37)-C(42)	1.392(4)
C(37)-C(38)	1.405(4)
C(38)-C(39)	1.390(4)
C(39)-C(40)	1.389(5)
C(40)-C(41)	1.374(4)
C(41)-C(42)	1.399(4)
C(43)-C(48)	1.392(4)
C(43)-C(44)	1.406(4)
C(44)-C(45)	1.388(4)
C(45)-C(46)	1.378(5)
C(46)-C(47)	1.375(5)
C(47)-C(48)	1.405(4)
C(49)-C(50)	1.391(4)
C(49)-C(54)	1.407(4)
C(50)-C(51)	1.399(4)
C(51)-C(52)	1.377(5)
C(52)-C(53)	1.382(5)
C(53)-C(54)	1.395(5)
C(55)-C(60)	1.387(4)
C(55)-C(56)	1.391(4)
C(56)-C(57)	1.386(4)
C(57)-C(58)	1.371(5)
C(58)-C(59)	1.375(5)
C(59)-C(60)	1.392(5)
C(61)-C(62)	1.396(4)
C(61)-C(66)	1.400(4)
C(62)-C(63)	1.395(4)
C(63)-C(64)	1.377(5)
C(64)-C(65)	1.371(5)
C(65)-C(66)	1.391(4)
C(67)-C(68)	1.396(4)
C(67)-C(72)	1.404(4)
C(68)-C(69)	1.387(4)
C(69)-C(70)	1.387(5)
C(70)-C(71)	1.382(5)
C(71)-C(72)	1.392(4)
C(73)-C(78)	1.385(5)
C(73)-C(74)	1.388(5)
C(74)-C(75)	1.408(5)
C(75)-C(76)	1.364(6)
C(76)-C(77)	1.362(6)
C(77)-C(78)	1.399(5)
C(79)-C(84)	1.399(4)
C(79)-C(80)	1.399(4)
C(80)-C(81)	1.407(4)
C(81)-C(82)	1.378(5)
C(82)-C(83)	1.397(5)
C(83)-C(84)	1.392(4)
C(85)-C(86)	1.400(4)
C(85)-C(90)	1.403(4)
C(86)-C(87)	1.390(4)
C(87)-C(88)	1.382(4)
C(88)-C(89)	1.396(4)
C(89)-C(90)	1.389(4)
C(91)-C(96)	1.392(4)
C(91)-C(92)	1.409(4)
C(92)-C(93)	1.396(4)
C(93)-C(94)	1.363(5)
C(94)-C(95)	1.383(5)
C(95)-C(96)	1.397(5)
N(1)-C(97)	1.488(4)
C(97)-C(98)	1.504(5)
C(98)-C(99)	1.537(5)
C(99)-C(100)	1.511(5)
C(100)-N(2)	1.501(4)
N(3)-C(1A1)	1.258(8)
C(1A1)-C(102)	1.624(8)
C(1B1)-C(102)	1.613(14)

C(102)-C(102)#1	1.408(13)
O(17)-C(106)	1.424(5)
O(17)-C(103)	1.431(4)
C(103)-C(104)	1.511(5)
C(104)-C(105)	1.516(5)
C(105)-C(106)	1.478(6)
O(18)-C(107)	1.441(4)
O(18)-C(110)	1.444(4)
C(107)-C(108)	1.517(5)
C(108)-C(109)	1.520(6)
C(109)-C(110)	1.517(5)
C(111)-C(116)	1.407(6)
C(111)-C(112)	1.424(6)
C(111)-C(117)	1.490(6)
C(112)-C(113)	1.364(6)
C(113)-C(114)	1.352(6)
C(114)-C(115)	1.376(6)
C(115)-C(116)	1.359(6)
C(118)-C(123)	1.308(7)
C(118)-C(124)	1.426(8)
C(118)-C(119)	1.497(8)
C(119)-C(120)	1.330(10)
C(120)-C(121)	1.356(9)
C(121)-C(122)	1.360(7)
C(122)-C(123)	1.366(7)
O(19)-C(125)	1.495(11)
O(19)-C(128)	1.627(15)
C(125)-C(126)	1.444(7)
C(126)-C(127)	1.433(7)
C(127)-C(128)	1.296(15)
C(129)-C(130)	1.266(15)
C(129)-C(133)#2	1.479(16)
C(129)-C(132)	1.533(15)
C(130)-C(133)#2	1.085(15)
C(130)-C(132)	1.323(16)
C(130)-C(131)#2	1.389(14)
C(130)-C(131)	1.483(13)
C(130)-C(130)#2	1.71(3)
C(131)-C(132)	1.095(13)
C(131)-C(133)	1.221(14)
C(131)-C(130)#2	1.389(14)
C(133)-C(130)#2	1.085(15)
C(133)-C(129)#2	1.479(16)

O(16)-Al(1)-O(4)	114.35(10)
O(16)-Al(1)-O(5)	111.92(10)
O(4)-Al(1)-O(5)	106.81(10)
O(16)-Al(1)-O(1)	105.99(9)
O(4)-Al(1)-O(1)	109.73(9)
O(5)-Al(1)-O(1)	107.88(9)
O(7)-Al(2)-O(8)	111.81(10)
O(7)-Al(2)-O(2)	110.62(10)
O(8)-Al(2)-O(2)	110.00(9)
O(7)-Al(2)-O(1)	106.63(10)
O(8)-Al(2)-O(1)	111.07(10)
O(2)-Al(2)-O(1)	106.54(9)
O(10)-Al(3)-O(11)	112.85(10)
O(10)-Al(3)-O(2)	113.42(10)
O(11)-Al(3)-O(2)	106.98(10)
O(10)-Al(3)-O(3)	105.53(10)
O(11)-Al(3)-O(3)	109.89(10)
O(2)-Al(3)-O(3)	108.06(9)
O(13)-Al(4)-O(14)	111.49(10)
O(13)-Al(4)-O(4)	108.75(10)
O(14)-Al(4)-O(4)	112.03(10)
O(13)-Al(4)-O(3)	108.96(10)
O(14)-Al(4)-O(3)	105.05(10)
O(4)-Al(4)-O(3)	110.50(10)
O(5)-Si(1)-O(6)	113.40(11)
O(5)-Si(1)-C(7)	110.14(12)
O(6)-Si(1)-C(7)	108.11(13)
O(5)-Si(1)-C(1)	108.16(12)
O(6)-Si(1)-C(1)	105.25(12)
C(7)-Si(1)-C(1)	111.74(13)
O(7)-Si(2)-O(6)	113.59(11)
O(7)-Si(2)-C(19)	110.22(12)
O(6)-Si(2)-C(19)	108.51(13)

O(7)-Si(2)-C(13)	109.72(12)
O(6)-Si(2)-C(13)	106.15(12)
C(19)-Si(2)-C(13)	108.47(13)
O(8)-Si(3)-O(9)	111.91(11)
O(8)-Si(3)-C(25)	107.64(13)
O(9)-Si(3)-C(25)	108.10(12)
O(8)-Si(3)-C(31)	112.81(12)
O(9)-Si(3)-C(31)	106.12(12)
C(25)-Si(3)-C(31)	110.17(14)
O(10)-Si(4)-O(9)	111.37(10)
O(10)-Si(4)-C(37)	108.51(12)
O(9)-Si(4)-C(37)	109.09(12)
O(10)-Si(4)-C(43)	112.51(12)
O(9)-Si(4)-C(43)	105.99(12)
C(37)-Si(4)-C(43)	109.30(13)
O(11)-Si(5)-O(12)	111.45(10)
O(11)-Si(5)-C(49)	110.12(12)
O(12)-Si(5)-C(49)	106.21(12)
O(11)-Si(5)-C(55)	110.99(12)
O(12)-Si(5)-C(55)	109.11(11)
C(49)-Si(5)-C(55)	108.81(13)
O(13)-Si(6)-O(12)	111.74(10)
O(13)-Si(6)-C(67)	108.45(11)
O(12)-Si(6)-C(67)	106.42(12)
O(13)-Si(6)-C(61)	111.54(12)
O(12)-Si(6)-C(61)	109.75(11)
C(67)-Si(6)-C(61)	108.76(12)
O(14)-Si(7)-O(15)	112.99(11)
O(14)-Si(7)-C(73)	109.15(12)
O(15)-Si(7)-C(73)	106.53(13)
O(14)-Si(7)-C(79)	108.65(12)
O(15)-Si(7)-C(79)	106.83(12)
C(73)-Si(7)-C(79)	112.74(13)
O(16)-Si(8)-O(15)	114.21(11)
O(16)-Si(8)-C(91)	111.92(12)
O(15)-Si(8)-C(91)	103.89(13)
O(16)-Si(8)-C(85)	108.88(12)
O(15)-Si(8)-C(85)	107.61(12)
C(91)-Si(8)-C(85)	110.16(13)
Al(2)-O(1)-Al(1)	128.60(11)
Al(2)-O(2)-Al(3)	129.23(11)
Al(4)-O(3)-Al(3)	126.12(11)
Al(1)-O(4)-Al(4)	135.53(12)
Si(1)-O(5)-Al(1)	154.37(13)
Si(2)-O(6)-Si(1)	147.19(13)
Si(2)-O(7)-Al(2)	154.74(14)
Si(3)-O(8)-Al(2)	132.56(12)
Si(4)-O(9)-Si(3)	140.56(13)
Si(4)-O(10)-Al(3)	148.06(13)
Si(5)-O(11)-Al(3)	154.66(13)
Si(6)-O(12)-Si(5)	137.49(13)
Si(6)-O(13)-Al(4)	151.99(13)
Si(7)-O(14)-Al(4)	136.52(12)
Si(7)-O(15)-Si(8)	146.57(14)
Si(8)-O(16)-Al(1)	148.27(13)
C(6)-C(1)-C(2)	116.6(3)
C(6)-C(1)-Si(1)	122.7(2)
C(2)-C(1)-Si(1)	120.7(2)
C(3)-C(2)-C(1)	121.4(3)
C(4)-C(3)-C(2)	120.3(3)
C(3)-C(4)-C(5)	119.8(3)
C(6)-C(5)-C(4)	119.8(3)
C(5)-C(6)-C(1)	122.2(3)
C(12)-C(7)-C(8)	116.8(3)
C(12)-C(7)-Si(1)	121.7(3)
C(8)-C(7)-Si(1)	121.4(2)
C(9)-C(8)-C(7)	120.4(3)
C(10)-C(9)-C(8)	121.2(4)
C(9)-C(10)-C(11)	119.0(4)
C(12)-C(11)-C(10)	119.9(4)
C(11)-C(12)-C(7)	122.6(4)
C(18)-C(13)-C(14)	116.7(3)
C(18)-C(13)-Si(2)	120.1(2)
C(14)-C(13)-Si(2)	123.2(2)
C(13)-C(14)-C(15)	121.7(3)
C(16)-C(15)-C(14)	119.8(3)
C(17)-C(16)-C(15)	119.3(3)

C(16)-C(17)-C(18)	120.4(3)
C(17)-C(18)-C(13)	122.2(3)
C(20)-C(19)-C(24)	116.8(3)
C(20)-C(19)-Si(2)	122.2(2)
C(24)-C(19)-Si(2)	120.9(2)
C(19)-C(20)-C(21)	122.2(3)
C(22)-C(21)-C(20)	119.0(3)
C(23)-C(22)-C(21)	119.9(3)
C(22)-C(23)-C(24)	120.4(3)
C(23)-C(24)-C(19)	121.7(3)
C(26)-C(25)-C(30)	117.4(3)
C(26)-C(25)-Si(3)	120.9(3)
C(30)-C(25)-Si(3)	121.7(3)
C(25)-C(26)-C(27)	120.1(4)
C(28)-C(27)-C(26)	120.0(5)
C(29)-C(28)-C(27)	120.1(4)
C(28)-C(29)-C(30)	120.8(5)
C(29)-C(30)-C(25)	121.5(4)
C(36)-C(31)-C(32)	117.0(3)
C(36)-C(31)-Si(3)	122.6(2)
C(32)-C(31)-Si(3)	120.4(2)
C(33)-C(32)-C(31)	122.1(3)
C(34)-C(33)-C(32)	120.3(3)
C(33)-C(34)-C(35)	119.4(3)
C(34)-C(35)-C(36)	120.3(3)
C(31)-C(36)-C(35)	120.9(3)
C(42)-C(37)-C(38)	117.0(3)
C(42)-C(37)-Si(4)	120.1(2)
C(38)-C(37)-Si(4)	122.9(2)
C(39)-C(38)-C(37)	121.1(3)
C(40)-C(39)-C(38)	120.5(3)
C(41)-C(40)-C(39)	119.5(3)
C(40)-C(41)-C(42)	119.8(3)
C(37)-C(42)-C(41)	122.0(3)
C(48)-C(43)-C(44)	117.0(3)
C(48)-C(43)-Si(4)	121.9(2)
C(44)-C(43)-Si(4)	121.0(2)
C(45)-C(44)-C(43)	121.2(3)
C(46)-C(45)-C(44)	120.5(3)
C(47)-C(46)-C(45)	120.1(3)
C(46)-C(47)-C(48)	119.4(3)
C(43)-C(48)-C(47)	121.8(3)
C(50)-C(49)-C(54)	116.6(3)
C(50)-C(49)-Si(5)	123.6(2)
C(54)-C(49)-Si(5)	119.7(2)
C(49)-C(50)-C(51)	121.6(3)
C(52)-C(51)-C(50)	120.4(3)
C(51)-C(52)-C(53)	119.7(3)
C(52)-C(53)-C(54)	119.7(3)
C(53)-C(54)-C(49)	122.0(3)
C(60)-C(55)-C(56)	116.2(3)
C(60)-C(55)-Si(5)	121.4(2)
C(56)-C(55)-Si(5)	122.2(2)
C(57)-C(56)-C(55)	122.0(3)
C(58)-C(57)-C(56)	120.4(3)
C(57)-C(58)-C(59)	119.2(3)
C(58)-C(59)-C(60)	120.0(3)
C(55)-C(60)-C(59)	122.2(3)
C(62)-C(61)-C(66)	117.2(3)
C(62)-C(61)-Si(6)	123.8(2)
C(66)-C(61)-Si(6)	119.0(2)
C(61)-C(62)-C(63)	121.0(3)
C(64)-C(63)-C(62)	120.1(3)
C(65)-C(64)-C(63)	120.3(3)
C(64)-C(65)-C(66)	119.7(3)
C(65)-C(66)-C(61)	121.6(3)
C(68)-C(67)-C(72)	117.5(3)
C(68)-C(67)-Si(6)	117.5(2)
C(72)-C(67)-Si(6)	125.0(2)
C(69)-C(68)-C(67)	121.3(3)
C(68)-C(69)-C(70)	120.5(3)
C(71)-C(70)-C(69)	119.2(3)
C(70)-C(71)-C(72)	120.6(3)
C(71)-C(72)-C(67)	120.9(3)
C(78)-C(73)-C(74)	116.0(3)
C(78)-C(73)-Si(7)	122.3(3)
C(74)-C(73)-Si(7)	121.7(2)

C(73)-C(74)-C(75)	122.0(3)
C(76)-C(75)-C(74)	119.8(4)
C(77)-C(76)-C(75)	119.9(3)
C(76)-C(77)-C(78)	120.1(4)
C(73)-C(78)-C(77)	122.3(4)
C(84)-C(79)-C(80)	117.1(3)
C(84)-C(79)-Si(7)	120.9(2)
C(80)-C(79)-Si(7)	122.0(2)
C(79)-C(80)-C(81)	121.7(3)
C(82)-C(81)-C(80)	119.5(3)
C(81)-C(82)-C(83)	120.3(3)
C(84)-C(83)-C(82)	119.4(3)
C(83)-C(84)-C(79)	122.1(3)
C(86)-C(85)-C(90)	116.8(3)
C(86)-C(85)-Si(8)	121.9(2)
C(90)-C(85)-Si(8)	121.2(2)
C(87)-C(86)-C(85)	122.1(3)
C(88)-C(87)-C(86)	119.8(3)
C(87)-C(88)-C(89)	119.6(3)
C(90)-C(89)-C(88)	120.0(3)
C(89)-C(90)-C(85)	121.6(3)
C(96)-C(91)-C(92)	116.8(3)
C(96)-C(91)-Si(8)	122.5(2)
C(92)-C(91)-Si(8)	120.7(2)
C(93)-C(92)-C(91)	121.1(3)
C(94)-C(93)-C(92)	120.8(3)
C(93)-C(94)-C(95)	119.5(3)
C(94)-C(95)-C(96)	120.1(3)
C(91)-C(96)-C(95)	121.6(3)
N(1)-C(97)-C(98)	112.6(3)
C(97)-C(98)-C(99)	116.1(3)
C(100)-C(99)-C(98)	114.4(3)
N(2)-C(100)-C(99)	110.8(3)
N(3)-C(1A1)-C(102)	113.4(6)
C(102)#1-C(102)-C(1B1)	145.0(8)
C(102)#1-C(102)-C(1A1)	102.0(7)
C(1B1)-C(102)-C(1A1)	51.7(5)
C(106)-O(17)-C(103)	109.2(3)
O(17)-C(103)-C(104)	104.7(3)
C(103)-C(104)-C(105)	102.8(3)
C(106)-C(105)-C(104)	103.0(3)
O(17)-C(106)-C(105)	108.6(3)
C(107)-O(18)-C(110)	109.3(3)
O(18)-C(107)-C(108)	106.3(3)
C(107)-C(108)-C(109)	101.3(3)
C(110)-C(109)-C(108)	102.4(3)
O(18)-C(110)-C(109)	105.6(3)
C(116)-C(111)-C(112)	116.9(4)
C(116)-C(111)-C(117)	121.4(4)
C(112)-C(111)-C(117)	121.7(5)
C(113)-C(112)-C(111)	121.1(4)
C(114)-C(113)-C(112)	120.1(4)
C(113)-C(114)-C(115)	120.5(4)
C(116)-C(115)-C(114)	121.2(4)
C(115)-C(116)-C(111)	120.2(4)
C(123)-C(118)-C(124)	125.0(6)
C(123)-C(118)-C(119)	113.7(6)
C(124)-C(118)-C(119)	121.3(6)
C(120)-C(119)-C(118)	116.8(7)
C(119)-C(120)-C(121)	128.2(8)
C(120)-C(121)-C(122)	113.3(7)
C(121)-C(122)-C(123)	121.9(6)
C(118)-C(123)-C(122)	126.0(5)
C(125)-O(19)-C(128)	102.2(9)
C(126)-C(125)-O(19)	102.0(6)
C(127)-C(126)-C(125)	109.5(5)
C(128)-C(127)-C(126)	111.7(9)
C(127)-C(128)-O(19)	105.9(12)
C(130)-C(129)-C(133)#2	45.8(8)
C(130)-C(129)-C(132)	55.4(9)
C(133)#2-C(129)-C(132)	101.1(10)
C(133)#2-C(130)-C(129)	77.5(12)
C(133)#2-C(130)-C(132)	149.9(15)
C(129)-C(130)-C(132)	72.6(10)
C(133)#2-C(130)-C(131)#2	57.6(10)
C(129)-C(130)-C(131)#2	135.1(13)
C(132)-C(130)-C(131)#2	152.2(12)

C(133)#2-C(130)-C(131)	164.0(15)
C(129)-C(130)-C(131)	118.1(12)
C(132)-C(130)-C(131)	45.5(7)
C(131)#2-C(130)-C(131)	106.8(9)
C(133)#2-C(130)-C(130)#2	113.4(16)
C(129)-C(130)-C(130)#2	168.9(16)
C(132)-C(130)-C(130)#2	96.3(12)
C(131)#2-C(130)-C(130)#2	55.9(8)
C(131)-C(130)-C(130)#2	50.9(7)
C(132)-C(131)-C(133)	178.3(13)
C(132)-C(131)-C(130)#2	132.7(11)
C(133)-C(131)-C(130)#2	48.6(8)
C(132)-C(131)-C(130)	59.5(8)
C(133)-C(131)-C(130)	121.7(10)
C(130)#2-C(131)-C(130)	73.2(9)
C(131)-C(132)-C(130)	75.0(10)
C(131)-C(132)-C(129)	127.0(12)
C(130)-C(132)-C(129)	52.0(7)
C(130)#2-C(133)-C(131)	73.8(12)
C(130)#2-C(133)-C(129)#2	56.7(10)
C(131)-C(133)-C(129)#2	130.5(13)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2333. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	15(1)	17(1)	16(1)	2(1)	-1(1)	-6(1)
Al(2)	16(1)	15(1)	18(1)	1(1)	-1(1)	-7(1)
Al(3)	17(1)	14(1)	19(1)	1(1)	-4(1)	-7(1)
Al(4)	14(1)	16(1)	16(1)	0(1)	-1(1)	-5(1)
Si(1)	20(1)	16(1)	18(1)	2(1)	0(1)	-7(1)
Si(2)	21(1)	18(1)	19(1)	-1(1)	3(1)	-9(1)
Si(3)	23(1)	18(1)	18(1)	0(1)	-3(1)	-9(1)
Si(4)	18(1)	15(1)	21(1)	0(1)	-2(1)	-8(1)
Si(5)	14(1)	17(1)	19(1)	0(1)	-2(1)	-5(1)
Si(6)	16(1)	18(1)	18(1)	0(1)	-2(1)	-7(1)
Si(7)	17(1)	20(1)	18(1)	-1(1)	1(1)	-4(1)
Si(8)	14(1)	19(1)	20(1)	1(1)	0(1)	-6(1)
O(1)	15(1)	20(1)	20(1)	1(1)	-2(1)	-9(1)
O(2)	18(1)	17(1)	19(1)	2(1)	-3(1)	-8(1)
O(3)	19(1)	16(1)	21(1)	-1(1)	-1(1)	-7(1)
O(4)	18(1)	17(1)	18(1)	1(1)	-3(1)	-6(1)
O(5)	21(1)	19(1)	19(1)	3(1)	0(1)	-8(1)
O(6)	25(1)	18(1)	23(1)	0(1)	5(1)	-7(1)
O(7)	22(1)	20(1)	22(1)	0(1)	2(1)	-11(1)
O(8)	23(1)	19(1)	22(1)	0(1)	-5(1)	-10(1)
O(9)	26(1)	19(1)	21(1)	0(1)	-2(1)	-11(1)
O(10)	23(1)	17(1)	24(1)	-1(1)	-2(1)	-10(1)
O(11)	22(1)	17(1)	26(1)	1(1)	-7(1)	-5(1)
O(12)	17(1)	21(1)	23(1)	0(1)	0(1)	-7(1)
O(13)	18(1)	20(1)	20(1)	1(1)	-3(1)	-7(1)
O(14)	18(1)	21(1)	19(1)	-1(1)	1(1)	-6(1)
O(15)	18(1)	23(1)	25(1)	-2(1)	0(1)	-6(1)
O(16)	16(1)	22(1)	22(1)	1(1)	0(1)	-8(1)
C(1)	20(1)	16(1)	23(1)	4(1)	-4(1)	-5(1)
C(2)	28(2)	22(2)	29(2)	1(1)	1(1)	-9(1)
C(3)	43(2)	24(2)	37(2)	-5(1)	1(2)	-13(2)
C(4)	41(2)	25(2)	49(2)	1(2)	-5(2)	-19(2)
C(5)	33(2)	31(2)	43(2)	6(2)	1(2)	-18(2)
C(6)	29(2)	20(2)	27(2)	1(1)	2(1)	-8(1)
C(7)	30(2)	25(2)	27(2)	3(1)	-7(1)	-14(1)
C(8)	39(2)	47(2)	40(2)	11(2)	-15(2)	-23(2)
C(9)	52(3)	72(3)	63(3)	23(2)	-25(2)	-43(2)
C(10)	70(3)	68(3)	56(3)	24(2)	-43(2)	-44(3)
C(11)	72(3)	76(3)	37(2)	19(2)	-26(2)	-35(3)
C(12)	42(2)	76(3)	31(2)	15(2)	-10(2)	-25(2)
C(13)	27(2)	26(2)	16(1)	1(1)	3(1)	-12(1)
C(14)	29(2)	25(2)	42(2)	2(1)	5(1)	-12(1)
C(15)	34(2)	34(2)	51(2)	3(2)	6(2)	-20(2)
C(16)	22(2)	44(2)	33(2)	0(2)	6(1)	-14(2)
C(17)	26(2)	33(2)	26(2)	-3(1)	2(1)	-9(1)
C(18)	27(2)	25(2)	23(1)	-2(1)	1(1)	-11(1)
C(19)	24(2)	27(2)	19(1)	-2(1)	3(1)	-10(1)
C(20)	25(2)	27(2)	26(2)	-2(1)	-2(1)	-9(1)
C(21)	32(2)	36(2)	32(2)	-8(1)	-2(1)	-14(2)
C(22)	49(2)	52(2)	29(2)	-3(2)	-10(2)	-25(2)
C(23)	90(3)	55(3)	33(2)	18(2)	-27(2)	-42(2)
C(24)	68(3)	38(2)	35(2)	9(2)	-17(2)	-33(2)
C(25)	42(2)	23(2)	23(2)	4(1)	-6(1)	-22(1)
C(26)	61(3)	37(2)	50(2)	8(2)	-32(2)	-27(2)
C(27)	117(5)	72(3)	64(3)	32(3)	-60(3)	-64(3)
C(28)	153(6)	66(3)	34(2)	1(2)	-16(3)	-82(4)
C(29)	112(4)	54(3)	30(2)	-14(2)	14(2)	-60(3)
C(30)	58(2)	34(2)	27(2)	-9(1)	9(2)	-31(2)
C(31)	23(2)	17(1)	25(2)	-5(1)	0(1)	-5(1)
C(32)	32(2)	25(2)	29(2)	5(1)	-3(1)	-11(1)
C(33)	31(2)	30(2)	42(2)	4(2)	8(2)	-12(2)
C(34)	22(2)	33(2)	54(2)	-7(2)	1(2)	-9(1)
C(35)	25(2)	50(2)	41(2)	-8(2)	-6(2)	-10(2)
C(36)	25(2)	36(2)	25(2)	-6(1)	1(1)	-8(1)
C(37)	18(1)	18(1)	23(1)	2(1)	1(1)	-9(1)
C(38)	36(2)	21(2)	31(2)	-3(1)	-7(1)	-11(1)
C(39)	48(2)	17(2)	43(2)	0(1)	-11(2)	-9(2)
C(40)	29(2)	22(2)	40(2)	10(1)	-11(1)	-8(1)
C(41)	32(2)	31(2)	31(2)	7(1)	-12(1)	-17(1)
C(42)	32(2)	21(2)	30(2)	4(1)	-9(1)	-13(1)
C(43)	19(1)	16(1)	33(2)	-3(1)	0(1)	-8(1)

C(44)	25(2)	37(2)	30(2)	-4(1)	-2(1)	-16(1)
C(45)	28(2)	48(2)	41(2)	-8(2)	-7(2)	-15(2)
C(46)	23(2)	32(2)	53(2)	-15(2)	3(2)	-13(1)
C(47)	26(2)	21(2)	52(2)	-5(1)	6(2)	-12(1)
C(48)	26(2)	22(2)	34(2)	2(1)	0(1)	-9(1)
C(49)	17(1)	22(2)	20(1)	-2(1)	0(1)	-4(1)
C(50)	23(2)	24(2)	34(2)	-7(1)	3(1)	-7(1)
C(51)	22(2)	39(2)	49(2)	-8(2)	7(2)	-13(2)
C(52)	20(2)	30(2)	49(2)	-12(2)	7(1)	-1(1)
C(53)	30(2)	25(2)	60(2)	-13(2)	7(2)	-5(2)
C(54)	22(2)	29(2)	53(2)	-10(2)	4(2)	-9(1)
C(55)	21(1)	18(1)	19(1)	0(1)	-2(1)	-7(1)
C(56)	21(2)	38(2)	34(2)	6(1)	0(1)	-5(1)
C(57)	29(2)	44(2)	38(2)	5(2)	12(2)	-10(2)
C(58)	45(2)	37(2)	27(2)	6(1)	4(2)	-18(2)
C(59)	50(2)	68(3)	37(2)	25(2)	-16(2)	-30(2)
C(60)	28(2)	55(2)	35(2)	18(2)	-9(1)	-20(2)
C(61)	22(1)	16(1)	20(1)	-1(1)	-1(1)	-7(1)
C(62)	24(2)	52(2)	26(2)	4(1)	-5(1)	-18(2)
C(63)	28(2)	63(2)	27(2)	1(2)	3(1)	-24(2)
C(64)	37(2)	39(2)	19(1)	4(1)	0(1)	-21(2)
C(65)	30(2)	49(2)	23(2)	7(1)	-6(1)	-10(2)
C(66)	20(2)	46(2)	22(2)	3(1)	-1(1)	-5(1)
C(67)	22(2)	23(2)	20(1)	4(1)	-6(1)	-12(1)
C(68)	25(2)	23(2)	29(2)	2(1)	-7(1)	-11(1)
C(69)	39(2)	20(2)	42(2)	3(1)	-11(2)	-13(1)
C(70)	41(2)	33(2)	40(2)	9(2)	-10(2)	-26(2)
C(71)	29(2)	44(2)	32(2)	0(2)	0(1)	-22(2)
C(72)	26(2)	29(2)	26(2)	-3(1)	-1(1)	-12(1)
C(73)	23(2)	22(2)	23(2)	-4(1)	3(1)	-1(1)
C(74)	41(2)	64(3)	27(2)	-11(2)	8(2)	-29(2)
C(75)	49(2)	75(3)	33(2)	-16(2)	19(2)	-35(2)
C(76)	44(2)	58(3)	26(2)	-2(2)	8(2)	-11(2)
C(77)	38(2)	128(4)	25(2)	-4(2)	-4(2)	-13(3)
C(78)	27(2)	102(4)	27(2)	-4(2)	0(2)	-10(2)
C(79)	22(2)	19(1)	23(1)	-6(1)	2(1)	-5(1)
C(80)	27(2)	23(2)	30(2)	-2(1)	-5(1)	-7(1)
C(81)	36(2)	23(2)	34(2)	1(1)	-3(1)	-7(1)
C(82)	41(2)	23(2)	40(2)	-6(1)	4(2)	-16(2)
C(83)	32(2)	37(2)	39(2)	-6(2)	-6(2)	-18(2)
C(84)	29(2)	28(2)	29(2)	-4(1)	-4(1)	-10(1)
C(85)	17(1)	24(2)	23(1)	3(1)	-3(1)	-9(1)
C(86)	31(2)	26(2)	30(2)	-6(1)	8(1)	-14(1)
C(87)	36(2)	32(2)	31(2)	-3(1)	12(1)	-20(2)
C(88)	31(2)	23(2)	33(2)	3(1)	2(1)	-12(1)
C(89)	38(2)	23(2)	44(2)	-4(1)	15(2)	-8(2)
C(90)	27(2)	20(2)	36(2)	0(1)	11(1)	-8(1)
C(91)	16(1)	23(2)	32(2)	4(1)	-2(1)	-8(1)
C(92)	21(2)	31(2)	39(2)	7(1)	0(1)	-2(1)
C(93)	22(2)	32(2)	56(2)	2(2)	6(2)	-1(1)
C(94)	23(2)	29(2)	69(3)	4(2)	-11(2)	-4(1)
C(95)	34(2)	44(2)	48(2)	6(2)	-18(2)	-10(2)
C(96)	28(2)	38(2)	40(2)	-1(2)	-8(2)	-6(2)
N(1)	34(2)	23(1)	35(2)	-2(1)	-1(1)	-17(1)
C(97)	38(2)	39(2)	47(2)	-7(2)	-3(2)	-23(2)
C(98)	39(2)	49(2)	47(2)	-3(2)	4(2)	-27(2)
C(99)	30(2)	46(2)	32(2)	-8(2)	2(1)	-20(2)
C(100)	36(2)	52(2)	31(2)	-2(2)	-1(1)	-31(2)
N(2)	24(2)	45(2)	45(2)	3(1)	-2(1)	-19(1)
N(3)	51(2)	158(5)	109(4)	96(3)	-36(2)	-73(3)
C(1A1)	28(3)	39(3)	43(4)	19(3)	12(3)	-5(3)
C(1B1)	35(6)	54(7)	95(9)	52(6)	-20(6)	-20(5)
C(102)	34(2)	154(6)	78(3)	62(4)	-4(3)	-9(3)
O(17)	26(1)	67(2)	38(1)	-15(1)	-3(1)	-22(1)
C(103)	37(2)	66(3)	34(2)	-8(2)	0(2)	-23(2)
C(104)	40(2)	76(3)	49(2)	-24(2)	-2(2)	-25(2)
C(105)	33(2)	80(3)	57(3)	-20(2)	0(2)	-24(2)
C(106)	40(3)	146(5)	65(3)	-52(3)	15(2)	-52(3)
O(18)	35(1)	36(1)	42(1)	0(1)	-7(1)	-10(1)
C(107)	50(2)	33(2)	44(2)	5(2)	-14(2)	-15(2)
C(108)	62(3)	40(2)	44(2)	4(2)	-12(2)	-25(2)
C(109)	56(3)	46(2)	56(3)	5(2)	-16(2)	-26(2)
C(110)	41(2)	37(2)	44(2)	1(2)	-3(2)	-14(2)
C(111)	33(2)	49(2)	74(3)	-6(2)	14(2)	-21(2)
C(112)	34(2)	61(3)	41(2)	3(2)	-4(2)	-20(2)
C(113)	44(2)	58(3)	40(2)	-4(2)	-2(2)	-23(2)
C(114)	64(3)	60(3)	50(3)	1(2)	-13(2)	-27(2)

C(115)	68(3)	66(3)	42(2)	4(2)	-15(2)	-36(2)
C(116)	38(2)	73(3)	39(2)	-10(2)	1(2)	-30(2)
C(117)	52(3)	70(4)	135(5)	-8(3)	0(3)	-34(3)

sh2338

Table 1. Crystal data and structure refinement for sh2338.

Identification code	sh2338	
Empirical formula	C122 H146 Al4 N6 O23 Si8	
Formula weight	2397.09	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.4253(14) Å	a= 93.363(5)°.
	b = 17.9309(14) Å	b= 102.747(5)°.
	c = 24.267(3) Å	g = 118.734(3)°.
Volume	6363.2(10) $Å^3$	
Z	2	
Density (calculated)	1.251 Mg/m^3	
Absorption coefficient	0.181 mm^{-1}	
F(000)	2536	
Crystal size	0.43 x 0.35 x 0.2 mm^3	
Theta range for data collection	1.32 to 28.93°.	
Index ranges	-23<=h<=23, -24<=k<=24, -19<=l<=33	
Reflections collected	81002	
Independent reflections	32898 [R(int) = 0.0447]	
Completeness to theta = 28.93°	97.9 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	32898 / 0 / 1483	
Goodness-of-fit on F^2	2.153	
Final R indices [I>2sigma(I)]	R1 = 0.1088, wR2 = 0.2808	
R indices (all data)	R1 = 0.1631, wR2 = 0.2953	
Largest diff. peak and hole	1.451 and -1.053 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2338. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	3565(1)	2643(1)	2326(1)	20(1)
Al(2)	4884(1)	2460(1)	3428(1)	22(1)
Al(3)	5332(1)	1427(1)	2503(1)	19(1)
Al(4)	3976(1)	1584(1)	1406(1)	17(1)
Si(1)	2189(1)	2386(1)	3084(1)	22(1)
Si(2)	3204(1)	1722(1)	3998(1)	24(1)
Si(3)	7043(1)	3632(1)	4096(1)	32(1)
Si(4)	7371(1)	2387(1)	3293(1)	27(1)
Si(5)	4447(1)	-572(1)	1907(1)	23(1)
Si(6)	2856(1)	-485(1)	1041(1)	22(1)
Si(7)	4378(1)	3082(1)	615(1)	19(1)
Si(8)	3714(1)	3915(1)	1427(1)	19(1)
O(1)	4514(2)	2868(2)	2874(1)	23(1)
O(2)	5009(2)	1594(2)	3133(1)	24(1)
O(3)	4946(2)	1805(2)	1931(1)	22(1)
O(4)	3253(2)	1778(2)	1751(1)	21(1)
O(5)	2600(2)	2349(2)	2563(1)	26(1)
O(6)	2591(3)	2104(2)	3658(1)	32(1)
O(7)	4141(3)	2021(2)	3846(1)	34(1)
O(8)	5972(3)	3278(3)	3854(1)	40(1)
O(9)	7404(3)	3160(2)	3710(1)	31(1)
O(10)	6532(2)	1985(2)	2715(1)	25(1)
O(11)	4883(2)	317(2)	2347(1)	26(1)
O(12)	3591(3)	-747(2)	1369(1)	33(1)
O(13)	3322(2)	526(2)	1015(1)	22(1)
O(14)	4306(2)	2306(2)	933(1)	23(1)
O(15)	4267(2)	3792(2)	996(1)	21(1)
O(16)	3850(2)	3566(2)	2015(1)	21(1)
C(1)	2422(4)	3503(3)	3323(2)	27(1)
C(2)	2632(4)	4122(3)	2969(2)	30(1)
C(3)	2772(4)	4950(4)	3140(2)	37(1)
C(4)	2710(4)	5171(4)	3677(2)	44(2)
C(5)	2498(5)	4572(5)	4035(2)	53(2)
C(6)	2364(4)	3758(4)	3866(2)	40(1)
C(7)	930(4)	1631(4)	2848(3)	58(2)
C(8A)	659(11)	751(10)	2459(6)	42(3)
C(9A)	-262(12)	129(12)	2190(7)	53(4)
C(10)	-704(7)	499(6)	2234(4)	79(2)
C(11A)	-630(14)	1221(13)	2409(8)	67(5)
C(12A)	256(13)	1781(13)	2668(7)	59(4)
C(8B)	397(8)	1112(8)	2411(5)	51(3)
C(9B)	-987(9)	608(8)	2713(5)	55(3)
C(11B)	-469(8)	1179(7)	3231(5)	53(3)
C(12B)	463(7)	1706(7)	3340(4)	45(2)
C(13)	3453(3)	2110(3)	4785(2)	20(1)
C(14)	4357(4)	2531(4)	5141(2)	42(1)
C(15)	4570(5)	2789(5)	5737(2)	51(2)
C(16)	3870(5)	2586(5)	5988(2)	57(2)
C(17)	2980(5)	2189(4)	5655(2)	43(2)
C(18)	2784(4)	1956(4)	5059(2)	36(1)
C(19)	2487(4)	516(4)	3846(2)	36(1)
C(20)	2866(5)	13(5)	3675(3)	65(2)
C(21)	2342(7)	-906(5)	3601(4)	92(3)
C(22)	1480(7)	-1308(5)	3680(3)	73(3)
C(23)	1118(7)	-837(5)	3804(3)	81(3)
C(24)	1606(6)	68(5)	3881(3)	67(2)
C(25)	7350(4)	3476(4)	4855(2)	32(1)
C(26)	8272(4)	3902(4)	5185(2)	39(1)
C(27)	8522(4)	3702(4)	5712(2)	40(1)
C(28)	7872(5)	3074(4)	5927(2)	42(2)
C(29)	6965(5)	2671(4)	5615(2)	43(2)
C(30)	6710(4)	2863(4)	5086(2)	35(1)
C(31)	7713(4)	4826(4)	4102(2)	37(1)
C(32)	8485(5)	5209(4)	3889(2)	47(2)
C(33)	9010(6)	6109(5)	3938(3)	66(2)
C(34)	8785(7)	6646(5)	4202(3)	76(2)
C(35)	8021(6)	6293(5)	4413(3)	67(2)
C(36)	7497(5)	5391(4)	4370(2)	46(2)
C(37)	8479(4)	2896(4)	3115(2)	34(1)
C(38)	8565(4)	2644(5)	2588(3)	50(2)
C(39)	9416(6)	2984(6)	2478(3)	79(3)

C(40)	10186(5)	3615(6)	2903(4)	80(3)
C(41)	10131(5)	3866(5)	3415(4)	67(2)
C(42)	9285(5)	3509(4)	3537(3)	50(2)
C(43)	7329(4)	1533(4)	3727(2)	37(1)
C(44)	7082(5)	699(4)	3447(3)	58(2)
C(45)	7069(6)	68(5)	3763(3)	69(2)
C(46)	7273(6)	244(5)	4358(3)	72(2)
C(47)	7533(6)	1052(5)	4646(3)	64(2)
C(48)	7569(5)	1695(5)	4329(3)	55(2)
C(49)	5356(4)	-569(3)	1612(2)	24(1)
C(50)	5206(4)	-1261(3)	1211(2)	30(1)
C(51)	5911(4)	-1238(4)	1018(2)	38(1)
C(52)	6777(4)	-518(4)	1206(2)	36(1)
C(53)	6951(4)	186(4)	1593(2)	34(1)
C(54)	6247(4)	162(3)	1792(2)	31(1)
C(55)	3996(4)	-1475(3)	2309(2)	30(1)
C(56)	3116(5)	-2155(4)	2143(3)	54(2)
C(57)	2814(6)	-2789(5)	2498(4)	82(3)
C(58)	3381(8)	-2715(5)	3000(4)	75(3)
C(59)	4267(8)	-2043(6)	3175(3)	74(3)
C(60)	4591(5)	-1419(4)	2829(2)	50(2)
C(61)	2319(3)	-1187(3)	307(2)	23(1)
C(62)	2038(3)	-919(3)	-196(2)	27(1)
C(63)	1581(4)	-1487(4)	-728(2)	34(1)
C(64)	1376(4)	-2347(4)	-762(2)	41(1)
C(65)	1639(4)	-2634(4)	-282(2)	37(1)
C(66)	2106(4)	-2055(3)	244(2)	33(1)
C(67)	1935(4)	-789(3)	1420(2)	28(1)
C(68)	1011(4)	-1328(3)	1122(2)	34(1)
C(69)	331(4)	-1490(4)	1389(3)	45(2)
C(70)	555(5)	-1107(5)	1959(3)	74(3)
C(71)	1471(6)	-561(6)	2258(3)	76(3)
C(72)	2143(5)	-426(4)	1999(2)	49(2)
C(73)	5544(3)	3706(3)	502(2)	22(1)
C(74)	6118(4)	4594(3)	690(2)	29(1)
C(75)	6993(4)	5023(4)	613(2)	35(1)
C(76)	7316(4)	4570(4)	356(2)	38(1)
C(77)	6756(4)	3687(4)	154(2)	34(1)
C(78)	5888(4)	3263(3)	226(2)	28(1)
C(79)	3497(3)	2662(3)	-107(2)	21(1)
C(80)	3579(4)	3194(3)	-514(2)	29(1)
C(81)	2922(4)	2915(4)	-1037(2)	35(1)
C(82)	2158(4)	2097(4)	-1166(2)	34(1)
C(83)	2062(4)	1551(4)	-772(2)	32(1)
C(84)	2734(4)	1831(3)	-246(2)	27(1)
C(85)	4172(3)	5109(3)	1607(2)	21(1)
C(86)	4401(4)	5652(3)	1203(2)	27(1)
C(87)	4661(4)	6511(3)	1328(2)	40(2)
C(88)	4707(4)	6879(4)	1867(2)	40(1)
C(89)	4498(4)	6361(3)	2281(2)	36(1)
C(90)	4237(4)	5491(3)	2152(2)	27(1)
C(91)	2474(3)	3363(3)	1020(2)	21(1)
C(92)	2182(4)	3409(3)	441(2)	30(1)
C(93)	1262(4)	3027(4)	148(2)	35(1)
C(94)	599(4)	2597(4)	418(2)	37(1)
C(95)	868(4)	2534(3)	996(2)	33(1)
C(96)	1783(3)	2911(3)	1289(2)	26(1)
N(1)	5802(3)	4543(3)	3085(2)	37(1)
C(97)	6218(5)	5036(4)	2650(2)	46(2)
C(98)	6316(5)	4459(5)	2196(2)	51(2)
C(99)	6915(5)	4117(4)	2449(2)	50(2)
C(100)	7158(4)	3705(4)	1993(2)	45(2)
N(2)	6337(3)	2948(3)	1582(2)	29(1)
N(3)	5016(4)	419(3)	3744(2)	51(2)
C(101)	5144(4)	632(4)	4366(2)	34(1)
C(102)	4906(4)	-143(3)	4675(2)	37(1)
N(4)	1458(3)	848(3)	1237(2)	32(1)
C(103)	1174(3)	663(3)	597(2)	28(1)
C(104)	127(3)	99(3)	336(2)	32(1)
N(5)	5066(5)	5129(4)	3834(2)	69(2)
C(105)	4824(6)	4479(6)	4222(3)	69(2)
C(106)	4677(7)	4762(8)	4772(3)	122(5)
N(6)	6513(3)	1750(3)	883(2)	36(1)
C(107)	5559(4)	1037(3)	589(2)	30(1)
C(108)	5481(4)	365(3)	136(2)	32(1)
O(17)	8553(4)	4296(4)	9473(2)	69(2)
C(109)	9202(5)	4201(5)	9274(3)	60(2)

C(110)	9705(6)	4922(6)	8985(3)	85(3)
O(18)	9065(4)	4942(4)	8502(2)	81(2)
C(111)	8400(7)	5030(6)	8696(3)	79(3)
C(112)	7919(6)	4319(6)	8998(3)	69(2)
O(19)	915(3)	4540(3)	8099(2)	71(2)
C(113)	542(6)	4836(6)	7609(4)	84(3)
C(114)	-410(6)	4224(5)	7332(3)	73(2)
O(20)	-554(5)	3407(4)	7134(2)	107(3)
C(115)	-226(10)	3092(7)	7599(5)	179(8)
C(116)	732(8)	3688(7)	7901(6)	144(6)
O(21)	2281(5)	2771(4)	7486(3)	94(2)
C(117)	3062(6)	2695(6)	7489(3)	73(2)
C(1A8)	2865(7)	1809(6)	7411(4)	54(2)
C(1B8)	2916(17)	2020(15)	7005(8)	58(7)
O(22)	2172(6)	1330(5)	6887(2)	96(2)
C(119)	1363(8)	1391(7)	6874(4)	102(3)
C(1A0)	1645(10)	2355(9)	7001(4)	66(4)
C(1B0)	1314(12)	1833(10)	7248(7)	49(4)
O(23)	498(6)	794(5)	5374(4)	130(3)
C(122)	39(13)	861(16)	4842(5)	246(12)
C(123)	746(11)	3(13)	5436(6)	214(9)

Table 3. Bond lengths [Å] and angles [°] for sh2338.

Al(1)-O(1)	1.730(3)
Al(1)-O(5)	1.746(4)
Al(1)-O(16)	1.755(3)
Al(1)-O(4)	1.802(3)
Al(2)-O(1)	1.715(3)
Al(2)-O(7)	1.736(4)
Al(2)-O(8)	1.760(4)
Al(2)-O(2)	1.799(3)
Al(3)-O(3)	1.726(3)
Al(3)-O(11)	1.732(3)
Al(3)-O(10)	1.757(4)
Al(3)-O(2)	1.799(3)
Al(4)-O(3)	1.727(3)
Al(4)-O(13)	1.741(3)
Al(4)-O(14)	1.753(3)
Al(4)-O(4)	1.806(3)
Si(1)-O(5)	1.596(3)
Si(1)-O(6)	1.637(3)
Si(1)-C(7)	1.864(7)
Si(1)-C(1)	1.869(5)
Si(2)-O(7)	1.594(4)
Si(2)-O(6)	1.634(3)
Si(2)-C(19)	1.865(6)
Si(2)-C(13)	1.872(4)
Si(3)-O(8)	1.601(4)
Si(3)-O(9)	1.634(3)
Si(3)-C(25)	1.879(5)
Si(3)-C(31)	1.879(6)
Si(4)-O(10)	1.610(3)
Si(4)-O(9)	1.638(3)
Si(4)-C(37)	1.863(6)
Si(4)-C(43)	1.890(6)
Si(5)-O(11)	1.592(3)
Si(5)-O(12)	1.633(4)
Si(5)-C(55)	1.869(5)
Si(5)-C(49)	1.877(5)
Si(6)-O(13)	1.603(3)
Si(6)-O(12)	1.634(4)
Si(6)-C(61)	1.872(4)
Si(6)-C(67)	1.894(5)
Si(7)-O(14)	1.597(3)
Si(7)-O(15)	1.642(3)
Si(7)-C(79)	1.881(5)
Si(7)-C(73)	1.883(5)
Si(8)-O(16)	1.606(3)
Si(8)-O(15)	1.641(3)
Si(8)-C(85)	1.874(5)
Si(8)-C(91)	1.874(5)
C(1)-C(2)	1.401(7)
C(1)-C(6)	1.410(6)
C(2)-C(3)	1.404(7)
C(3)-C(4)	1.381(7)
C(4)-C(5)	1.385(9)
C(5)-C(6)	1.383(8)
C(7)-C(8B)	1.212(12)
C(7)-C(12A)	1.315(19)
C(7)-C(8A)	1.586(16)
C(7)-C(12B)	1.619(12)
C(8A)-C(9A)	1.41(2)
C(9A)-C(10)	1.249(18)
C(10)-C(11A)	1.27(2)
C(10)-C(9B)	1.398(13)
C(10)-C(8B)	1.620(15)
C(11A)-C(12A)	1.34(3)
C(9B)-C(11B)	1.378(14)
C(11B)-C(12B)	1.380(15)
C(13)-C(18)	1.390(7)
C(13)-C(14)	1.405(7)
C(14)-C(15)	1.400(7)
C(15)-C(16)	1.385(9)
C(16)-C(17)	1.371(9)
C(17)-C(18)	1.399(7)
C(19)-C(24)	1.374(9)
C(19)-C(20)	1.439(8)
C(20)-C(21)	1.424(10)

C(21)-C(22)	1.385(13)
C(22)-C(23)	1.330(11)
C(23)-C(24)	1.399(10)
C(25)-C(30)	1.391(8)
C(25)-C(26)	1.409(8)
C(26)-C(27)	1.383(7)
C(27)-C(28)	1.388(9)
C(28)-C(29)	1.379(9)
C(29)-C(30)	1.383(8)
C(31)-C(36)	1.409(7)
C(31)-C(32)	1.418(9)
C(32)-C(33)	1.402(9)
C(33)-C(34)	1.376(11)
C(34)-C(35)	1.399(12)
C(35)-C(36)	1.407(10)
C(37)-C(38)	1.393(7)
C(37)-C(42)	1.407(8)
C(38)-C(39)	1.403(9)
C(39)-C(40)	1.392(11)
C(40)-C(41)	1.336(11)
C(41)-C(42)	1.406(10)
C(43)-C(48)	1.399(7)
C(43)-C(44)	1.420(8)
C(44)-C(45)	1.397(9)
C(45)-C(46)	1.387(10)
C(46)-C(47)	1.380(10)
C(47)-C(48)	1.408(9)
C(49)-C(50)	1.408(6)
C(49)-C(54)	1.413(7)
C(50)-C(51)	1.393(8)
C(51)-C(52)	1.381(8)
C(52)-C(53)	1.390(7)
C(53)-C(54)	1.397(7)
C(55)-C(56)	1.368(9)
C(55)-C(60)	1.409(8)
C(56)-C(57)	1.431(10)
C(57)-C(58)	1.343(12)
C(58)-C(59)	1.370(13)
C(59)-C(60)	1.409(9)
C(61)-C(66)	1.405(7)
C(61)-C(62)	1.410(6)
C(62)-C(63)	1.398(6)
C(63)-C(64)	1.399(8)
C(64)-C(65)	1.377(8)
C(65)-C(66)	1.395(7)
C(67)-C(68)	1.400(7)
C(67)-C(72)	1.402(7)
C(68)-C(69)	1.391(8)
C(69)-C(70)	1.390(8)
C(70)-C(71)	1.392(10)
C(71)-C(72)	1.377(9)
C(73)-C(74)	1.388(7)
C(73)-C(78)	1.419(6)
C(74)-C(75)	1.401(7)
C(75)-C(76)	1.378(7)
C(76)-C(77)	1.384(8)
C(77)-C(78)	1.386(7)
C(79)-C(84)	1.393(7)
C(79)-C(80)	1.395(6)
C(80)-C(81)	1.382(7)
C(81)-C(82)	1.380(8)
C(82)-C(83)	1.386(7)
C(83)-C(84)	1.397(7)
C(85)-C(86)	1.406(6)
C(85)-C(90)	1.407(6)
C(86)-C(87)	1.372(7)
C(87)-C(88)	1.398(7)
C(88)-C(89)	1.397(7)
C(89)-C(90)	1.392(7)
C(91)-C(92)	1.406(6)
C(91)-C(96)	1.416(7)
C(92)-C(93)	1.388(7)
C(93)-C(94)	1.376(8)
C(94)-C(95)	1.408(7)
C(95)-C(96)	1.384(7)
N(1)-C(97)	1.501(7)
C(97)-C(98)	1.560(8)

C(98)-C(99)	1.491(8)
C(99)-C(100)	1.537(8)
C(100)-N(2)	1.493(7)
N(3)-C(101)	1.474(6)
C(101)-C(102)	1.540(7)
C(102)-C(102)#1	1.542(9)
N(4)-C(103)	1.486(6)
C(103)-C(104)	1.546(7)
C(104)-C(104)#2	1.565(10)
N(5)-C(105)	1.502(10)
C(105)-C(106)	1.516(9)
C(106)-C(106)#3	1.278(16)
N(6)-C(107)	1.495(7)
C(107)-C(108)	1.516(7)
C(108)-C(108)#4	1.503(11)
O(17)-C(109)	1.400(8)
O(17)-C(112)	1.427(8)
C(109)-C(110)	1.489(11)
C(110)-O(18)	1.444(10)
O(18)-C(111)	1.413(9)
C(111)-C(112)	1.490(11)
O(19)-C(116)	1.430(11)
O(19)-C(113)	1.476(9)
C(113)-C(114)	1.442(11)
C(114)-O(20)	1.396(9)
O(20)-C(115)	1.423(11)
C(115)-C(116)	1.455(15)
O(21)-C(1A0)	1.302(12)
O(21)-C(117)	1.430(9)
O(21)-C(1B0)	1.653(18)
C(117)-C(1A8)	1.446(12)
C(117)-C(1B8)	1.52(2)
C(1A8)-O(22)	1.418(11)
C(1B8)-O(22)	1.24(2)
O(22)-C(119)	1.458(11)
C(119)-C(1B0)	1.213(17)
C(119)-C(1A0)	1.542(16)
O(23)-C(122)	1.406(12)
O(23)-C(123)	1.676(17)
C(122)-C(123)#5	1.47(2)
C(123)-C(122)#5	1.47(2)

O(1)-Al(1)-O(5)	112.79(16)
O(1)-Al(1)-O(16)	107.43(16)
O(5)-Al(1)-O(16)	111.10(16)
O(1)-Al(1)-O(4)	113.00(15)
O(5)-Al(1)-O(4)	106.67(16)
O(16)-Al(1)-O(4)	105.66(14)
O(1)-Al(2)-O(7)	114.61(18)
O(1)-Al(2)-O(8)	108.71(19)
O(7)-Al(2)-O(8)	111.10(19)
O(1)-Al(2)-O(2)	108.90(14)
O(7)-Al(2)-O(2)	106.02(17)
O(8)-Al(2)-O(2)	107.21(18)
O(3)-Al(3)-O(11)	112.20(16)
O(3)-Al(3)-O(10)	109.65(17)
O(11)-Al(3)-O(10)	111.24(17)
O(3)-Al(3)-O(2)	113.58(15)
O(11)-Al(3)-O(2)	104.06(16)
O(10)-Al(3)-O(2)	105.85(16)
O(3)-Al(4)-O(13)	115.44(16)
O(3)-Al(4)-O(14)	108.13(17)
O(13)-Al(4)-O(14)	109.33(15)
O(3)-Al(4)-O(4)	108.15(14)
O(13)-Al(4)-O(4)	106.95(16)
O(14)-Al(4)-O(4)	108.67(15)
O(5)-Si(1)-O(6)	114.53(18)
O(5)-Si(1)-C(7)	109.4(3)
O(6)-Si(1)-C(7)	106.6(2)
O(5)-Si(1)-C(1)	111.3(2)
O(6)-Si(1)-C(1)	106.22(19)
C(7)-Si(1)-C(1)	108.6(3)
O(7)-Si(2)-O(6)	114.58(18)
O(7)-Si(2)-C(19)	110.6(2)
O(6)-Si(2)-C(19)	108.1(2)
O(7)-Si(2)-C(13)	109.1(2)
O(6)-Si(2)-C(13)	106.46(19)

C(19)-Si(2)-C(13)	107.7(2)
O(8)-Si(3)-O(9)	112.99(18)
O(8)-Si(3)-C(25)	111.6(2)
O(9)-Si(3)-C(25)	107.4(2)
O(8)-Si(3)-C(31)	110.2(2)
O(9)-Si(3)-C(31)	107.2(2)
C(25)-Si(3)-C(31)	107.3(2)
O(10)-Si(4)-O(9)	112.46(18)
O(10)-Si(4)-C(37)	110.5(2)
O(9)-Si(4)-C(37)	105.6(2)
O(10)-Si(4)-C(43)	111.8(2)
O(9)-Si(4)-C(43)	108.1(2)
C(37)-Si(4)-C(43)	108.1(2)
O(11)-Si(5)-O(12)	114.08(18)
O(11)-Si(5)-C(55)	107.8(2)
O(12)-Si(5)-C(55)	106.9(2)
O(11)-Si(5)-C(49)	108.7(2)
O(12)-Si(5)-C(49)	108.58(19)
C(55)-Si(5)-C(49)	110.8(2)
O(13)-Si(6)-O(12)	112.60(19)
O(13)-Si(6)-C(61)	112.12(19)
O(12)-Si(6)-C(61)	104.85(19)
O(13)-Si(6)-C(67)	109.7(2)
O(12)-Si(6)-C(67)	109.3(2)
C(61)-Si(6)-C(67)	108.1(2)
O(14)-Si(7)-O(15)	112.65(16)
O(14)-Si(7)-C(79)	111.1(2)
O(15)-Si(7)-C(79)	108.91(18)
O(14)-Si(7)-C(73)	109.90(19)
O(15)-Si(7)-C(73)	105.53(19)
C(79)-Si(7)-C(73)	108.56(19)
O(16)-Si(8)-O(15)	114.23(17)
O(16)-Si(8)-C(85)	108.79(17)
O(15)-Si(8)-C(85)	105.81(19)
O(16)-Si(8)-C(91)	110.65(19)
O(15)-Si(8)-C(91)	108.25(18)
C(85)-Si(8)-C(91)	108.9(2)
Al(2)-O(1)-Al(1)	142.7(2)
Al(3)-O(2)-Al(2)	131.55(18)
Al(3)-O(3)-Al(4)	142.7(2)
Al(1)-O(4)-Al(4)	129.13(19)
Si(1)-O(5)-Al(1)	148.1(2)
Si(2)-O(6)-Si(1)	151.9(2)
Si(2)-O(7)-Al(2)	153.6(2)
Si(3)-O(8)-Al(2)	149.2(2)
Si(3)-O(9)-Si(4)	158.2(3)
Si(4)-O(10)-Al(3)	139.6(2)
Si(5)-O(11)-Al(3)	152.0(2)
Si(6)-O(12)-Si(5)	151.0(2)
Si(6)-O(13)-Al(4)	146.3(2)
Si(7)-O(14)-Al(4)	157.2(2)
Si(8)-O(15)-Si(7)	144.6(2)
Si(8)-O(16)-Al(1)	145.3(2)
C(2)-C(1)-C(6)	116.3(4)
C(2)-C(1)-Si(1)	122.2(3)
C(6)-C(1)-Si(1)	121.4(4)
C(1)-C(2)-C(3)	122.3(4)
C(4)-C(3)-C(2)	119.3(5)
C(3)-C(4)-C(5)	119.8(5)
C(6)-C(5)-C(4)	120.6(5)
C(5)-C(6)-C(1)	121.6(5)
C(8B)-C(7)-C(12A)	70.8(10)
C(8B)-C(7)-C(8A)	37.0(7)
C(12A)-C(7)-C(8A)	106.9(11)
C(8B)-C(7)-C(12B)	114.4(9)
C(12A)-C(7)-C(12B)	65.9(9)
C(8A)-C(7)-C(12B)	124.9(8)
C(8B)-C(7)-Si(1)	134.1(8)
C(12A)-C(7)-Si(1)	130.6(10)
C(8A)-C(7)-Si(1)	111.7(7)
C(12B)-C(7)-Si(1)	111.5(6)
C(9A)-C(8A)-C(7)	120.7(13)
C(10)-C(9A)-C(8A)	106.0(15)
C(9A)-C(10)-C(11A)	143.9(16)
C(9A)-C(10)-C(9B)	126.0(11)
C(11A)-C(10)-C(9B)	59.7(10)
C(9A)-C(10)-C(8B)	63.6(10)

C(11A)-C(10)-C(8B)	80.5(12)
C(9B)-C(10)-C(8B)	107.4(9)
C(10)-C(11A)-C(12A)	107.3(18)
C(7)-C(12A)-C(11A)	129.5(18)
C(7)-C(8B)-C(10)	130.8(10)
C(11B)-C(9B)-C(10)	128.3(12)
C(9B)-C(11B)-C(12B)	120.6(11)
C(11B)-C(12B)-C(7)	118.4(9)
C(18)-C(13)-C(14)	116.2(4)
C(18)-C(13)-Si(2)	123.8(4)
C(14)-C(13)-Si(2)	119.8(4)
C(15)-C(14)-C(13)	121.8(5)
C(16)-C(15)-C(14)	119.2(6)
C(17)-C(16)-C(15)	120.7(5)
C(16)-C(17)-C(18)	119.1(6)
C(13)-C(18)-C(17)	122.8(5)
C(24)-C(19)-C(20)	117.1(6)
C(24)-C(19)-Si(2)	124.1(5)
C(20)-C(19)-Si(2)	118.8(5)
C(21)-C(20)-C(19)	118.5(8)
C(22)-C(21)-C(20)	120.8(8)
C(23)-C(22)-C(21)	119.9(8)
C(22)-C(23)-C(24)	121.3(9)
C(19)-C(24)-C(23)	122.1(7)
C(30)-C(25)-C(26)	117.3(5)
C(30)-C(25)-Si(3)	122.1(4)
C(26)-C(25)-Si(3)	120.0(4)
C(27)-C(26)-C(25)	120.8(6)
C(26)-C(27)-C(28)	120.8(6)
C(29)-C(28)-C(27)	118.9(5)
C(28)-C(29)-C(30)	120.6(6)
C(29)-C(30)-C(25)	121.6(5)
C(36)-C(31)-C(32)	117.1(6)
C(36)-C(31)-Si(3)	119.6(5)
C(32)-C(31)-Si(3)	123.1(4)
C(33)-C(32)-C(31)	121.7(6)
C(34)-C(33)-C(32)	120.0(8)
C(33)-C(34)-C(35)	120.1(8)
C(34)-C(35)-C(36)	120.3(7)
C(35)-C(36)-C(31)	120.9(7)
C(38)-C(37)-C(42)	117.3(6)
C(38)-C(37)-Si(4)	122.6(4)
C(42)-C(37)-Si(4)	119.9(4)
C(37)-C(38)-C(39)	121.9(6)
C(40)-C(39)-C(38)	118.3(7)
C(41)-C(40)-C(39)	121.4(8)
C(40)-C(41)-C(42)	120.7(7)
C(37)-C(42)-C(41)	120.3(6)
C(48)-C(43)-C(44)	117.1(5)
C(48)-C(43)-Si(4)	122.5(5)
C(44)-C(43)-Si(4)	120.4(4)
C(45)-C(44)-C(43)	121.0(6)
C(46)-C(45)-C(44)	120.0(7)
C(47)-C(46)-C(45)	120.7(6)
C(46)-C(47)-C(48)	119.3(6)
C(43)-C(48)-C(47)	121.9(6)
C(50)-C(49)-C(54)	116.9(5)
C(50)-C(49)-Si(5)	123.8(4)
C(54)-C(49)-Si(5)	119.3(3)
C(51)-C(50)-C(49)	121.5(5)
C(52)-C(51)-C(50)	120.1(5)
C(51)-C(52)-C(53)	120.3(5)
C(52)-C(53)-C(54)	119.7(5)
C(53)-C(54)-C(49)	121.4(5)
C(56)-C(55)-C(60)	118.7(5)
C(56)-C(55)-Si(5)	123.8(4)
C(60)-C(55)-Si(5)	117.4(4)
C(55)-C(56)-C(57)	120.0(7)
C(58)-C(57)-C(56)	120.6(8)
C(57)-C(58)-C(59)	120.5(7)
C(58)-C(59)-C(60)	120.2(8)
C(59)-C(60)-C(55)	119.9(7)
C(66)-C(61)-C(62)	116.6(4)
C(66)-C(61)-Si(6)	119.6(3)
C(62)-C(61)-Si(6)	123.6(4)
C(63)-C(62)-C(61)	121.5(5)
C(62)-C(63)-C(64)	119.4(5)

C(65)-C(64)-C(63)	120.9(5)
C(64)-C(65)-C(66)	118.9(5)
C(65)-C(66)-C(61)	122.8(5)
C(68)-C(67)-C(72)	117.0(5)
C(68)-C(67)-Si(6)	121.3(4)
C(72)-C(67)-Si(6)	121.5(4)
C(69)-C(68)-C(67)	121.2(5)
C(70)-C(69)-C(68)	120.6(6)
C(69)-C(70)-C(71)	118.8(6)
C(72)-C(71)-C(70)	120.4(6)
C(71)-C(72)-C(67)	121.9(6)
C(74)-C(73)-C(78)	116.4(5)
C(74)-C(73)-Si(7)	123.6(4)
C(78)-C(73)-Si(7)	120.0(4)
C(73)-C(74)-C(75)	121.4(5)
C(76)-C(75)-C(74)	120.8(5)
C(75)-C(76)-C(77)	119.4(5)
C(76)-C(77)-C(78)	119.8(5)
C(77)-C(78)-C(73)	122.2(5)
C(84)-C(79)-C(80)	118.0(4)
C(84)-C(79)-Si(7)	121.7(3)
C(80)-C(79)-Si(7)	120.2(4)
C(81)-C(80)-C(79)	121.4(5)
C(82)-C(81)-C(80)	120.1(5)
C(81)-C(82)-C(83)	119.8(5)
C(82)-C(83)-C(84)	120.0(5)
C(79)-C(84)-C(83)	120.6(5)
C(86)-C(85)-C(90)	117.0(4)
C(86)-C(85)-Si(8)	122.7(3)
C(90)-C(85)-Si(8)	120.2(3)
C(87)-C(86)-C(85)	121.8(4)
C(86)-C(87)-C(88)	120.8(5)
C(89)-C(88)-C(87)	118.9(5)
C(90)-C(89)-C(88)	120.0(4)
C(89)-C(90)-C(85)	121.6(4)
C(92)-C(91)-C(96)	116.6(4)
C(92)-C(91)-Si(8)	121.9(4)
C(96)-C(91)-Si(8)	121.4(3)
C(93)-C(92)-C(91)	121.6(5)
C(94)-C(93)-C(92)	121.0(5)
C(93)-C(94)-C(95)	118.8(5)
C(96)-C(95)-C(94)	120.4(5)
C(95)-C(96)-C(91)	121.5(4)
N(1)-C(97)-C(98)	111.8(5)
C(99)-C(98)-C(97)	113.7(5)
C(98)-C(99)-C(100)	113.0(5)
N(2)-C(100)-C(99)	112.6(5)
N(3)-C(101)-C(102)	114.4(4)
C(101)-C(102)-C(102)#1	111.0(5)
N(4)-C(103)-C(104)	112.8(4)
C(103)-C(104)-C(104)#2	110.4(5)
N(5)-C(105)-C(106)	115.3(7)
C(106)#3-C(106)-C(105)	124.0(12)
N(6)-C(107)-C(108)	114.6(4)
C(108)#4-C(108)-C(107)	113.7(5)
C(109)-O(17)-C(112)	109.0(5)
O(17)-C(109)-C(110)	112.0(7)
O(18)-C(110)-C(109)	109.4(6)
C(111)-O(18)-C(110)	109.4(6)
O(18)-C(111)-C(112)	111.4(6)
O(17)-C(112)-C(111)	110.9(7)
C(116)-O(19)-C(113)	108.5(7)
C(114)-C(113)-O(19)	111.8(7)
O(20)-C(114)-C(113)	111.7(8)
C(114)-O(20)-C(115)	110.0(6)
O(20)-C(115)-C(116)	112.2(11)
O(19)-C(116)-C(115)	112.7(9)
C(1A0)-O(21)-C(117)	110.6(8)
C(1A0)-O(21)-C(1B0)	42.7(8)
C(117)-O(21)-C(1B0)	112.6(8)
O(21)-C(117)-C(1A8)	113.4(8)
O(21)-C(117)-C(1B8)	115.3(12)
C(1A8)-C(117)-C(1B8)	42.8(9)
O(22)-C(1A8)-C(117)	109.3(8)
O(22)-C(1B8)-C(117)	115.0(15)
C(1B8)-O(22)-C(1A8)	47.5(10)
C(1B8)-O(22)-C(119)	117.4(15)

C(1A8)-O(22)-C(119)	110.8(7)
C(1B0)-C(119)-O(22)	124.3(13)
C(1B0)-C(119)-C(1A0)	46.3(9)
O(22)-C(119)-C(1A0)	109.0(10)
O(21)-C(1A0)-C(119)	112.3(9)
C(119)-C(1B0)-O(21)	110.3(13)
C(122)-O(23)-C(123)	121.8(10)
O(23)-C(122)-C(123)#5	108.1(17)
C(122)#5-C(123)-O(23)	112.9(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x,-y,-z #3 -x+1,-y+1,-z+1
#4 -x+1,-y,-z #5 -x,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2338. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	28(1)	18(1)	12(1)	3(1)	4(1)	11(1)
Al(2)	30(1)	31(1)	10(1)	4(1)	5(1)	20(1)
Al(3)	25(1)	22(1)	13(1)	3(1)	4(1)	14(1)
Al(4)	22(1)	16(1)	12(1)	2(1)	2(1)	9(1)
Si(1)	24(1)	26(1)	19(1)	10(1)	8(1)	14(1)
Si(2)	37(1)	30(1)	15(1)	10(1)	11(1)	21(1)
Si(3)	39(1)	41(1)	17(1)	-6(1)	-3(1)	26(1)
Si(4)	32(1)	33(1)	19(1)	-1(1)	2(1)	20(1)
Si(5)	31(1)	19(1)	19(1)	5(1)	4(1)	14(1)
Si(6)	27(1)	18(1)	17(1)	1(1)	1(1)	10(1)
Si(7)	24(1)	20(1)	14(1)	6(1)	7(1)	11(1)
Si(8)	24(1)	18(1)	14(1)	5(1)	5(1)	10(1)
O(1)	32(2)	20(2)	11(1)	1(1)	-1(1)	12(2)
O(2)	38(2)	32(2)	14(1)	9(1)	10(1)	25(2)
O(3)	28(2)	27(2)	12(1)	6(1)	6(1)	14(2)
O(4)	26(2)	19(2)	13(1)	0(1)	3(1)	10(2)
O(5)	39(2)	27(2)	18(2)	7(1)	10(1)	20(2)
O(6)	46(2)	45(2)	20(2)	17(2)	15(2)	32(2)
O(7)	53(3)	47(2)	28(2)	24(2)	26(2)	38(2)
O(8)	43(2)	56(3)	21(2)	-12(2)	-5(2)	33(2)
O(9)	36(2)	40(2)	17(2)	-5(1)	-2(2)	23(2)
O(10)	29(2)	31(2)	17(2)	2(1)	6(1)	17(2)
O(11)	34(2)	22(2)	20(2)	3(1)	5(1)	15(2)
O(12)	36(2)	25(2)	32(2)	3(1)	-4(2)	16(2)
O(13)	27(2)	18(2)	18(1)	1(1)	4(1)	9(2)
O(14)	33(2)	25(2)	17(1)	10(1)	12(1)	17(2)
O(15)	24(2)	19(2)	18(1)	4(1)	6(1)	10(2)
O(16)	29(2)	19(2)	13(1)	4(1)	3(1)	10(2)
C(1)	35(3)	30(3)	21(2)	6(2)	8(2)	20(3)
C(2)	37(3)	22(3)	27(2)	0(2)	10(2)	12(2)
C(3)	41(4)	31(3)	43(3)	9(2)	17(3)	19(3)
C(4)	56(4)	42(4)	39(3)	-1(3)	8(3)	33(3)
C(5)	81(5)	75(5)	32(3)	6(3)	16(3)	61(5)
C(6)	62(4)	53(4)	27(3)	15(2)	20(3)	41(4)
C(7)	27(3)	37(4)	101(6)	40(4)	4(4)	13(3)
C(13)	22(3)	25(3)	14(2)	6(2)	6(2)	11(2)
C(14)	36(3)	52(4)	36(3)	-1(3)	4(3)	25(3)
C(15)	44(4)	65(5)	32(3)	-9(3)	-9(3)	30(4)
C(16)	83(6)	73(5)	19(3)	-1(3)	3(3)	49(5)
C(17)	55(4)	51(4)	31(3)	10(3)	21(3)	28(3)
C(18)	34(3)	43(3)	26(2)	0(2)	10(2)	17(3)
C(19)	51(4)	34(3)	18(2)	5(2)	2(2)	23(3)
C(20)	57(5)	41(4)	82(5)	-15(4)	-7(4)	26(4)
C(21)	88(7)	32(4)	121(7)	-12(4)	-27(6)	31(5)
C(22)	99(7)	35(4)	55(4)	14(3)	6(5)	17(5)
C(23)	105(7)	39(4)	83(6)	3(4)	53(5)	13(5)
C(24)	71(6)	46(4)	80(5)	-4(4)	42(4)	19(4)
C(25)	34(3)	39(3)	20(2)	-6(2)	1(2)	21(3)
C(26)	40(4)	43(3)	22(2)	1(2)	-1(2)	17(3)
C(27)	39(4)	51(4)	24(3)	2(2)	-2(2)	24(3)
C(28)	62(4)	38(3)	28(3)	1(2)	5(3)	31(3)
C(29)	58(4)	27(3)	39(3)	-1(2)	22(3)	14(3)
C(30)	32(3)	33(3)	32(3)	-7(2)	6(2)	14(3)
C(31)	50(4)	42(3)	16(2)	-4(2)	-9(2)	29(3)
C(32)	54(4)	50(4)	39(3)	9(3)	4(3)	33(4)
C(33)	68(5)	59(5)	62(4)	27(4)	15(4)	27(4)
C(34)	95(7)	47(5)	76(5)	14(4)	8(5)	35(5)
C(35)	101(7)	48(5)	55(4)	0(3)	5(4)	47(5)
C(36)	60(4)	49(4)	32(3)	0(3)	1(3)	35(4)
C(37)	35(3)	32(3)	29(3)	-1(2)	-2(2)	20(3)
C(38)	33(4)	70(5)	39(3)	9(3)	10(3)	20(3)
C(39)	52(5)	125(8)	58(5)	26(5)	28(4)	37(5)
C(40)	31(4)	90(7)	93(6)	37(5)	13(4)	10(4)
C(41)	33(4)	51(5)	86(6)	2(4)	-15(4)	13(4)
C(42)	44(4)	43(4)	47(3)	-11(3)	-13(3)	22(3)
C(43)	38(3)	44(3)	29(3)	6(2)	1(2)	26(3)
C(44)	76(5)	48(4)	42(3)	-1(3)	-8(3)	37(4)
C(45)	91(6)	47(4)	64(5)	7(3)	-3(4)	42(5)
C(46)	94(7)	72(6)	69(5)	40(4)	20(5)	55(5)
C(47)	93(6)	89(6)	39(3)	30(4)	21(4)	66(5)
C(48)	88(6)	75(5)	40(3)	25(3)	28(4)	64(5)

C(49)	35(3)	22(3)	18(2)	7(2)	4(2)	17(2)
C(50)	44(3)	22(3)	26(2)	5(2)	9(2)	18(3)
C(51)	63(4)	26(3)	34(3)	8(2)	23(3)	26(3)
C(52)	51(4)	35(3)	31(3)	8(2)	23(3)	24(3)
C(53)	39(3)	30(3)	34(3)	7(2)	16(2)	16(3)
C(54)	42(3)	32(3)	21(2)	3(2)	9(2)	21(3)
C(55)	44(3)	24(3)	35(3)	12(2)	20(2)	22(3)
C(56)	53(5)	34(4)	78(5)	24(3)	29(4)	18(3)
C(57)	81(7)	37(4)	129(8)	25(5)	71(6)	13(4)
C(58)	147(9)	48(5)	75(5)	40(4)	80(6)	60(6)
C(59)	151(9)	65(5)	47(4)	35(4)	47(5)	74(6)
C(60)	74(5)	46(4)	43(3)	26(3)	25(3)	36(4)
C(61)	29(3)	26(3)	13(2)	-3(2)	-1(2)	16(2)
C(62)	27(3)	28(3)	22(2)	5(2)	8(2)	10(2)
C(63)	28(3)	50(4)	19(2)	3(2)	4(2)	17(3)
C(64)	28(3)	49(4)	32(3)	-11(2)	8(2)	11(3)
C(65)	28(3)	28(3)	45(3)	-10(2)	9(3)	9(3)
C(66)	31(3)	25(3)	37(3)	2(2)	7(2)	12(3)
C(67)	31(3)	22(3)	25(2)	10(2)	8(2)	9(2)
C(68)	35(3)	25(3)	31(3)	2(2)	10(2)	8(3)
C(69)	32(3)	36(3)	46(3)	4(3)	17(3)	0(3)
C(70)	57(5)	83(6)	44(4)	4(4)	33(4)	0(4)
C(71)	70(6)	99(6)	24(3)	11(3)	23(3)	12(5)
C(72)	41(4)	55(4)	22(3)	6(2)	6(3)	3(3)
C(73)	25(3)	29(3)	13(2)	7(2)	5(2)	15(2)
C(74)	35(3)	32(3)	23(2)	11(2)	10(2)	18(3)
C(75)	28(3)	32(3)	35(3)	4(2)	10(2)	7(3)
C(76)	26(3)	44(4)	39(3)	11(3)	14(2)	12(3)
C(77)	41(3)	47(4)	30(3)	17(2)	19(2)	29(3)
C(78)	35(3)	27(3)	23(2)	8(2)	10(2)	16(2)
C(79)	26(3)	24(3)	15(2)	3(2)	8(2)	12(2)
C(80)	31(3)	28(3)	23(2)	5(2)	5(2)	13(2)
C(81)	44(4)	44(3)	16(2)	8(2)	5(2)	23(3)
C(82)	28(3)	51(4)	19(2)	-2(2)	1(2)	21(3)
C(83)	20(3)	34(3)	29(3)	-5(2)	8(2)	5(2)
C(84)	34(3)	31(3)	20(2)	3(2)	11(2)	19(3)
C(85)	24(3)	19(2)	16(2)	6(2)	4(2)	9(2)
C(86)	34(3)	24(3)	17(2)	5(2)	6(2)	12(2)
C(87)	67(4)	21(3)	29(3)	10(2)	12(3)	20(3)
C(88)	58(4)	19(3)	41(3)	4(2)	12(3)	18(3)
C(89)	49(4)	29(3)	29(3)	2(2)	14(3)	19(3)
C(90)	34(3)	21(3)	23(2)	5(2)	9(2)	11(2)
C(91)	24(3)	19(2)	15(2)	1(2)	3(2)	9(2)
C(92)	32(3)	40(3)	17(2)	6(2)	5(2)	20(3)
C(93)	35(3)	47(4)	18(2)	0(2)	1(2)	20(3)
C(94)	25(3)	48(4)	22(2)	-6(2)	-3(2)	13(3)
C(95)	26(3)	35(3)	30(3)	1(2)	10(2)	9(3)
C(96)	30(3)	24(3)	23(2)	4(2)	7(2)	13(2)
N(1)	42(3)	25(2)	31(2)	1(2)	0(2)	12(2)
C(97)	48(4)	35(3)	42(3)	14(3)	6(3)	13(3)
C(98)	53(4)	71(5)	36(3)	20(3)	16(3)	36(4)
C(99)	59(5)	43(4)	41(3)	5(3)	6(3)	24(4)
C(100)	51(4)	34(3)	34(3)	8(2)	9(3)	11(3)
N(2)	32(3)	30(2)	20(2)	9(2)	8(2)	11(2)
N(3)	99(5)	61(4)	37(3)	31(2)	38(3)	64(4)
C(101)	52(4)	36(3)	24(2)	16(2)	15(2)	27(3)
C(102)	56(4)	29(3)	23(2)	11(2)	10(3)	21(3)
N(4)	21(2)	31(2)	32(2)	-3(2)	6(2)	6(2)
C(103)	28(3)	20(3)	28(2)	2(2)	8(2)	5(2)
C(104)	20(3)	29(3)	34(3)	1(2)	4(2)	6(2)
N(5)	71(5)	79(5)	62(4)	-22(3)	-6(3)	55(4)
C(105)	85(6)	107(7)	44(4)	-2(4)	3(4)	79(6)
C(106)	144(10)	238(14)	53(5)	-20(6)	-8(5)	168(11)
N(6)	32(3)	34(3)	40(3)	9(2)	12(2)	13(2)
C(107)	28(3)	31(3)	33(3)	12(2)	13(2)	15(3)
C(108)	33(3)	36(3)	32(3)	14(2)	14(2)	19(3)
O(17)	81(4)	98(4)	58(3)	33(3)	39(3)	59(4)
C(109)	60(5)	70(5)	50(4)	10(3)	15(4)	34(4)
C(110)	50(5)	89(7)	61(5)	-24(4)	6(4)	1(5)
O(18)	108(5)	89(4)	56(3)	25(3)	44(3)	49(4)
C(111)	128(8)	93(7)	54(4)	21(4)	36(5)	79(7)
C(112)	83(6)	87(6)	65(5)	22(4)	34(4)	58(5)
O(19)	48(3)	59(3)	69(3)	-2(3)	-2(3)	8(3)
C(113)	59(6)	68(6)	87(6)	20(5)	3(5)	9(5)
C(114)	72(6)	53(5)	54(4)	-2(4)	4(4)	7(4)
O(20)	152(7)	69(4)	62(3)	-30(3)	-42(4)	61(4)
C(115)	213(16)	60(7)	146(10)	-25(7)	-112(10)	53(9)

C(116)	102(9)	85(8)	197(13)	-28(8)	-61(9)	58(7)
O(21)	126(6)	85(5)	119(5)	50(4)	70(5)	73(5)
C(117)	86(6)	93(7)	66(5)	22(4)	37(5)	58(6)
C(1A8)	56(7)	48(6)	62(6)	9(5)	20(5)	28(5)
C(1B8)	61(16)	53(14)	28(10)	13(9)	34(11)	-5(12)
O(22)	148(7)	98(5)	66(4)	6(3)	39(4)	77(5)
C(119)	113(9)	124(10)	91(7)	15(6)	43(6)	72(8)
C(1A0)	95(11)	97(11)	20(5)	-4(6)	-8(6)	72(10)
C(1B0)	59(12)	38(9)	44(9)	15(7)	27(8)	14(9)
O(23)	122(7)	120(7)	150(7)	15(5)	39(6)	64(6)
C(122)	260(20)	550(40)	44(7)	63(12)	9(9)	300(20)
C(123)	195(16)	350(20)	103(10)	-66(12)	-73(10)	200(17)

sh2072

Table 1. Crystal data and structure refinement for sh2072.

Identification code	sh2072	
Empirical formula	C135.50 H147 Al4 N2 O20 Si8	
Formula weight	2456.19	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.405(3) Å	α= 110.69(3)°.
	b = 18.160(4) Å	β= 97.91(3)°.
	c = 25.165(5) Å	γ = 91.98(3)°.
Volume	7340(3) $Å^3$	
Z	2	
Density (calculated)	1.111 Mg/m^3	
Absorption coefficient	0.156 mm^{-1}	
F(000)	2596	
Crystal size	0.53 x 0.4 x 0.23 mm^3	
Theta range for data collection	1.95 to 24.04°.	
Index ranges	-19<=h<=18, -20<=k<=20, -28<=l<=28	
Reflections collected	46726	
Independent reflections	21490 [R(int) = 0.1140]	
Completeness to theta = 24.04°	92.8 %	
Absorption correction	N/A	
Refinement method	Full-matrix-block least-squares on F^2	
Data / restraints / parameters	21490 / 0 / 1497	
Goodness-of-fit on F^2	1.893	
Final R indices [I>2sigma(I)]	R1 = 0.1216, wR2 = 0.3022	
R indices (all data)	R1 = 0.1695, wR2 = 0.3184	
Largest diff. peak and hole	1.677 and -0.646 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2072. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	6431(1)	4778(1)	3015(1)	24(1)
Al(2)	5917(1)	3501(1)	1712(1)	23(1)
Al(3)	7566(2)	2777(1)	1787(1)	25(1)
Al(4)	8192(1)	4352(1)	2928(1)	25(1)
Si(1)	4836(1)	4147(1)	3327(1)	27(1)
Si(2)	4232(1)	3129(1)	2030(1)	28(1)
Si(3)	5973(1)	3202(1)	383(1)	27(1)
Si(4)	7170(1)	1979(1)	467(1)	29(1)
Si(5)	8589(1)	1776(1)	2415(1)	29(1)
Si(6)	9345(2)	3331(1)	3424(1)	30(1)
Si(7)	8516(2)	6167(1)	3037(1)	31(1)
Si(8)	7192(2)	6485(1)	3761(1)	31(1)
O(1)	6127(3)	4482(3)	2250(2)	25(1)
O(2)	6602(3)	2900(3)	1867(2)	27(1)
O(3)	8134(3)	3703(3)	2183(2)	28(1)
O(4)	7269(3)	4342(3)	3130(2)	28(1)
O(5)	5707(3)	4432(3)	3302(2)	33(1)
O(6)	4422(3)	3438(3)	2735(2)	34(1)
O(7)	5006(3)	3133(3)	1755(2)	33(1)
O(8)	5963(3)	3613(3)	1058(2)	30(1)
O(9)	6514(3)	2473(3)	242(2)	31(1)
O(10)	7690(3)	2500(3)	1068(2)	32(1)
O(11)	7903(3)	2105(3)	2093(2)	32(1)
O(12)	8975(3)	2428(3)	3032(2)	35(1)
O(13)	8776(3)	3977(3)	3366(2)	32(1)
O(14)	8563(4)	5244(3)	2939(2)	37(2)
O(15)	8014(4)	6604(3)	3545(2)	39(2)
O(16)	6582(3)	5801(3)	3288(2)	31(1)
C(1)	4223(5)	4985(5)	3488(3)	34(2)
C(2)	3496(6)	4939(5)	3628(4)	46(2)
C(3)	3035(6)	5578(7)	3758(5)	65(3)
C(4)	3310(7)	6288(7)	3746(5)	71(3)
C(5)	4033(8)	6365(6)	3607(5)	71(4)
C(6)	4499(6)	5743(5)	3488(4)	52(3)
C(7)	4843(6)	3716(5)	3905(3)	36(2)
C(8)	5262(6)	4125(5)	4448(3)	39(2)
C(9)	5318(6)	3802(6)	4879(4)	54(3)
C(10)	4939(7)	3080(6)	4773(4)	63(3)
C(11)	4490(7)	2664(6)	4237(4)	60(3)
C(12)	4452(6)	2979(5)	3814(4)	47(3)
C(13)	3504(5)	3760(5)	1834(3)	39(2)
C(14)	2774(7)	3459(7)	1550(5)	70(3)
C(15)	2226(9)	4016(13)	1453(7)	124(7)
C(16)	2416(11)	4777(9)	1641(7)	107(6)
C(17)	3161(11)	5065(9)	1917(7)	113(6)
C(18)	3684(8)	4579(6)	2018(5)	79(4)
C(19)	3744(5)	2101(4)	1761(3)	32(2)
C(20)	3237(6)	1865(6)	2061(4)	53(3)
C(21)	2793(7)	1120(6)	1820(5)	68(3)
C(22)	2879(7)	634(6)	1279(5)	62(3)
C(23)	3378(6)	832(5)	975(4)	56(3)
C(24)	3812(6)	1581(5)	1213(4)	49(3)
C(25)	4966(5)	2819(4)	3(3)	31(2)
C(26)	4792(7)	2419(5)	-603(4)	51(3)
C(27)	4042(7)	2159(5)	-880(4)	57(3)
C(28)	3430(7)	2254(5)	-579(5)	58(3)
C(29)	3573(7)	2626(6)	21(5)	61(3)
C(30)	4324(6)	2893(6)	294(4)	48(3)
C(31)	6383(5)	3931(5)	89(3)	36(2)
C(32)	5972(6)	4557(5)	79(4)	50(3)
C(33)	6263(7)	5128(6)	-104(4)	55(3)
C(34)	6947(8)	5076(6)	-293(5)	67(3)
C(35)	7368(9)	4426(8)	-321(6)	91(5)
C(36)	7061(7)	3874(6)	-119(5)	64(3)
C(37)	6621(6)	1113(4)	556(3)	37(2)
C(38)	5843(6)	1057(5)	570(5)	59(3)
C(39)	5461(8)	428(7)	650(6)	83(4)
C(40)	5904(8)	-166(6)	721(5)	69(4)
C(41)	6669(9)	-122(6)	703(5)	77(4)
C(42)	7051(7)	500(6)	628(5)	66(3)
C(43)	7810(6)	1644(5)	-105(3)	37(2)

C(44)	7589(6)	1668(5)	-659(3)	45(2)
C(45)	8078(7)	1445(6)	-1063(4)	62(3)
C(46)	8795(8)	1201(6)	-947(5)	72(4)
C(47)	8991(8)	1123(8)	-430(5)	82(4)
C(48)	8516(6)	1353(6)	-6(4)	57(3)
C(49)	8197(6)	919(5)	2582(4)	40(2)
C(50)	8171(7)	937(6)	3139(4)	58(3)
C(51)	7889(8)	304(7)	3257(5)	82(4)
C(52)	7605(8)	-391(8)	2807(6)	87(4)
C(53)	7603(8)	-435(6)	2250(5)	82(4)
C(54)	7893(7)	215(5)	2139(4)	56(3)
C(55)	9375(6)	1462(5)	1978(4)	43(2)
C(56)	9936(6)	964(6)	2104(4)	55(3)
C(57)	10563(7)	772(7)	1820(5)	71(4)
C(58)	10668(8)	1051(9)	1375(6)	92(5)
C(59)	10119(7)	1513(8)	1232(5)	80(4)
C(60)	9504(7)	1716(6)	1529(4)	57(3)
C(61)	9457(5)	3379(5)	4185(3)	35(2)
C(62)	9630(7)	2734(6)	4345(4)	53(3)
C(63)	9685(8)	2771(7)	4908(5)	80(4)
C(64)	9552(8)	3482(7)	5342(4)	75(4)
C(65)	9381(7)	4112(7)	5194(4)	65(3)
C(66)	9317(6)	4076(6)	4630(4)	50(3)
C(67)	10289(5)	3526(5)	3206(3)	39(2)
C(68)	10515(7)	4279(6)	3210(4)	58(3)
C(69)	11195(8)	4405(8)	3013(5)	76(4)
C(70)	11662(7)	3847(9)	2821(4)	80(4)
C(71)	11454(8)	3100(9)	2801(6)	96(5)
C(72)	10801(7)	2935(7)	3003(5)	68(3)
C(73)	8052(6)	6277(5)	2360(4)	39(2)
C(74)	7681(6)	5651(5)	1892(4)	46(2)
C(75)	7343(7)	5728(6)	1383(4)	68(4)
C(76)	7358(8)	6447(6)	1332(5)	80(4)
C(77)	7720(9)	7124(7)	1809(6)	93(5)
C(78)	8046(8)	7028(6)	2313(4)	69(4)
C(79)	9515(5)	6679(5)	3258(3)	33(2)
C(80)	9662(6)	7492(5)	3609(4)	51(3)
C(81)	10383(7)	7886(7)	3750(5)	73(4)
C(82)	10994(8)	7480(8)	3527(5)	86(4)
C(83)	10903(8)	6670(7)	3171(5)	73(3)
C(84)	10152(6)	6293(6)	3037(4)	54(3)
C(85)	7435(5)	6218(4)	4426(3)	34(2)
C(86)	8186(6)	6188(5)	4659(4)	46(2)
C(87)	8356(6)	5990(6)	5146(4)	56(3)
C(88)	7750(7)	5828(5)	5411(4)	53(3)
C(89)	7000(7)	5838(6)	5186(4)	51(3)
C(90)	6840(6)	6025(5)	4694(4)	42(2)
C(91)	6747(6)	7437(4)	3917(3)	37(2)
C(92)	7163(9)	8102(7)	3899(6)	93(5)
C(93)	6798(13)	8818(8)	4009(8)	131(7)
C(94)	6023(12)	8836(9)	4101(7)	116(6)
C(95)	5646(10)	8223(8)	4136(7)	112(6)
C(96)	6012(8)	7518(6)	4025(5)	75(4)
N(1)	6077(7)	1711(5)	2084(4)	75(3)
C(97)	6118(11)	1856(9)	2692(6)	128(7)
C(98)	6613(11)	2531(7)	3117(5)	106(6)
C(99)	6693(9)	2675(7)	3725(4)	84(4)
C(100)	7273(9)	3282(7)	4104(6)	90(4)
N(2)	7290(7)	4030(5)	4061(4)	74(3)
O(17)	5448(5)	5632(4)	2027(3)	74(2)
C(101)	5609(11)	6452(6)	2365(5)	104(6)
C(102)	5338(13)	6888(8)	2022(7)	136(8)
C(103)	5005(16)	6310(10)	1451(8)	193(12)
C(104)	5136(10)	5514(8)	1445(5)	95(5)
O(18)	9071(5)	4129(5)	1589(3)	73(2)
C(105)	8770(9)	4030(9)	1020(6)	97(5)
C(106)	9991(12)	3612(12)	953(8)	148(8)
C(107)	9213(13)	3535(15)	642(8)	182(11)
C(108)	9826(10)	3944(10)	1596(6)	112(5)
C(109)	8881(11)	8138(9)	713(6)	109(5)
C(110)	9021(9)	8917(10)	980(6)	101(5)
C(111)	8901(9)	9417(8)	680(5)	92(5)
C(112)	8617(8)	9122(8)	100(5)	87(4)
C(113)	8482(8)	8302(9)	-168(6)	100(5)
C(114)	8604(10)	7816(9)	144(7)	111(6)
C(115)	4608(10)	243(10)	2234(9)	116(6)
C(116)	5102(14)	-269(11)	2108(9)	143(8)

C(117)	5584(14)	-444(14)	2510(12)	172(11)
C(118)	5573(12)	4(12)	3055(11)	149(9)
C(119)	5074(14)	512(12)	3219(8)	136(8)
C(120)	4555(11)	642(10)	2803(10)	129(7)
C(121)	2203(15)	1524(14)	3440(10)	163(9)
C(122)	2672(15)	909(14)	3374(8)	159(10)
C(123)	2971(13)	729(10)	3833(10)	148(8)
C(124)	2785(16)	1172(10)	4359(9)	164(10)
C(125)	2232(16)	1776(10)	4384(8)	169(11)
C(126)	1975(15)	1911(12)	3905(8)	165(10)
C(127)	9350(20)	9526(19)	4864(15)	113(10)
C(128)	10130(20)	10340(19)	4623(14)	102(9)
C(129)	9580(20)	9910(20)	4543(14)	106(10)
O(19)	9695(15)	8705(14)	2501(10)	257(8)
C(130)	9975(14)	9557(13)	2963(9)	145(7)
C(131)	10816(16)	9757(14)	3104(10)	163(8)
C(132)	11258(15)	9032(14)	2743(10)	167(8)
C(133)	10571(15)	8325(13)	2309(10)	159(8)
C(134)	6752(16)	1886(13)	4936(9)	66(6)
O(20)	7425(14)	1855(12)	4919(9)	106(5)
C(135)	7879(17)	1215(15)	5029(11)	78(7)
C(136)	7173(19)	803(16)	5293(12)	93(8)
C(137)	6247(19)	1350(17)	5027(12)	97(8)
C(140)	2792(18)	7338(16)	2564(12)	86(8)
C(138)	3140(20)	7925(18)	3005(13)	99(9)
C(139)	3663(19)	8524(16)	2630(12)	91(8)
O(21)	3513(15)	8042(13)	2060(10)	125(6)
C(141)	2924(18)	7262(16)	2011(12)	91(8)

Table 3. Bond lengths [Å] and angles [°] for sh2072.

Al(1)-O(4)	1.723(6)
Al(1)-O(16)	1.733(5)
Al(1)-O(5)	1.738(6)
Al(1)-O(1)	1.800(5)
Al(2)-O(7)	1.731(6)
Al(2)-O(8)	1.739(5)
Al(2)-O(2)	1.740(5)
Al(2)-O(1)	1.804(5)
Al(3)-O(2)	1.730(6)
Al(3)-O(11)	1.737(5)
Al(3)-O(10)	1.744(5)
Al(3)-O(3)	1.798(6)
Al(4)-O(14)	1.713(6)
Al(4)-O(13)	1.725(6)
Al(4)-O(4)	1.752(6)
Al(4)-O(3)	1.814(5)
Si(1)-O(5)	1.603(6)
Si(1)-O(6)	1.637(5)
Si(1)-C(1)	1.846(9)
Si(1)-C(7)	1.879(8)
Si(2)-O(7)	1.599(6)
Si(2)-O(6)	1.641(5)
Si(2)-C(13)	1.868(9)
Si(2)-C(19)	1.871(8)
Si(3)-O(8)	1.598(5)
Si(3)-O(9)	1.616(5)
Si(3)-C(25)	1.859(9)
Si(3)-C(31)	1.894(9)
Si(4)-O(10)	1.600(6)
Si(4)-O(9)	1.637(5)
Si(4)-C(43)	1.884(9)
Si(4)-C(37)	1.907(9)
Si(5)-O(11)	1.601(6)
Si(5)-O(12)	1.620(5)
Si(5)-C(55)	1.852(10)
Si(5)-C(49)	1.878(9)
Si(6)-O(13)	1.593(6)
Si(6)-O(12)	1.639(6)
Si(6)-C(67)	1.864(10)
Si(6)-C(61)	1.869(8)
Si(7)-O(14)	1.612(5)
Si(7)-O(15)	1.633(6)
Si(7)-C(79)	1.858(9)
Si(7)-C(73)	1.863(9)
Si(8)-O(16)	1.613(6)
Si(8)-O(15)	1.633(7)
Si(8)-C(91)	1.855(8)
Si(8)-C(85)	1.897(9)
C(1)-C(2)	1.368(13)
C(1)-C(6)	1.443(13)
C(2)-C(3)	1.403(13)
C(3)-C(4)	1.370(16)
C(4)-C(5)	1.367(17)
C(5)-C(6)	1.383(14)
C(7)-C(8)	1.386(12)
C(7)-C(12)	1.408(12)
C(8)-C(9)	1.397(12)
C(9)-C(10)	1.368(15)
C(10)-C(11)	1.396(16)
C(11)-C(12)	1.372(13)
C(13)-C(14)	1.361(15)
C(13)-C(18)	1.402(14)
C(14)-C(15)	1.472(19)
C(15)-C(16)	1.31(2)
C(16)-C(17)	1.37(2)
C(17)-C(18)	1.349(19)
C(19)-C(20)	1.386(13)
C(19)-C(24)	1.394(11)
C(20)-C(21)	1.419(14)
C(21)-C(22)	1.369(15)
C(22)-C(23)	1.351(15)
C(23)-C(24)	1.416(14)
C(25)-C(30)	1.403(13)
C(25)-C(26)	1.420(11)
C(26)-C(27)	1.373(15)

C(27)-C(28)	1.371(15)
C(28)-C(29)	1.400(15)
C(29)-C(30)	1.374(14)
C(31)-C(36)	1.348(14)
C(31)-C(32)	1.369(12)
C(32)-C(33)	1.382(14)
C(33)-C(34)	1.336(15)
C(34)-C(35)	1.397(17)
C(35)-C(36)	1.396(15)
C(37)-C(38)	1.361(14)
C(37)-C(42)	1.411(13)
C(38)-C(39)	1.391(15)
C(39)-C(40)	1.396(17)
C(40)-C(41)	1.338(18)
C(41)-C(42)	1.374(16)
C(43)-C(48)	1.381(13)
C(43)-C(44)	1.410(12)
C(44)-C(45)	1.376(13)
C(45)-C(46)	1.367(17)
C(46)-C(47)	1.357(17)
C(47)-C(48)	1.395(14)
C(49)-C(54)	1.394(13)
C(49)-C(50)	1.398(13)
C(50)-C(51)	1.375(14)
C(51)-C(52)	1.382(18)
C(52)-C(53)	1.375(17)
C(53)-C(54)	1.399(15)
C(55)-C(60)	1.406(13)
C(55)-C(56)	1.432(13)
C(56)-C(57)	1.374(15)
C(57)-C(58)	1.410(17)
C(58)-C(59)	1.387(17)
C(59)-C(60)	1.375(14)
C(61)-C(62)	1.394(12)
C(61)-C(66)	1.418(12)
C(62)-C(63)	1.386(14)
C(63)-C(64)	1.417(17)
C(64)-C(65)	1.354(16)
C(65)-C(66)	1.386(13)
C(67)-C(68)	1.406(13)
C(67)-C(72)	1.418(13)
C(68)-C(69)	1.385(16)
C(69)-C(70)	1.320(18)
C(70)-C(71)	1.375(19)
C(71)-C(72)	1.371(18)
C(73)-C(74)	1.375(12)
C(73)-C(78)	1.409(12)
C(74)-C(75)	1.389(13)
C(75)-C(76)	1.356(15)
C(76)-C(77)	1.431(17)
C(77)-C(78)	1.387(15)
C(79)-C(84)	1.405(14)
C(79)-C(80)	1.420(12)
C(80)-C(81)	1.361(16)
C(81)-C(82)	1.384(19)
C(82)-C(83)	1.416(17)
C(83)-C(84)	1.394(16)
C(85)-C(86)	1.367(13)
C(85)-C(90)	1.409(13)
C(86)-C(87)	1.392(13)
C(87)-C(88)	1.397(15)
C(88)-C(89)	1.353(15)
C(89)-C(90)	1.391(12)
C(91)-C(96)	1.347(15)
C(91)-C(92)	1.405(15)
C(92)-C(93)	1.423(18)
C(93)-C(94)	1.40(2)
C(94)-C(95)	1.31(2)
C(95)-C(96)	1.405(16)
N(1)-C(97)	1.448(16)
C(97)-C(98)	1.461(19)
C(98)-C(99)	1.445(15)
C(99)-C(100)	1.434(18)
C(100)-N(2)	1.401(13)
O(17)-C(101)	1.424(13)
O(17)-C(104)	1.426(13)
C(101)-C(102)	1.411(16)

C(102)-C(103)	1.47(2)
C(103)-C(104)	1.467(19)
O(18)-C(108)	1.367(18)
O(18)-C(105)	1.400(15)
C(105)-C(107)	1.40(2)
C(106)-C(107)	1.44(3)
C(106)-C(108)	1.59(2)
C(109)-C(110)	1.33(2)
C(109)-C(114)	1.35(2)
C(110)-C(111)	1.376(19)
C(111)-C(112)	1.376(18)
C(112)-C(113)	1.40(2)
C(113)-C(114)	1.38(2)
C(115)-C(116)	1.28(3)
C(115)-C(120)	1.38(3)
C(116)-C(117)	1.36(3)
C(117)-C(118)	1.33(3)
C(118)-C(119)	1.29(3)
C(119)-C(120)	1.38(3)
C(121)-C(126)	1.26(3)
C(121)-C(122)	1.38(3)
C(122)-C(123)	1.35(3)
C(123)-C(124)	1.38(3)
C(124)-C(125)	1.47(3)
C(125)-C(126)	1.33(3)
C(127)-C(129)	1.33(4)
C(127)-C(128)#1	1.41(4)
C(128)-C(129)	1.16(4)
C(128)-C(127)#1	1.41(4)
O(19)-C(130)	1.58(3)
O(19)-C(133)	1.75(3)
C(130)-C(131)	1.46(3)
C(131)-C(132)	1.60(3)
C(132)-C(133)	1.68(3)
C(134)-O(20)	1.18(3)
C(134)-C(137)	1.39(4)
O(20)-C(135)	1.51(3)
C(135)-C(136)	1.74(4)
C(140)-C(138)	1.29(4)
C(140)-C(141)	1.40(3)
C(138)-C(139)	1.95(4)
C(139)-O(21)	1.37(3)
O(21)-C(141)	1.68(4)

O(4)-Al(1)-O(16)	112.1(3)
O(4)-Al(1)-O(5)	108.7(3)
O(16)-Al(1)-O(5)	112.3(3)
O(4)-Al(1)-O(1)	108.2(3)
O(16)-Al(1)-O(1)	107.0(2)
O(5)-Al(1)-O(1)	108.5(3)
O(7)-Al(2)-O(8)	113.2(3)
O(7)-Al(2)-O(2)	108.3(3)
O(8)-Al(2)-O(2)	112.7(3)
O(7)-Al(2)-O(1)	108.2(3)
O(8)-Al(2)-O(1)	105.5(3)
O(2)-Al(2)-O(1)	108.6(3)
O(2)-Al(3)-O(11)	109.3(3)
O(2)-Al(3)-O(10)	111.7(3)
O(11)-Al(3)-O(10)	112.4(3)
O(2)-Al(3)-O(3)	108.5(3)
O(11)-Al(3)-O(3)	106.9(3)
O(10)-Al(3)-O(3)	107.8(3)
O(14)-Al(4)-O(13)	113.6(3)
O(14)-Al(4)-O(4)	115.5(3)
O(13)-Al(4)-O(4)	105.2(3)
O(14)-Al(4)-O(3)	103.9(3)
O(13)-Al(4)-O(3)	109.4(3)
O(4)-Al(4)-O(3)	109.1(3)
O(5)-Si(1)-O(6)	113.3(3)
O(5)-Si(1)-C(1)	110.8(4)
O(6)-Si(1)-C(1)	109.3(4)
O(5)-Si(1)-C(7)	109.9(4)
O(6)-Si(1)-C(7)	104.9(3)
C(1)-Si(1)-C(7)	108.5(4)
O(7)-Si(2)-O(6)	111.7(3)
O(7)-Si(2)-C(13)	112.8(4)
O(6)-Si(2)-C(13)	107.7(3)

O(7)-Si(2)-C(19)	109.8(3)
O(6)-Si(2)-C(19)	108.0(3)
C(13)-Si(2)-C(19)	106.7(4)
O(8)-Si(3)-O(9)	112.0(3)
O(8)-Si(3)-C(25)	109.5(4)
O(9)-Si(3)-C(25)	108.3(3)
O(8)-Si(3)-C(31)	110.6(3)
O(9)-Si(3)-C(31)	106.6(4)
C(25)-Si(3)-C(31)	109.7(4)
O(10)-Si(4)-O(9)	112.8(3)
O(10)-Si(4)-C(43)	109.5(4)
O(9)-Si(4)-C(43)	106.3(3)
O(10)-Si(4)-C(37)	109.1(3)
O(9)-Si(4)-C(37)	106.9(4)
C(43)-Si(4)-C(37)	112.3(4)
O(11)-Si(5)-O(12)	112.1(3)
O(11)-Si(5)-C(55)	111.7(4)
O(12)-Si(5)-C(55)	108.0(4)
O(11)-Si(5)-C(49)	110.3(4)
O(12)-Si(5)-C(49)	105.2(3)
C(55)-Si(5)-C(49)	109.3(4)
O(13)-Si(6)-O(12)	112.5(3)
O(13)-Si(6)-C(67)	109.3(4)
O(12)-Si(6)-C(67)	109.4(4)
O(13)-Si(6)-C(61)	107.7(3)
O(12)-Si(6)-C(61)	105.2(3)
C(67)-Si(6)-C(61)	112.7(4)
O(14)-Si(7)-O(15)	112.0(3)
O(14)-Si(7)-C(79)	109.4(4)
O(15)-Si(7)-C(79)	107.4(3)
O(14)-Si(7)-C(73)	110.0(3)
O(15)-Si(7)-C(73)	108.4(4)
C(79)-Si(7)-C(73)	109.6(4)
O(16)-Si(8)-O(15)	113.8(3)
O(16)-Si(8)-C(91)	108.2(4)
O(15)-Si(8)-C(91)	106.4(4)
O(16)-Si(8)-C(85)	109.0(3)
O(15)-Si(8)-C(85)	107.0(4)
C(91)-Si(8)-C(85)	112.5(4)
Al(1)-O(1)-Al(2)	129.3(3)
Al(3)-O(2)-Al(2)	135.2(3)
Al(3)-O(3)-Al(4)	130.3(3)
Al(1)-O(4)-Al(4)	134.6(3)
Si(1)-O(5)-Al(1)	155.5(4)
Si(1)-O(6)-Si(2)	146.0(4)
Si(2)-O(7)-Al(2)	155.6(3)
Si(3)-O(8)-Al(2)	147.9(3)
Si(3)-O(9)-Si(4)	149.4(3)
Si(4)-O(10)-Al(3)	134.4(4)
Si(5)-O(11)-Al(3)	151.2(4)
Si(5)-O(12)-Si(6)	150.0(4)
Si(6)-O(13)-Al(4)	148.8(3)
Si(7)-O(14)-Al(4)	152.9(4)
Si(7)-O(15)-Si(8)	140.9(4)
Si(8)-O(16)-Al(1)	138.6(4)
C(2)-C(1)-C(6)	115.6(8)
C(2)-C(1)-Si(1)	123.0(7)
C(6)-C(1)-Si(1)	121.4(7)
C(1)-C(2)-C(3)	123.0(10)
C(4)-C(3)-C(2)	119.8(11)
C(5)-C(4)-C(3)	119.6(10)
C(4)-C(5)-C(6)	121.2(11)
C(5)-C(6)-C(1)	120.8(10)
C(8)-C(7)-C(12)	117.4(8)
C(8)-C(7)-Si(1)	119.5(7)
C(12)-C(7)-Si(1)	123.1(7)
C(7)-C(8)-C(9)	121.1(9)
C(10)-C(9)-C(8)	120.0(10)
C(9)-C(10)-C(11)	120.4(9)
C(12)-C(11)-C(10)	119.1(10)
C(11)-C(12)-C(7)	122.0(9)
C(14)-C(13)-C(18)	117.9(10)
C(14)-C(13)-Si(2)	122.0(8)
C(18)-C(13)-Si(2)	119.9(8)
C(13)-C(14)-C(15)	117.7(13)
C(16)-C(15)-C(14)	122.2(17)
C(15)-C(16)-C(17)	119.0(15)

C(18)-C(17)-C(16)	121.0(15)
C(17)-C(18)-C(13)	122.1(14)
C(20)-C(19)-C(24)	117.9(8)
C(20)-C(19)-Si(2)	121.9(6)
C(24)-C(19)-Si(2)	119.7(7)
C(19)-C(20)-C(21)	121.5(9)
C(22)-C(21)-C(20)	118.1(11)
C(23)-C(22)-C(21)	122.4(10)
C(22)-C(23)-C(24)	119.3(9)
C(19)-C(24)-C(23)	120.7(9)
C(30)-C(25)-C(26)	115.1(9)
C(30)-C(25)-Si(3)	122.5(6)
C(26)-C(25)-Si(3)	122.4(7)
C(27)-C(26)-C(25)	121.8(10)
C(28)-C(27)-C(26)	121.1(10)
C(27)-C(28)-C(29)	119.3(11)
C(30)-C(29)-C(28)	119.2(11)
C(29)-C(30)-C(25)	123.5(9)
C(36)-C(31)-C(32)	116.9(9)
C(36)-C(31)-Si(3)	124.1(7)
C(32)-C(31)-Si(3)	119.0(7)
C(31)-C(32)-C(33)	121.4(11)
C(34)-C(33)-C(32)	120.9(10)
C(33)-C(34)-C(35)	119.9(11)
C(34)-C(35)-C(36)	117.1(13)
C(31)-C(36)-C(35)	123.6(11)
C(38)-C(37)-C(42)	117.7(9)
C(38)-C(37)-Si(4)	124.2(7)
C(42)-C(37)-Si(4)	118.1(8)
C(37)-C(38)-C(39)	123.0(10)
C(38)-C(39)-C(40)	117.7(13)
C(41)-C(40)-C(39)	119.9(11)
C(40)-C(41)-C(42)	122.7(11)
C(41)-C(42)-C(37)	119.0(12)
C(48)-C(43)-C(44)	116.4(8)
C(48)-C(43)-Si(4)	121.7(7)
C(44)-C(43)-Si(4)	121.8(7)
C(45)-C(44)-C(43)	120.7(10)
C(46)-C(45)-C(44)	122.1(10)
C(47)-C(46)-C(45)	117.6(10)
C(46)-C(47)-C(48)	121.8(11)
C(43)-C(48)-C(47)	121.1(10)
C(54)-C(49)-C(50)	115.5(9)
C(54)-C(49)-Si(5)	120.5(7)
C(50)-C(49)-Si(5)	124.0(7)
C(51)-C(50)-C(49)	123.5(10)
C(50)-C(51)-C(52)	119.4(11)
C(53)-C(52)-C(51)	119.4(11)
C(52)-C(53)-C(54)	120.3(11)
C(49)-C(54)-C(53)	121.8(10)
C(60)-C(55)-C(56)	114.5(9)
C(60)-C(55)-Si(5)	124.4(7)
C(56)-C(55)-Si(5)	121.0(8)
C(57)-C(56)-C(55)	122.5(11)
C(56)-C(57)-C(58)	120.5(11)
C(59)-C(58)-C(57)	118.1(11)
C(60)-C(59)-C(58)	120.8(12)
C(59)-C(60)-C(55)	123.4(10)
C(62)-C(61)-C(66)	116.4(8)
C(62)-C(61)-Si(6)	123.1(6)
C(66)-C(61)-Si(6)	120.4(6)
C(63)-C(62)-C(61)	122.5(10)
C(62)-C(63)-C(64)	119.5(10)
C(65)-C(64)-C(63)	118.8(9)
C(64)-C(65)-C(66)	121.9(10)
C(65)-C(66)-C(61)	120.9(10)
C(68)-C(67)-C(72)	115.9(10)
C(68)-C(67)-Si(6)	120.6(7)
C(72)-C(67)-Si(6)	123.4(8)
C(69)-C(68)-C(67)	120.1(11)
C(70)-C(69)-C(68)	123.2(13)
C(69)-C(70)-C(71)	118.3(13)
C(72)-C(71)-C(70)	121.7(12)
C(71)-C(72)-C(67)	120.5(12)
C(74)-C(73)-C(78)	116.5(8)
C(74)-C(73)-Si(7)	122.9(6)
C(78)-C(73)-Si(7)	120.6(7)

C(73)-C(74)-C(75)	123.1(9)
C(76)-C(75)-C(74)	120.3(10)
C(75)-C(76)-C(77)	119.1(10)
C(78)-C(77)-C(76)	119.1(10)
C(77)-C(78)-C(73)	121.8(10)
C(84)-C(79)-C(80)	116.8(9)
C(84)-C(79)-Si(7)	120.9(6)
C(80)-C(79)-Si(7)	122.0(8)
C(81)-C(80)-C(79)	122.8(11)
C(80)-C(81)-C(82)	118.3(11)
C(81)-C(82)-C(83)	122.8(12)
C(84)-C(83)-C(82)	116.6(12)
C(83)-C(84)-C(79)	122.6(10)
C(86)-C(85)-C(90)	117.0(8)
C(86)-C(85)-Si(8)	122.2(7)
C(90)-C(85)-Si(8)	120.8(7)
C(85)-C(86)-C(87)	121.5(10)
C(86)-C(87)-C(88)	119.7(10)
C(89)-C(88)-C(87)	120.3(9)
C(88)-C(89)-C(90)	119.2(10)
C(89)-C(90)-C(85)	122.1(10)
C(96)-C(91)-C(92)	117.0(10)
C(96)-C(91)-Si(8)	122.5(7)
C(92)-C(91)-Si(8)	120.4(9)
C(91)-C(92)-C(93)	118.8(14)
C(94)-C(93)-C(92)	119.7(15)
C(95)-C(94)-C(93)	121.2(14)
C(94)-C(95)-C(96)	118.4(15)
C(91)-C(96)-C(95)	124.6(13)
N(1)-C(97)-C(98)	120.0(11)
C(99)-C(98)-C(97)	121.5(13)
C(100)-C(99)-C(98)	117.7(13)
N(2)-C(100)-C(99)	118.8(11)
C(101)-O(17)-C(104)	111.2(8)
C(102)-C(101)-O(17)	108.4(11)
C(101)-C(102)-C(103)	106.9(11)
C(104)-C(103)-C(102)	108.6(11)
O(17)-C(104)-C(103)	104.5(11)
C(108)-O(18)-C(105)	107.0(11)
C(107)-C(105)-O(18)	110.2(16)
C(107)-C(106)-C(108)	100.5(14)
C(105)-C(107)-C(106)	107.4(16)
O(18)-C(108)-C(106)	108.4(13)
C(110)-C(109)-C(114)	121.3(16)
C(109)-C(110)-C(111)	120.7(14)
C(110)-C(111)-C(112)	120.5(14)
C(111)-C(112)-C(113)	117.3(15)
C(114)-C(113)-C(112)	120.9(14)
C(109)-C(114)-C(113)	119.3(15)
C(116)-C(115)-C(120)	119(2)
C(115)-C(116)-C(117)	123(2)
C(118)-C(117)-C(116)	116(2)
C(119)-C(118)-C(117)	124(2)
C(118)-C(119)-C(120)	118(2)
C(119)-C(120)-C(115)	118.7(19)
C(126)-C(121)-C(122)	124(3)
C(123)-C(122)-C(121)	120(2)
C(122)-C(123)-C(124)	118(2)
C(123)-C(124)-C(125)	118(2)
C(126)-C(125)-C(124)	119.1(19)
C(121)-C(126)-C(125)	120(3)
C(129)-C(127)-C(128)#1	114(3)
C(129)-C(128)-C(127)#1	116(3)
C(128)-C(129)-C(127)	130(4)
C(130)-O(19)-C(133)	102.9(19)
C(131)-C(130)-O(19)	116(2)
C(130)-C(131)-C(132)	110(2)
C(131)-C(132)-C(133)	107(2)
C(132)-C(133)-O(19)	103.9(17)
O(20)-C(134)-C(137)	128(3)
C(134)-O(20)-C(135)	123(2)
O(20)-C(135)-C(136)	98(2)
C(138)-C(140)-C(141)	120(3)
C(140)-C(138)-C(139)	101(2)
O(21)-C(139)-C(138)	103(2)
C(139)-O(21)-C(141)	107(2)
C(140)-C(141)-O(21)	109(2)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2072. 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}
Al(1)	27(2)	20(1)	21(1)	3(1)	5(1)	4(1)
Al(2)	23(2)	22(1)	21(1)	5(1)	1(1)	4(1)
Al(3)	28(2)	22(1)	21(1)	5(1)	1(1)	7(1)
Al(4)	25(2)	23(1)	24(1)	7(1)	0(1)	3(1)
Si(1)	28(2)	30(1)	21(1)	4(1)	5(1)	1(1)
Si(2)	26(2)	29(1)	23(1)	2(1)	3(1)	0(1)
Si(3)	32(2)	27(1)	21(1)	8(1)	3(1)	9(1)
Si(4)	35(2)	27(1)	22(1)	3(1)	3(1)	11(1)
Si(5)	29(2)	26(1)	28(1)	7(1)	0(1)	7(1)
Si(6)	31(2)	30(1)	26(1)	6(1)	-2(1)	5(1)
Si(7)	35(2)	23(1)	32(1)	9(1)	-1(1)	-4(1)
Si(8)	36(2)	22(1)	28(1)	3(1)	2(1)	1(1)
O(1)	37(4)	17(2)	21(3)	5(2)	4(2)	4(2)
O(2)	20(4)	27(3)	32(3)	7(2)	6(2)	7(2)
O(3)	33(4)	27(3)	22(3)	7(2)	5(2)	2(2)
O(4)	31(4)	25(3)	27(3)	8(2)	8(2)	9(2)
O(5)	33(4)	33(3)	34(3)	8(2)	19(3)	8(3)
O(6)	38(4)	32(3)	23(3)	1(2)	-2(3)	-5(3)
O(7)	29(4)	37(3)	26(3)	5(2)	1(3)	-1(3)
O(8)	43(4)	28(3)	23(3)	12(2)	9(3)	14(3)
O(9)	30(4)	32(3)	26(3)	6(2)	4(2)	17(3)
O(10)	39(4)	27(3)	26(3)	6(2)	7(3)	10(3)
O(11)	32(4)	30(3)	32(3)	12(2)	2(3)	11(3)
O(12)	39(4)	29(3)	30(3)	8(2)	-9(3)	2(3)
O(13)	25(4)	33(3)	34(3)	11(2)	-4(3)	5(3)
O(14)	50(5)	19(3)	36(3)	7(2)	-1(3)	-6(3)
O(15)	46(5)	29(3)	39(3)	7(2)	8(3)	-4(3)
O(16)	40(4)	18(3)	27(3)	2(2)	-3(3)	-1(2)
C(1)	29(6)	42(5)	24(4)	3(4)	4(4)	1(4)
C(2)	39(7)	45(5)	47(5)	6(4)	14(5)	9(5)
C(3)	26(7)	87(9)	77(8)	17(6)	21(6)	23(6)
C(4)	64(10)	59(7)	92(9)	27(6)	18(7)	35(7)
C(5)	81(11)	39(6)	95(9)	28(6)	12(8)	17(6)
C(6)	45(8)	48(6)	62(6)	14(5)	18(5)	4(5)
C(7)	41(7)	37(5)	28(4)	11(4)	5(4)	3(4)
C(8)	39(7)	40(5)	36(5)	13(4)	2(4)	2(4)
C(9)	57(8)	75(7)	33(5)	21(5)	9(5)	24(6)
C(10)	81(10)	71(8)	58(7)	41(6)	28(7)	24(7)
C(11)	64(9)	55(6)	67(7)	30(6)	17(6)	0(6)
C(12)	52(8)	42(5)	43(5)	13(4)	2(5)	-8(5)
C(13)	32(7)	51(5)	32(4)	11(4)	10(4)	13(4)
C(14)	37(9)	74(8)	92(9)	31(7)	-14(6)	-3(6)
C(15)	36(11)	230(20)	127(14)	90(15)	-9(9)	41(12)
C(16)	147(19)	96(12)	124(14)	77(11)	56(13)	72(13)
C(17)	140(19)	75(10)	125(13)	45(9)	-3(12)	38(11)
C(18)	96(12)	46(6)	83(8)	26(6)	-35(7)	0(6)
C(19)	31(6)	25(4)	33(4)	3(4)	1(4)	0(4)
C(20)	53(8)	53(6)	45(6)	9(5)	5(5)	-8(5)
C(21)	60(9)	55(7)	86(8)	29(6)	2(7)	-18(6)
C(22)	53(9)	36(6)	76(8)	3(5)	-6(6)	-14(5)
C(23)	45(8)	38(5)	60(6)	-7(5)	-9(6)	-3(5)
C(24)	45(7)	48(6)	43(5)	1(4)	10(5)	4(5)
C(25)	36(6)	30(4)	28(4)	14(3)	-3(4)	8(4)
C(26)	64(9)	42(5)	39(5)	8(4)	-2(5)	3(5)
C(27)	66(10)	46(6)	41(6)	7(5)	-24(6)	-9(5)
C(28)	46(8)	45(6)	79(8)	28(6)	-17(6)	-7(5)
C(29)	40(8)	68(7)	71(7)	27(6)	-4(6)	-7(6)
C(30)	42(8)	60(6)	38(5)	14(5)	-1(5)	9(5)
C(31)	39(7)	49(5)	25(4)	19(4)	7(4)	7(4)
C(32)	62(8)	46(5)	54(6)	38(5)	-8(5)	15(5)
C(33)	54(9)	59(6)	57(6)	35(5)	-10(6)	6(5)
C(34)	84(11)	61(7)	72(8)	41(6)	17(7)	0(7)
C(35)	100(13)	89(10)	98(10)	42(8)	46(9)	-7(9)
C(36)	68(9)	63(7)	77(8)	39(6)	28(7)	13(6)
C(37)	56(8)	27(4)	21(4)	1(3)	5(4)	11(4)
C(38)	45(9)	33(5)	97(8)	19(5)	16(6)	9(5)
C(39)	54(10)	62(8)	140(12)	37(8)	33(9)	2(6)

C(40)	102(13)	37(6)	65(7)	20(5)	5(7)	-14(7)
C(41)	105(13)	35(6)	94(9)	39(6)	-19(8)	-4(7)
C(42)	53(9)	57(7)	95(9)	41(6)	4(7)	12(6)
C(43)	46(7)	31(4)	32(5)	5(4)	10(4)	10(4)
C(44)	58(8)	46(5)	31(5)	11(4)	10(5)	15(5)
C(45)	89(11)	60(7)	41(6)	19(5)	25(6)	13(7)
C(46)	85(11)	64(7)	67(8)	10(6)	54(8)	14(7)
C(47)	53(10)	108(10)	82(9)	18(8)	31(7)	38(8)
C(48)	54(8)	74(7)	42(5)	15(5)	13(5)	29(6)
C(49)	44(7)	30(5)	42(5)	11(4)	2(4)	5(4)
C(50)	76(9)	51(6)	54(6)	28(5)	6(6)	4(6)
C(51)	106(13)	74(8)	74(8)	48(7)	-9(8)	-23(8)
C(52)	82(11)	80(9)	126(12)	74(9)	13(9)	-5(8)
C(53)	98(12)	46(7)	88(9)	18(6)	-8(8)	-16(7)
C(54)	69(9)	38(5)	57(6)	15(5)	2(6)	-4(5)
C(55)	34(7)	39(5)	45(5)	5(4)	-3(4)	9(4)
C(56)	45(8)	50(6)	63(6)	8(5)	13(5)	20(5)
C(57)	51(9)	72(7)	78(8)	10(6)	13(6)	34(6)
C(58)	45(10)	140(13)	91(10)	33(9)	29(8)	40(9)
C(59)	56(10)	128(11)	64(7)	36(7)	29(7)	33(8)
C(60)	55(8)	76(7)	50(6)	31(5)	20(5)	25(6)
C(61)	33(6)	36(5)	31(4)	12(4)	-12(4)	3(4)
C(62)	70(9)	53(6)	32(5)	15(4)	-5(5)	4(5)
C(63)	102(12)	83(9)	67(8)	54(7)	-19(7)	1(8)
C(64)	87(11)	104(10)	35(6)	34(7)	-4(6)	-3(8)
C(65)	75(10)	77(8)	31(5)	7(5)	2(5)	12(6)
C(66)	51(8)	56(6)	34(5)	7(4)	3(5)	11(5)
C(67)	22(6)	56(6)	31(4)	10(4)	-3(4)	1(4)
C(68)	52(9)	64(7)	63(7)	33(5)	0(6)	-3(6)
C(69)	59(10)	94(9)	79(8)	37(7)	10(7)	-14(7)
C(70)	43(9)	135(13)	49(7)	13(8)	19(6)	3(9)
C(71)	39(10)	114(12)	108(11)	-3(9)	33(8)	24(8)
C(72)	35(8)	63(7)	87(8)	0(6)	20(6)	15(6)
C(73)	43(7)	29(4)	44(5)	17(4)	-11(4)	-4(4)
C(74)	52(8)	37(5)	43(5)	14(4)	-7(5)	4(5)
C(75)	92(11)	52(6)	45(6)	13(5)	-31(6)	12(6)
C(76)	101(12)	60(7)	66(7)	24(6)	-35(7)	7(7)
C(77)	119(13)	50(7)	115(10)	54(7)	-31(9)	4(7)
C(78)	112(12)	35(5)	51(6)	17(5)	-16(6)	2(6)
C(79)	33(6)	37(5)	22(4)	7(3)	-6(4)	-6(4)
C(80)	51(8)	36(5)	58(6)	13(4)	-2(5)	-15(5)
C(81)	52(10)	60(7)	88(9)	11(6)	-2(7)	-21(6)
C(82)	67(12)	98(10)	83(9)	39(8)	-22(8)	-57(8)
C(83)	53(10)	84(9)	75(8)	22(7)	11(7)	-9(7)
C(84)	39(8)	64(7)	51(6)	17(5)	-4(5)	-19(5)
C(85)	35(7)	26(4)	28(4)	-4(3)	-1(4)	-1(4)
C(86)	34(7)	56(6)	41(5)	11(4)	3(5)	0(5)
C(87)	38(8)	79(7)	52(6)	25(5)	-3(5)	17(6)
C(88)	71(9)	53(6)	32(5)	12(4)	4(5)	12(6)
C(89)	50(8)	64(6)	42(5)	28(5)	-5(5)	-3(5)
C(90)	36(7)	47(5)	41(5)	13(4)	5(4)	6(4)
C(91)	49(7)	26(4)	28(4)	-2(3)	10(4)	10(4)
C(92)	114(13)	53(7)	134(12)	45(8)	56(10)	17(7)
C(93)	200(20)	49(8)	167(17)	51(9)	69(16)	41(11)
C(94)	160(20)	76(11)	138(14)	48(10)	53(13)	67(12)
C(95)	95(14)	78(10)	176(16)	46(11)	60(12)	59(10)
C(96)	85(11)	42(6)	103(9)	23(6)	29(8)	19(6)
N(1)	121(10)	37(5)	68(6)	21(4)	18(6)	-16(5)
C(97)	175(19)	106(11)	108(12)	74(10)	-31(11)	-79(12)
C(98)	204(19)	64(8)	63(8)	31(7)	38(10)	35(10)
C(99)	146(15)	64(8)	54(7)	31(6)	20(8)	38(9)
C(100)	101(13)	82(9)	109(11)	67(9)	0(9)	1(8)
N(2)	107(10)	78(6)	55(5)	45(5)	8(5)	4(6)
O(17)	103(7)	45(4)	66(5)	22(4)	-20(4)	24(4)
C(101)	176(18)	50(7)	72(8)	17(6)	-19(9)	29(8)
C(102)	210(20)	52(8)	127(13)	35(9)	-44(13)	24(10)
C(103)	320(30)	98(13)	132(15)	67(12)	-125(18)	-38(16)
C(104)	132(15)	88(9)	60(7)	30(7)	-14(8)	27(9)
O(18)	60(7)	88(6)	71(5)	25(4)	28(5)	-3(5)
C(105)	96(14)	122(12)	80(10)	49(9)	4(9)	-25(10)
C(106)	90(18)	171(18)	152(18)	13(14)	35(14)	45(14)
C(107)	120(20)	290(30)	83(12)	5(15)	36(14)	-49(19)
C(108)	98(16)	118(13)	97(11)	23(9)	-10(10)	-24(11)
C(109)	138(17)	91(11)	89(11)	23(9)	17(11)	2(10)
C(110)	90(13)	138(14)	64(9)	26(10)	1(8)	26(11)
C(111)	91(12)	84(9)	73(9)	-8(8)	18(8)	33(8)
C(112)	77(11)	97(10)	69(8)	7(8)	12(7)	26(8)

C(113)	55(11)	137(14)	66(9)	-12(10)	3(7)	-6(9)
C(114)	104(16)	88(11)	123(15)	14(11)	22(12)	-9(10)
C(115)	86(15)	122(15)	158(18)	85(14)	-9(13)	-5(11)
C(116)	190(30)	120(16)	142(18)	41(14)	96(19)	46(16)
C(117)	150(20)	200(20)	230(30)	110(20)	110(20)	110(20)
C(118)	130(20)	160(20)	210(30)	120(20)	48(18)	74(17)
C(119)	160(20)	149(18)	100(14)	49(13)	32(16)	-33(16)
C(120)	97(17)	110(14)	190(20)	53(16)	62(17)	34(12)
C(121)	170(30)	180(30)	160(30)	80(20)	25(19)	10(20)
C(122)	200(30)	190(30)	86(14)	40(16)	41(16)	-20(20)
C(123)	160(20)	98(13)	170(20)	7(15)	71(18)	15(13)
C(124)	270(30)	84(13)	132(17)	44(13)	15(18)	-8(16)
C(125)	280(30)	93(14)	94(15)	-24(11)	57(17)	-16(16)
C(126)	250(30)	132(17)	85(13)	6(13)	12(17)	36(17)

sh2139

Table 1. Crystal data and structure refinement for sh2139.

Identification code	sh2139	
Empirical formula	C128 H132 Al4 N4 O16 Si8	
Formula weight	2315.02	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 29.148(6) Å	α= 90°.
	b = 14.500(3) Å	β= 115.12(3)°.
	c = 33.036(7) Å	γ = 90°.
Volume	12642(5) $Å^3$	
Z	4	
Density (calculated)	1.216 Mg/m^3	
Absorption coefficient	0.176 mm^{-1}	
F(000)	4880	
Crystal size	0.57 x 0.44 x 0.2 mm^3	
Theta range for data collection	1.86 to 24.02°.	
Index ranges	-30<=h<=32, -16<=k<=12, -37<=l<=37	
Reflections collected	24928	
Independent reflections	9432 [R(int) = 0.1148]	
Completeness to theta = 24.02°	94.6 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9432 / 0 / 721	
Goodness-of-fit on F^2	0.806	
Final R indices [I>2sigma(I)]	R1 = 0.0556, wR2 = 0.1160	
R indices (all data)	R1 = 0.1201, wR2 = 0.1353	
Largest diff. peak and hole	0.312 and -0.326 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2139. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	271(1)	7692(1)	1928(1)	27(1)
Al(2)	-800(1)	7871(1)	1975(1)	26(1)
Si(1)	1197(1)	8917(1)	1958(1)	31(1)
Si(2)	1517(1)	9526(1)	2942(1)	31(1)
Si(3)	-201(1)	6055(1)	1184(1)	30(1)
Si(4)	-1281(1)	6500(1)	1134(1)	31(1)
O(1)	-277(1)	8245(2)	1888(1)	29(1)
O(2)	607(1)	7292(2)	2495(1)	29(1)
O(3)	647(1)	8485(2)	1818(1)	33(1)
O(4)	1383(1)	9583(2)	2402(1)	36(1)
O(5)	1135(1)	8858(2)	3031(1)	33(1)
O(6)	143(1)	6730(2)	1584(1)	33(1)
O(7)	-789(1)	5991(2)	1118(1)	36(1)
O(8)	-1148(1)	7039(2)	1596(1)	36(1)
C(1)	1180(2)	9673(3)	1496(1)	35(1)
C(2)	1263(2)	10610(4)	1533(2)	50(1)
C(3)	1229(2)	11160(4)	1170(2)	60(2)
C(4)	1119(2)	10741(5)	762(2)	67(2)
C(5)	1029(2)	9828(5)	708(2)	69(2)
C(6)	1062(2)	9299(4)	1072(2)	56(2)
C(7)	1686(2)	7994(3)	2078(1)	40(1)
C(8)	2196(2)	8207(4)	2241(2)	68(2)
C(9)	2567(2)	7529(6)	2354(2)	93(3)
C(10)	2440(3)	6621(6)	2310(2)	91(2)
C(11)	1933(3)	6384(5)	2148(2)	86(2)
C(12)	1567(2)	7051(4)	2035(2)	60(2)
C(13)	1447(2)	10734(3)	3110(1)	35(1)
C(14)	1307(2)	11475(3)	2806(2)	47(1)
C(15)	1245(2)	12354(4)	2928(2)	63(2)
C(16)	1323(2)	12539(4)	3366(2)	67(2)
C(17)	1457(2)	11829(4)	3674(2)	58(2)
C(18)	1524(2)	10947(4)	3552(1)	45(1)
C(19)	2184(2)	9136(3)	3282(1)	34(1)
C(20)	2294(2)	8196(3)	3355(2)	49(1)
C(21)	2778(2)	7883(4)	3621(2)	60(2)
C(22)	3169(2)	8509(4)	3823(2)	60(2)
C(23)	3069(2)	9424(4)	3763(2)	71(2)
C(24)	2584(2)	9730(4)	3492(2)	55(2)
C(25)	52(2)	4855(3)	1308(1)	36(1)
C(26)	-245(2)	4107(3)	1316(2)	48(1)
C(27)	-54(3)	3217(4)	1425(2)	65(2)
C(28)	444(3)	3058(4)	1533(2)	68(2)
C(29)	752(2)	3760(4)	1531(2)	62(2)
C(30)	557(2)	4654(4)	1418(1)	48(1)
C(31)	-212(2)	6446(3)	640(1)	33(1)
C(32)	-367(2)	5851(3)	271(1)	46(1)
C(33)	-425(2)	6151(4)	-150(1)	56(2)
C(34)	-322(2)	7038(4)	-212(2)	57(2)
C(35)	-160(2)	7657(4)	148(2)	63(2)
C(36)	-109(2)	7346(3)	566(1)	45(1)
C(37)	-1750(2)	5581(3)	1081(1)	36(1)
C(38)	-1846(2)	4816(4)	796(2)	51(1)
C(39)	-2218(2)	4184(4)	733(2)	68(2)
C(40)	-2517(2)	4294(4)	957(2)	74(2)
C(41)	-2446(2)	5022(4)	1241(2)	66(2)
C(42)	-2063(2)	5641(4)	1300(2)	51(1)
C(43)	-1567(2)	7318(3)	654(1)	35(1)
C(44)	-1540(2)	7180(4)	243(1)	50(1)
C(45)	-1793(2)	7760(5)	-123(2)	65(2)
C(46)	-2084(2)	8479(5)	-86(2)	74(2)
C(47)	-2122(2)	8629(4)	312(2)	66(2)
C(48)	-1857(2)	8058(3)	679(2)	49(1)
N(1)	-403(2)	9903(3)	1598(1)	65(1)
C(49)	-59(4)	10594(8)	1742(4)	52(3)
C(50A)	-63(4)	10982(9)	2168(3)	45(3)
C(50B)	-86(4)	10664(9)	2018(4)	48(3)
C(51)	0	10254(5)	2500	54(2)
N(2)	951(2)	5599(3)	2555(1)	69(1)
C(52A)	922(4)	4878(8)	2789(3)	50(3)
C(53A)	373(4)	4529(8)	2555(3)	44(3)
C(53B)	564(5)	4868(9)	2647(4)	54(3)

C(54)	0	5241(5)	2500	55(2)
C(55)	4740(3)	5919(6)	607(2)	81(2)
C(56)	4374(3)	6590(5)	467(2)	80(2)
C(57)	3873(3)	6368(5)	312(2)	81(2)
C(58)	3731(3)	5458(6)	303(2)	77(2)
C(59)	4087(3)	4775(5)	446(2)	76(2)
C(60)	4597(3)	5003(5)	593(2)	77(2)
C(61)	1894(4)	6299(6)	366(3)	118(3)
C(62)	2080(3)	6779(5)	776(3)	93(2)
C(63)	1760(3)	7008(5)	959(2)	77(2)
C(64)	1263(3)	6784(5)	753(2)	84(2)
C(65)	1083(3)	6307(5)	362(3)	96(2)
C(66)	1383(4)	6089(7)	165(3)	122(3)

Table 3. Bond lengths [Å] and angles [°] for sh2139.

Al(1)-O(3)	1.728(3)
Al(1)-O(6)	1.737(3)
Al(1)-O(1)	1.742(3)
Al(1)-O(2)	1.802(3)
Al(2)-O(8)	1.725(3)
Al(2)-O(5)#1	1.729(3)
Al(2)-O(1)	1.752(3)
Al(2)-O(2)#1	1.803(3)
Si(1)-O(3)	1.597(3)
Si(1)-O(4)	1.645(3)
Si(1)-C(1)	1.864(4)
Si(1)-C(7)	1.872(5)
Si(2)-O(5)	1.592(3)
Si(2)-O(4)	1.657(3)
Si(2)-C(19)	1.873(4)
Si(2)-C(13)	1.874(5)
Si(3)-O(6)	1.607(3)
Si(3)-O(7)	1.636(3)
Si(3)-C(25)	1.865(5)
Si(3)-C(31)	1.872(4)
Si(4)-O(8)	1.609(3)
Si(4)-O(7)	1.634(3)
Si(4)-C(37)	1.863(5)
Si(4)-C(43)	1.869(4)
O(2)-Al(2)#1	1.802(3)
O(5)-Al(2)#1	1.729(3)
C(1)-C(2)	1.376(7)
C(1)-C(6)	1.401(6)
C(2)-C(3)	1.407(7)
C(3)-C(4)	1.387(8)
C(4)-C(5)	1.347(8)
C(5)-C(6)	1.395(7)
C(7)-C(8)	1.384(7)
C(7)-C(12)	1.402(7)
C(8)-C(9)	1.390(8)
C(9)-C(10)	1.358(10)
C(10)-C(11)	1.386(9)
C(11)-C(12)	1.369(8)
C(13)-C(14)	1.408(6)
C(13)-C(18)	1.414(6)
C(14)-C(15)	1.371(7)
C(15)-C(16)	1.394(7)
C(16)-C(17)	1.382(8)
C(17)-C(18)	1.380(7)
C(19)-C(24)	1.376(6)
C(19)-C(20)	1.398(6)
C(20)-C(21)	1.385(7)
C(21)-C(22)	1.386(7)
C(22)-C(23)	1.355(8)
C(23)-C(24)	1.388(7)
C(25)-C(30)	1.390(7)
C(25)-C(26)	1.395(7)
C(26)-C(27)	1.391(7)
C(27)-C(28)	1.361(8)
C(28)-C(29)	1.359(8)
C(29)-C(30)	1.400(7)
C(31)-C(36)	1.383(6)
C(31)-C(32)	1.401(6)
C(32)-C(33)	1.397(6)
C(33)-C(34)	1.358(7)
C(34)-C(35)	1.403(7)
C(35)-C(36)	1.399(6)
C(37)-C(42)	1.388(7)
C(37)-C(38)	1.404(6)
C(38)-C(39)	1.368(7)
C(39)-C(40)	1.370(8)
C(40)-C(41)	1.368(8)
C(41)-C(42)	1.380(7)
C(43)-C(48)	1.390(7)
C(43)-C(44)	1.409(6)
C(44)-C(45)	1.396(7)
C(45)-C(46)	1.381(9)
C(46)-C(47)	1.381(8)
C(47)-C(48)	1.399(7)
N(1)-C(49)	1.352(11)

C(49)-C(50A)	1.520(14)
C(50A)-C(51)	1.476(11)
C(51)-C(50A)#1	1.476(11)
N(2)-C(52A)	1.324(11)
C(52A)-C(53A)	1.537(15)
C(53A)-C(54)	1.454(11)
C(54)-C(53A)#1	1.454(11)
C(55)-C(56)	1.370(9)
C(55)-C(60)	1.387(9)
C(56)-C(57)	1.365(9)
C(57)-C(58)	1.380(9)
C(58)-C(59)	1.365(9)
C(59)-C(60)	1.393(9)
C(61)-C(66)	1.382(12)
C(61)-C(62)	1.410(11)
C(62)-C(63)	1.350(10)
C(63)-C(64)	1.354(9)
C(64)-C(65)	1.361(9)
C(65)-C(66)	1.328(11)

O(3)-Al(1)-O(6)	112.18(15)
O(3)-Al(1)-O(1)	108.67(15)
O(6)-Al(1)-O(1)	112.58(14)
O(3)-Al(1)-O(2)	108.59(13)
O(6)-Al(1)-O(2)	106.97(14)
O(1)-Al(1)-O(2)	107.68(13)
O(8)-Al(2)-O(5)#1	114.51(15)
O(8)-Al(2)-O(1)	112.41(14)
O(5)#1-Al(2)-O(1)	105.63(15)
O(8)-Al(2)-O(2)#1	102.92(14)
O(5)#1-Al(2)-O(2)#1	109.75(14)
O(1)-Al(2)-O(2)#1	111.76(13)
O(3)-Si(1)-O(4)	113.40(16)
O(3)-Si(1)-C(1)	108.71(17)
O(4)-Si(1)-C(1)	105.68(18)
O(3)-Si(1)-C(7)	111.21(19)
O(4)-Si(1)-C(7)	107.34(17)
C(1)-Si(1)-C(7)	110.3(2)
O(5)-Si(2)-O(4)	111.36(15)
O(5)-Si(2)-C(19)	109.55(18)
O(4)-Si(2)-C(19)	111.82(18)
O(5)-Si(2)-C(13)	110.03(19)
O(4)-Si(2)-C(13)	105.38(18)
C(19)-Si(2)-C(13)	108.60(19)
O(6)-Si(3)-O(7)	113.36(16)
O(6)-Si(3)-C(25)	109.73(17)
O(7)-Si(3)-C(25)	105.7(2)
O(6)-Si(3)-C(31)	110.87(18)
O(7)-Si(3)-C(31)	107.39(17)
C(25)-Si(3)-C(31)	109.7(2)
O(8)-Si(4)-O(7)	112.91(15)
O(8)-Si(4)-C(37)	107.96(18)
O(7)-Si(4)-C(37)	106.96(19)
O(8)-Si(4)-C(43)	109.77(19)
O(7)-Si(4)-C(43)	109.92(19)
C(37)-Si(4)-C(43)	109.21(18)
Al(1)-O(1)-Al(2)	132.71(17)
Al(1)-O(2)-Al(2)#1	131.82(17)
Si(1)-O(3)-Al(1)	148.05(18)
Si(1)-O(4)-Si(2)	140.21(19)
Si(2)-O(5)-Al(2)#1	159.6(2)
Si(3)-O(6)-Al(1)	155.9(2)
Si(4)-O(7)-Si(3)	148.6(2)
Si(4)-O(8)-Al(2)	149.2(2)
C(2)-C(1)-C(6)	115.5(4)
C(2)-C(1)-Si(1)	124.4(3)
C(6)-C(1)-Si(1)	120.0(4)
C(1)-C(2)-C(3)	122.5(5)
C(4)-C(3)-C(2)	118.9(5)
C(5)-C(4)-C(3)	120.8(5)
C(4)-C(5)-C(6)	119.2(5)
C(5)-C(6)-C(1)	123.1(5)
C(8)-C(7)-C(12)	115.9(5)
C(8)-C(7)-Si(1)	121.2(4)
C(12)-C(7)-Si(1)	122.8(4)
C(7)-C(8)-C(9)	122.1(6)
C(10)-C(9)-C(8)	120.7(7)

C(9)-C(10)-C(11)	118.6(6)
C(12)-C(11)-C(10)	120.7(7)
C(11)-C(12)-C(7)	122.0(6)
C(14)-C(13)-C(18)	116.2(4)
C(14)-C(13)-Si(2)	122.5(3)
C(18)-C(13)-Si(2)	121.3(3)
C(15)-C(14)-C(13)	122.3(5)
C(14)-C(15)-C(16)	120.1(5)
C(17)-C(16)-C(15)	119.4(5)
C(18)-C(17)-C(16)	120.4(5)
C(17)-C(18)-C(13)	121.6(5)
C(24)-C(19)-C(20)	116.2(4)
C(24)-C(19)-Si(2)	123.7(4)
C(20)-C(19)-Si(2)	120.0(3)
C(21)-C(20)-C(19)	121.7(4)
C(20)-C(21)-C(22)	119.9(5)
C(23)-C(22)-C(21)	119.3(5)
C(22)-C(23)-C(24)	120.3(5)
C(19)-C(24)-C(23)	122.5(5)
C(30)-C(25)-C(26)	115.3(4)
C(30)-C(25)-Si(3)	122.0(4)
C(26)-C(25)-Si(3)	122.6(4)
C(27)-C(26)-C(25)	123.0(5)
C(28)-C(27)-C(26)	119.3(6)
C(29)-C(28)-C(27)	120.4(5)
C(28)-C(29)-C(30)	120.1(6)
C(25)-C(30)-C(29)	122.0(5)
C(36)-C(31)-C(32)	116.2(4)
C(36)-C(31)-Si(3)	122.6(3)
C(32)-C(31)-Si(3)	121.0(4)
C(33)-C(32)-C(31)	122.1(5)
C(34)-C(33)-C(32)	120.4(5)
C(33)-C(34)-C(35)	119.6(4)
C(36)-C(35)-C(34)	119.1(5)
C(31)-C(36)-C(35)	122.6(4)
C(42)-C(37)-C(38)	114.3(4)
C(42)-C(37)-Si(4)	121.6(4)
C(38)-C(37)-Si(4)	123.9(4)
C(39)-C(38)-C(37)	123.4(5)
C(38)-C(39)-C(40)	119.1(5)
C(41)-C(40)-C(39)	120.9(6)
C(40)-C(41)-C(42)	118.5(6)
C(41)-C(42)-C(37)	123.8(5)
C(48)-C(43)-C(44)	116.7(4)
C(48)-C(43)-Si(4)	120.3(3)
C(44)-C(43)-Si(4)	122.8(4)
C(45)-C(44)-C(43)	121.5(5)
C(46)-C(45)-C(44)	119.9(5)
C(47)-C(46)-C(45)	120.1(5)
C(46)-C(47)-C(48)	119.6(6)
C(43)-C(48)-C(47)	122.2(5)
N(1)-C(49)-C(50A)	107.8(10)
C(51)-C(50A)-C(49)	112.1(10)
C(50A)#1-C(51)-C(50A)	88.7(11)
N(2)-C(52A)-C(53A)	106.1(9)
C(54)-C(53A)-C(52A)	113.2(9)
C(53A)-C(54)-C(53A)#1	89.5(11)
C(56)-C(55)-C(60)	119.2(7)
C(57)-C(56)-C(55)	121.0(7)
C(56)-C(57)-C(58)	119.8(7)
C(59)-C(58)-C(57)	120.6(7)
C(58)-C(59)-C(60)	119.3(7)
C(55)-C(60)-C(59)	120.0(7)
C(66)-C(61)-C(62)	117.8(8)
C(63)-C(62)-C(61)	119.6(7)
C(62)-C(63)-C(64)	120.7(7)
C(63)-C(64)-C(65)	119.9(7)
C(66)-C(65)-C(64)	121.1(8)
C(65)-C(66)-C(61)	120.7(8)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2139. 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}
Al(1)	29(1)	22(1)	29(1)	0(1)	12(1)	-1(1)
Al(2)	26(1)	22(1)	30(1)	-1(1)	11(1)	1(1)
Si(1)	33(1)	26(1)	38(1)	-1(1)	19(1)	-2(1)
Si(2)	32(1)	24(1)	37(1)	-3(1)	17(1)	-4(1)
Si(3)	33(1)	24(1)	33(1)	-4(1)	14(1)	-2(1)
Si(4)	30(1)	28(1)	32(1)	-2(1)	10(1)	-3(1)
O(1)	29(2)	24(2)	32(1)	1(1)	13(1)	-1(1)
O(2)	31(2)	26(2)	27(1)	1(1)	9(1)	0(1)
O(3)	36(2)	28(2)	39(2)	1(1)	20(1)	-3(1)
O(4)	44(2)	32(2)	35(2)	-3(1)	20(1)	-6(2)
O(5)	36(2)	28(2)	39(2)	-2(1)	18(1)	-8(1)
O(6)	41(2)	24(2)	32(1)	-7(1)	15(1)	-3(1)
O(7)	32(2)	35(2)	44(2)	0(1)	18(1)	-1(1)
O(8)	38(2)	35(2)	31(1)	-9(1)	10(1)	-5(1)
C(1)	32(3)	36(3)	39(2)	0(2)	16(2)	-6(2)
C(2)	52(3)	48(4)	51(3)	3(2)	22(2)	-7(3)
C(3)	70(4)	41(3)	75(4)	19(3)	37(3)	-10(3)
C(4)	70(4)	74(5)	63(4)	26(3)	34(3)	-2(3)
C(5)	97(5)	76(5)	40(3)	5(3)	34(3)	-4(4)
C(6)	74(4)	50(4)	50(3)	4(2)	33(3)	0(3)
C(7)	37(3)	43(3)	43(2)	-8(2)	22(2)	-1(2)
C(8)	42(4)	70(4)	89(4)	-27(3)	27(3)	0(3)
C(9)	41(4)	116(7)	114(5)	-33(5)	24(3)	26(4)
C(10)	78(6)	101(7)	96(5)	6(4)	37(4)	49(5)
C(11)	86(5)	49(4)	143(6)	17(4)	67(5)	26(4)
C(12)	55(4)	47(4)	88(4)	7(3)	41(3)	11(3)
C(13)	26(3)	28(3)	53(3)	-6(2)	20(2)	-2(2)
C(14)	56(3)	31(3)	59(3)	-3(2)	30(2)	-2(2)
C(15)	80(4)	31(3)	87(4)	1(3)	46(3)	10(3)
C(16)	64(4)	41(4)	97(4)	-25(3)	36(3)	0(3)
C(17)	56(4)	55(4)	63(3)	-24(3)	27(3)	-1(3)
C(18)	43(3)	46(3)	45(3)	-6(2)	18(2)	1(2)
C(19)	31(3)	32(3)	39(2)	-6(2)	16(2)	-6(2)
C(20)	37(3)	28(3)	73(3)	4(2)	12(2)	-1(2)
C(21)	47(3)	39(3)	87(4)	10(3)	21(3)	6(3)
C(22)	30(3)	59(4)	76(3)	-2(3)	8(3)	7(3)
C(23)	31(3)	56(4)	106(4)	-16(3)	10(3)	-6(3)
C(24)	38(3)	35(3)	85(4)	-5(3)	18(3)	-7(2)
C(25)	49(3)	27(3)	32(2)	-7(2)	18(2)	1(2)
C(26)	53(3)	33(3)	59(3)	-3(2)	23(2)	-1(2)
C(27)	81(5)	28(3)	89(4)	7(3)	39(3)	9(3)
C(28)	107(6)	27(3)	77(4)	7(3)	45(4)	24(4)
C(29)	64(4)	56(4)	73(3)	2(3)	35(3)	25(3)
C(30)	46(3)	45(3)	54(3)	1(2)	23(2)	4(3)
C(31)	28(3)	34(3)	37(2)	-4(2)	15(2)	2(2)
C(32)	66(4)	33(3)	43(3)	-4(2)	27(2)	-7(2)
C(33)	67(4)	67(4)	33(3)	-7(3)	20(2)	-3(3)
C(34)	63(4)	73(4)	37(3)	11(3)	23(2)	3(3)
C(35)	93(5)	43(3)	56(3)	9(3)	35(3)	-8(3)
C(36)	60(3)	35(3)	42(3)	-1(2)	23(2)	-8(2)
C(37)	31(3)	38(3)	38(2)	2(2)	12(2)	0(2)
C(38)	56(3)	44(3)	55(3)	-9(2)	24(2)	-17(3)
C(39)	71(4)	40(4)	86(4)	-21(3)	28(3)	-22(3)
C(40)	62(4)	48(4)	101(5)	12(3)	23(4)	-24(3)
C(41)	62(4)	51(4)	96(4)	1(3)	46(3)	-13(3)
C(42)	46(3)	46(4)	63(3)	-2(2)	26(3)	-6(3)
C(43)	25(3)	36(3)	37(2)	0(2)	8(2)	-9(2)
C(44)	47(3)	54(3)	39(3)	6(2)	9(2)	-6(3)
C(45)	66(4)	74(5)	39(3)	18(3)	7(3)	-16(4)
C(46)	50(4)	79(5)	59(4)	30(3)	-9(3)	-19(4)
C(47)	49(4)	48(4)	89(4)	25(3)	17(3)	2(3)
C(48)	49(3)	37(3)	59(3)	10(2)	20(2)	0(3)
N(1)	98(4)	46(3)	64(3)	17(2)	46(3)	16(3)
C(51)	86(6)	29(4)	56(4)	0	38(4)	0
N(2)	84(4)	43(3)	63(3)	-8(2)	16(2)	11(3)
C(54)	57(5)	36(5)	62(4)	0	16(4)	0
C(55)	72(5)	101(6)	72(4)	-11(4)	34(3)	-22(5)
C(56)	99(6)	72(5)	80(4)	-20(4)	49(4)	-37(5)
C(57)	88(6)	76(5)	88(4)	-7(4)	46(4)	-12(4)
C(58)	66(4)	97(6)	69(4)	-4(4)	29(3)	-20(4)
C(59)	87(5)	77(5)	63(4)	-11(3)	33(4)	-35(4)

C(60)	103(6)	69(5)	60(4)	1(3)	36(4)	-7(4)
C(61)	130(8)	102(7)	164(8)	-24(6)	104(7)	-8(6)
C(62)	55(5)	61(5)	146(7)	18(5)	27(5)	-1(4)
C(63)	80(5)	56(4)	90(4)	-2(3)	30(4)	-6(4)
C(64)	79(5)	55(4)	124(6)	-16(4)	48(4)	-5(4)
C(65)	73(5)	79(6)	116(6)	-14(4)	22(5)	-8(4)
C(66)	130(9)	135(9)	112(6)	-45(5)	62(6)	-45(7)

sh 2024

Table 1. Crystal data and structure refinement for sh2024.

Identification code	sh2024	
Empirical formula	C106 H114 Al4 N5 O16 Si8	
Formula weight	2046.66	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 15.132(3) Å	α= 84.87(3)°.
	b = 17.175(3) Å	β= 71.83(3)°.
	c = 24.217(5) Å	γ = 64.66(3)°.
Volume	5397.5(18) $Å^3$	
Z	2	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.197 mm^{-1}	
F(000)	2154	
Crystal size	0.44 x 0.28 x 0.2 mm^3	
Theta range for data collection	2.03 to 25.20°.	
Index ranges	-16<=h<=17, -18<=k<=18, -27<=l<=27	
Reflections collected	33570	
Independent reflections	15752 [R(int) = 0.1736]	
Completeness to theta = 25.20°	81.1 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15752 / 0 / 1269	
Goodness-of-fit on F^2	2.679	
Final R indices [I>2sigma(I)]	R1 = 0.1865, wR2 = 0.4050	
R indices (all data)	R1 = 0.2482, wR2 = 0.4219	
Largest diff. peak and hole	0.636 and -0.611 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2024. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	11750(3)	1045(2)	2329(1)	48(1)
Al(2)	11227(3)	2612(2)	1428(1)	45(1)
Al(3)	9691(3)	3905(2)	2556(1)	49(1)
Al(4)	10031(3)	2305(2)	3435(1)	47(1)
Si(1)	11655(3)	-212(2)	1407(1)	51(1)
Si(2)	11062(3)	1314(2)	569(1)	54(1)
Si(3)	11960(3)	4089(2)	887(1)	55(1)
Si(4)	10489(3)	5304(2)	1997(1)	53(1)
Si(5)	7232(3)	4632(2)	3198(1)	54(1)
Si(6)	7578(3)	3089(3)	4017(1)	55(1)
Si(7)	11765(3)	1702(2)	4046(1)	50(1)
Si(8)	13247(3)	193(2)	3119(1)	54(1)
O(1)	12013(6)	1812(5)	1819(3)	48(2)
O(2)	10060(6)	3242(5)	1929(3)	53(2)
O(3)	10057(6)	3297(5)	3150(3)	55(2)
O(4)	10583(6)	1538(5)	2872(3)	52(2)
O(5)	11683(7)	291(5)	1918(3)	58(2)
O(6)	11224(7)	435(5)	924(3)	59(2)
O(7)	11017(7)	2071(5)	944(3)	59(2)
O(8)	11893(6)	3182(6)	1047(3)	55(2)
O(9)	11050(6)	4895(5)	1329(3)	53(2)
O(10)	10254(7)	4620(5)	2449(3)	56(2)
O(11)	8371(6)	4389(6)	2765(3)	58(2)
O(12)	7124(7)	3822(5)	3569(3)	58(2)
O(13)	8767(7)	2462(6)	3740(3)	60(2)
O(14)	10666(6)	2070(6)	3970(3)	55(2)
O(15)	12502(7)	732(5)	3753(3)	59(2)
O(16)	12787(7)	602(5)	2591(3)	59(2)
C(1)	12957(10)	-1083(9)	1049(5)	59(4)
C(2)	13270(12)	-1389(9)	483(6)	65(4)
C(3)	14083(15)	-2094(13)	244(8)	101(6)
C(4)	14732(16)	-2546(12)	606(10)	114(7)
C(5)	14477(15)	-2246(11)	1203(9)	109(7)
C(6)	13561(12)	-1548(11)	1407(7)	86(5)
C(7)	10786(11)	-742(8)	1705(5)	56(3)
C(8)	10122(15)	-759(12)	1455(7)	90(6)
C(9)	9414(15)	-1128(13)	1713(7)	101(6)
C(10)	9453(13)	-1566(10)	2208(6)	72(4)
C(11)	10213(13)	-1639(12)	2453(6)	87(5)
C(12)	10823(13)	-1229(10)	2225(6)	76(4)
C(13)	12132(11)	1046(8)	-141(4)	54(3)
C(14)	12764(11)	1470(9)	-306(5)	66(4)
C(15)	13519(12)	1303(11)	-845(6)	83(5)
C(16)	13663(13)	651(12)	-1210(6)	87(6)
C(17)	13048(15)	223(11)	-1061(5)	93(6)
C(18)	12225(13)	412(11)	-513(5)	79(5)
C(19)	9830(10)	1683(10)	391(5)	60(4)
C(20)	9591(14)	2352(13)	28(8)	110(7)
C(21)	8698(16)	2671(15)	-115(9)	117(7)
C(22)	7955(18)	2368(14)	122(12)	126(8)
C(23)	8144(19)	1706(15)	512(10)	132(9)
C(24)	9071(15)	1419(12)	621(9)	101(6)
C(25)	11771(10)	4401(9)	152(5)	58(4)
C(26)	12246(13)	3794(10)	-328(5)	76(5)
C(27)	12048(14)	3991(13)	-845(5)	80(5)
C(28)	11320(16)	4789(14)	-903(7)	101(6)
C(29)	10820(13)	5411(11)	-447(5)	82(5)
C(30)	11086(13)	5199(10)	71(6)	73(4)
C(31)	13243(11)	3967(8)	895(5)	59(3)
C(32)	13763(13)	4410(12)	620(8)	91(5)
C(33)	14693(16)	4360(17)	655(10)	126(8)
C(34)	15123(19)	3769(19)	1026(8)	129(8)
C(35)	14602(15)	3288(14)	1371(9)	104(6)
C(36)	13665(12)	3401(11)	1287(5)	80(5)
C(37)	11315(11)	5733(8)	2183(5)	60(4)
C(38)	11864(14)	6090(10)	1754(6)	84(5)
C(39)	12425(16)	6479(14)	1882(11)	117(7)
C(40)	12470(15)	6552(12)	2413(8)	87(5)
C(41)	11993(15)	6186(13)	2835(8)	96(6)
C(42)	11400(14)	5785(12)	2741(6)	88(5)
C(43)	9287(12)	6249(9)	2019(5)	69(4)

C(44)	8415(11)	6417(9)	2488(6)	71(4)
C(45)	8234(12)	7514(9)	1618(7)	67(4)
C(46)	7464(13)	7680(10)	2072(6)	78(5)
C(47)	7479(14)	7153(10)	2528(8)	100(6)
C(48)	9144(11)	6801(8)	1578(5)	62(4)
C(49)	6350(13)	4924(9)	2736(5)	73(5)
C(50)	6551(12)	5356(10)	2223(5)	70(4)
C(51)	5975(13)	5540(11)	1844(6)	79(5)
C(52)	5237(14)	5303(12)	1943(6)	80(5)
C(53)	4990(14)	4923(13)	2461(9)	105(6)
C(54)	5533(14)	4686(11)	2859(6)	76(5)
C(55)	6853(11)	5552(9)	3708(5)	65(4)
C(56)	7544(12)	5599(11)	3951(6)	82(5)
C(57)	7320(20)	6243(14)	4343(8)	113(7)
C(58)	6340(20)	6877(16)	4503(8)	118(8)
C(59)	5650(20)	6855(14)	4289(9)	132(8)
C(60)	5890(14)	6190(11)	3885(6)	98(6)
C(61)	6830(11)	2430(10)	4155(6)	67(4)
C(62)	6151(13)	2480(11)	3886(6)	77(4)
C(63)	5668(16)	1937(16)	3964(10)	118(7)
C(64)	5900(18)	1307(15)	4411(10)	108(7)
C(65)	6520(20)	1238(16)	4696(11)	125(8)
C(66)	6966(13)	1814(12)	4588(7)	86(5)
C(67)	7362(11)	3655(9)	4716(5)	58(3)
C(68)	6489(13)	4325(10)	4986(6)	84(5)
C(69)	6253(16)	4734(12)	5477(7)	110(7)
C(70)	7004(16)	4440(11)	5766(6)	98(6)
C(71)	7944(12)	3798(12)	5513(5)	87(5)
C(72)	8090(12)	3433(10)	4984(5)	69(4)
C(73)	11716(10)	1631(8)	4830(5)	52(3)
C(74)	10769(11)	2202(10)	5265(5)	69(4)
C(75)	10846(14)	2248(12)	5846(5)	91(6)
C(76)	11681(17)	1733(13)	6012(7)	106(7)
C(77)	12482(18)	1181(14)	5597(7)	124(8)
C(78)	12529(16)	1138(12)	5017(6)	97(6)
C(79)	14523(11)	179(9)	2991(5)	67(4)
C(80)	14778(13)	793(13)	2648(7)	86(5)
C(81)	15723(18)	826(18)	2545(8)	129(9)
C(82)	16490(18)	290(20)	2705(11)	145(11)
C(83)	16190(17)	-387(19)	3079(11)	138(10)
C(84)	15278(13)	-401(13)	3185(7)	96(6)
C(85)	13375(11)	-932(8)	3230(5)	59(4)
C(86)	12779(13)	-1159(11)	3746(6)	84(5)
C(87)	12867(16)	-1989(14)	3778(8)	110(7)
C(88)	13544(19)	-2631(12)	3374(9)	106(7)
C(89)	14154(18)	-2438(12)	2858(9)	111(7)
C(90)	14062(14)	-1612(10)	2823(6)	87(5)
C(91)	12435(10)	2427(9)	3731(5)	58(4)
C(92)	12759(12)	2789(10)	4078(7)	70(4)
C(93)	13160(16)	3384(12)	3871(7)	100(6)
C(94)	13260(17)	3589(13)	3295(9)	111(7)
C(95)	12888(14)	3255(14)	2923(7)	101(6)
C(96)	12515(11)	2689(9)	3157(5)	67(4)
N(1)	8595(11)	3349(9)	1600(5)	89(4)
C(97)	7998(14)	2812(12)	1928(9)	99(6)
C(98)	8666(14)	2041(12)	2202(7)	92(5)
C(99)	8086(14)	1548(13)	2506(8)	94(5)
C(100)	8549(17)	898(13)	2839(11)	118(7)
N(2A)	9240(40)	860(40)	3090(20)	106(13)
N(2B)	9530(30)	500(40)	2877(18)	33(16)
N(3)	13918(9)	1290(7)	1113(4)	72(4)
C(101)	14916(10)	358(8)	175(5)	60(4)
C(102)	14090(10)	556(8)	770(5)	57(4)
N(4)	10354(11)	4345(8)	3750(4)	86(4)
C(103)	10003(12)	4388(10)	4347(6)	78(5)
C(104)	10187(14)	4980(11)	4668(5)	80(5)
N(5)	9770(40)	-380(20)	3841(10)	239(17)
C(105)	9930(19)	60(20)	4240(12)	160(12)
C(106)	9960(20)	-250(18)	4794(10)	157(11)

Table 3. Bond lengths [Å] and angles [°] for sh2024.

Al(1)-O(16)	1.720(9)
Al(1)-O(4)	1.742(8)
Al(1)-O(5)	1.755(9)
Al(1)-O(1)	1.809(8)
Al(2)-O(8)	1.711(9)
Al(2)-O(7)	1.737(9)
Al(2)-O(2)	1.739(8)
Al(2)-O(1)	1.807(8)
Al(3)-O(11)	1.720(9)
Al(3)-O(10)	1.735(10)
Al(3)-O(2)	1.774(8)
Al(3)-O(3)	1.790(8)
Al(4)-O(4)	1.723(8)
Al(4)-O(13)	1.729(10)
Al(4)-O(14)	1.764(8)
Al(4)-O(3)	1.791(9)
Si(1)-O(5)	1.594(8)
Si(1)-O(6)	1.627(8)
Si(1)-C(7)	1.842(15)
Si(1)-C(1)	1.875(13)
Si(2)-O(7)	1.617(9)
Si(2)-O(6)	1.631(8)
Si(2)-C(19)	1.872(14)
Si(2)-C(13)	1.886(12)
Si(3)-O(8)	1.610(9)
Si(3)-O(9)	1.636(8)
Si(3)-C(31)	1.869(16)
Si(3)-C(25)	1.884(12)
Si(4)-O(10)	1.609(8)
Si(4)-O(9)	1.632(8)
Si(4)-C(43)	1.836(16)
Si(4)-C(37)	1.873(16)
Si(5)-O(11)	1.606(8)
Si(5)-O(12)	1.627(9)
Si(5)-C(55)	1.866(15)
Si(5)-C(49)	1.882(16)
Si(6)-O(13)	1.602(9)
Si(6)-O(12)	1.646(8)
Si(6)-C(61)	1.861(17)
Si(6)-C(67)	1.898(13)
Si(7)-O(14)	1.572(9)
Si(7)-O(15)	1.627(9)
Si(7)-C(73)	1.872(11)
Si(7)-C(91)	1.895(15)
Si(8)-O(16)	1.608(8)
Si(8)-O(15)	1.662(8)
Si(8)-C(79)	1.847(17)
Si(8)-C(85)	1.861(14)
C(1)-C(2)	1.374(17)
C(1)-C(6)	1.404(19)
C(2)-C(3)	1.31(2)
C(3)-C(4)	1.45(3)
C(4)-C(5)	1.45(3)
C(5)-C(6)	1.36(2)
C(7)-C(8)	1.34(2)
C(7)-C(12)	1.452(18)
C(8)-C(9)	1.43(2)
C(9)-C(10)	1.36(2)
C(10)-C(11)	1.41(2)
C(11)-C(12)	1.35(2)
C(13)-C(14)	1.382(19)
C(13)-C(18)	1.409(19)
C(14)-C(15)	1.397(19)
C(15)-C(16)	1.39(2)
C(16)-C(17)	1.37(3)
C(17)-C(18)	1.45(2)
C(19)-C(24)	1.36(2)
C(19)-C(20)	1.37(2)
C(20)-C(21)	1.37(2)
C(21)-C(22)	1.38(3)
C(22)-C(23)	1.40(3)
C(23)-C(24)	1.38(2)
C(25)-C(30)	1.361(19)
C(25)-C(26)	1.419(19)
C(26)-C(27)	1.357(18)

C(27)-C(28)	1.37(2)
C(28)-C(29)	1.39(2)
C(29)-C(30)	1.406(18)
C(31)-C(32)	1.32(2)
C(31)-C(36)	1.391(19)
C(32)-C(33)	1.40(2)
C(33)-C(34)	1.38(3)
C(34)-C(35)	1.42(3)
C(35)-C(36)	1.42(2)
C(37)-C(38)	1.39(2)
C(37)-C(42)	1.409(17)
C(38)-C(39)	1.40(2)
C(39)-C(40)	1.33(2)
C(40)-C(41)	1.33(2)
C(41)-C(42)	1.42(2)
C(43)-C(48)	1.369(16)
C(43)-C(44)	1.382(19)
C(44)-C(47)	1.42(2)
C(45)-C(46)	1.27(2)
C(45)-C(48)	1.379(18)
C(46)-C(47)	1.36(2)
C(49)-C(54)	1.40(2)
C(49)-C(50)	1.408(19)
C(50)-C(51)	1.38(2)
C(51)-C(52)	1.29(2)
C(52)-C(53)	1.38(2)
C(53)-C(54)	1.38(2)
C(55)-C(60)	1.355(19)
C(55)-C(56)	1.38(2)
C(56)-C(57)	1.38(2)
C(57)-C(58)	1.36(3)
C(58)-C(59)	1.32(3)
C(59)-C(60)	1.42(2)
C(61)-C(62)	1.35(2)
C(61)-C(66)	1.42(2)
C(62)-C(63)	1.38(2)
C(63)-C(64)	1.47(3)
C(64)-C(65)	1.29(3)
C(65)-C(66)	1.39(3)
C(67)-C(68)	1.338(19)
C(67)-C(72)	1.350(19)
C(68)-C(69)	1.31(2)
C(69)-C(70)	1.40(2)
C(70)-C(71)	1.36(2)
C(71)-C(72)	1.389(18)
C(73)-C(78)	1.35(2)
C(73)-C(74)	1.471(17)
C(74)-C(75)	1.459(17)
C(75)-C(76)	1.36(2)
C(76)-C(77)	1.34(2)
C(77)-C(78)	1.39(2)
C(79)-C(84)	1.339(19)
C(79)-C(80)	1.39(2)
C(80)-C(81)	1.40(2)
C(81)-C(82)	1.28(3)
C(82)-C(83)	1.54(3)
C(83)-C(84)	1.33(3)
C(85)-C(90)	1.395(18)
C(85)-C(86)	1.43(2)
C(86)-C(87)	1.37(2)
C(87)-C(88)	1.35(3)
C(88)-C(89)	1.41(3)
C(89)-C(90)	1.36(2)
C(91)-C(92)	1.393(19)
C(91)-C(96)	1.407(16)
C(92)-C(93)	1.38(2)
C(93)-C(94)	1.39(2)
C(94)-C(95)	1.46(3)
C(95)-C(96)	1.33(2)
N(1)-C(97)	1.56(2)
C(97)-C(98)	1.53(2)
C(98)-C(99)	1.47(2)
C(99)-C(100)	1.38(2)
C(100)-N(2A)	1.34(3)
C(100)-N(2B)	1.38(5)
N(3)-C(102)	1.455(16)
C(101)-C(101)#1	1.44(3)

C(101)-C(102)	1.535(17)
N(4)-C(103)	1.372(15)
C(103)-C(104)	1.49(2)
C(104)-C(104)#2	1.53(3)
N(5)-C(105)	1.42(3)
C(105)-C(106)	1.41(3)
C(106)-C(106)#3	1.44(5)

O(16)-Al(1)-O(4)	113.3(4)
O(16)-Al(1)-O(5)	112.5(4)
O(4)-Al(1)-O(5)	109.2(5)
O(16)-Al(1)-O(1)	104.4(4)
O(4)-Al(1)-O(1)	111.5(4)
O(5)-Al(1)-O(1)	105.6(4)
O(8)-Al(2)-O(7)	109.3(4)
O(8)-Al(2)-O(2)	113.9(4)
O(7)-Al(2)-O(2)	109.3(5)
O(8)-Al(2)-O(1)	108.2(4)
O(7)-Al(2)-O(1)	107.8(4)
O(2)-Al(2)-O(1)	108.2(3)
O(11)-Al(3)-O(10)	114.3(5)
O(11)-Al(3)-O(2)	105.1(4)
O(10)-Al(3)-O(2)	113.8(4)
O(11)-Al(3)-O(3)	107.1(4)
O(10)-Al(3)-O(3)	104.0(4)
O(2)-Al(3)-O(3)	112.7(4)
O(4)-Al(4)-O(13)	107.6(4)
O(4)-Al(4)-O(14)	115.2(4)
O(13)-Al(4)-O(14)	111.0(4)
O(4)-Al(4)-O(3)	109.0(4)
O(13)-Al(4)-O(3)	108.8(4)
O(14)-Al(4)-O(3)	105.1(4)
O(5)-Si(1)-O(6)	112.0(5)
O(5)-Si(1)-C(7)	109.8(5)
O(6)-Si(1)-C(7)	106.8(5)
O(5)-Si(1)-C(1)	110.8(6)
O(6)-Si(1)-C(1)	110.2(5)
C(7)-Si(1)-C(1)	107.0(6)
O(7)-Si(2)-O(6)	112.1(4)
O(7)-Si(2)-C(19)	109.5(6)
O(6)-Si(2)-C(19)	107.9(6)
O(7)-Si(2)-C(13)	111.1(6)
O(6)-Si(2)-C(13)	108.6(5)
C(19)-Si(2)-C(13)	107.5(5)
O(8)-Si(3)-O(9)	113.4(4)
O(8)-Si(3)-C(31)	107.9(5)
O(9)-Si(3)-C(31)	110.0(5)
O(8)-Si(3)-C(25)	110.1(6)
O(9)-Si(3)-C(25)	104.2(5)
C(31)-Si(3)-C(25)	111.3(6)
O(10)-Si(4)-O(9)	112.3(5)
O(10)-Si(4)-C(43)	109.9(6)
O(9)-Si(4)-C(43)	108.4(5)
O(10)-Si(4)-C(37)	112.5(5)
O(9)-Si(4)-C(37)	107.9(5)
C(43)-Si(4)-C(37)	105.6(7)
O(11)-Si(5)-O(12)	112.7(5)
O(11)-Si(5)-C(55)	109.9(6)
O(12)-Si(5)-C(55)	109.5(5)
O(11)-Si(5)-C(49)	107.3(6)
O(12)-Si(5)-C(49)	106.4(7)
C(55)-Si(5)-C(49)	111.1(6)
O(13)-Si(6)-O(12)	112.7(4)
O(13)-Si(6)-C(61)	108.2(6)
O(12)-Si(6)-C(61)	105.7(6)
O(13)-Si(6)-C(67)	110.6(5)
O(12)-Si(6)-C(67)	108.7(5)
C(61)-Si(6)-C(67)	110.8(6)
O(14)-Si(7)-O(15)	113.0(5)
O(14)-Si(7)-C(73)	112.1(5)
O(15)-Si(7)-C(73)	105.9(5)
O(14)-Si(7)-C(91)	111.7(5)
O(15)-Si(7)-C(91)	108.6(5)
C(73)-Si(7)-C(91)	105.1(6)
O(16)-Si(8)-O(15)	112.8(4)
O(16)-Si(8)-C(79)	111.6(5)
O(15)-Si(8)-C(79)	107.0(5)

O(16)-Si(8)-C(85)	111.5(5)
O(15)-Si(8)-C(85)	105.6(5)
C(79)-Si(8)-C(85)	108.0(7)
Al(2)-O(1)-Al(1)	131.0(5)
Al(2)-O(2)-Al(3)	134.5(5)
Al(3)-O(3)-Al(4)	132.9(5)
Al(4)-O(4)-Al(1)	138.6(6)
Si(1)-O(5)-Al(1)	164.0(5)
Si(1)-O(6)-Si(2)	151.1(6)
Si(2)-O(7)-Al(2)	162.3(5)
Si(3)-O(8)-Al(2)	150.0(6)
Si(4)-O(9)-Si(3)	147.3(5)
Si(4)-O(10)-Al(3)	141.3(5)
Si(5)-O(11)-Al(3)	155.9(5)
Si(5)-O(12)-Si(6)	144.9(6)
Si(6)-O(13)-Al(4)	150.5(6)
Si(7)-O(14)-Al(4)	142.2(5)
Si(7)-O(15)-Si(8)	142.5(5)
Si(8)-O(16)-Al(1)	149.2(6)
C(2)-C(1)-C(6)	118.1(14)
C(2)-C(1)-Si(1)	123.2(11)
C(6)-C(1)-Si(1)	117.6(10)
C(3)-C(2)-C(1)	125.8(16)
C(2)-C(3)-C(4)	115.7(15)
C(3)-C(4)-C(5)	121.8(16)
C(6)-C(5)-C(4)	115.7(18)
C(5)-C(6)-C(1)	122.4(16)
C(8)-C(7)-C(12)	114.3(15)
C(8)-C(7)-Si(1)	124.4(10)
C(12)-C(7)-Si(1)	121.3(11)
C(7)-C(8)-C(9)	123.1(14)
C(10)-C(9)-C(8)	120.8(16)
C(9)-C(10)-C(11)	117.7(15)
C(12)-C(11)-C(10)	120.2(14)
C(11)-C(12)-C(7)	123.3(16)
C(14)-C(13)-C(18)	121.1(12)
C(14)-C(13)-Si(2)	122.7(10)
C(18)-C(13)-Si(2)	116.2(11)
C(13)-C(14)-C(15)	122.5(15)
C(16)-C(15)-C(14)	117.6(17)
C(17)-C(16)-C(15)	121.2(14)
C(16)-C(17)-C(18)	122.2(16)
C(13)-C(18)-C(17)	115.2(16)
C(24)-C(19)-C(20)	113.5(15)
C(24)-C(19)-Si(2)	127.6(12)
C(20)-C(19)-Si(2)	118.7(12)
C(21)-C(20)-C(19)	122.4(19)
C(20)-C(21)-C(22)	121.7(19)
C(21)-C(22)-C(23)	118.2(19)
C(24)-C(23)-C(22)	116(2)
C(19)-C(24)-C(23)	128.4(19)
C(30)-C(25)-C(26)	116.3(12)
C(30)-C(25)-Si(3)	121.5(10)
C(26)-C(25)-Si(3)	121.9(11)
C(27)-C(26)-C(25)	122.5(15)
C(26)-C(27)-C(28)	119.6(16)
C(27)-C(28)-C(29)	120.6(16)
C(28)-C(29)-C(30)	118.1(16)
C(25)-C(30)-C(29)	122.7(14)
C(32)-C(31)-C(36)	114.7(15)
C(32)-C(31)-Si(3)	128.4(12)
C(36)-C(31)-Si(3)	116.5(12)
C(31)-C(32)-C(33)	128.6(18)
C(34)-C(33)-C(32)	116(2)
C(33)-C(34)-C(35)	120(2)
C(34)-C(35)-C(36)	117.5(19)
C(31)-C(36)-C(35)	122.7(18)
C(38)-C(37)-C(42)	114.2(14)
C(38)-C(37)-Si(4)	119.4(10)
C(42)-C(37)-Si(4)	126.3(11)
C(37)-C(38)-C(39)	121.4(16)
C(40)-C(39)-C(38)	124.0(19)
C(39)-C(40)-C(41)	116.8(18)
C(40)-C(41)-C(42)	122.6(15)
C(37)-C(42)-C(41)	121.0(15)
C(48)-C(43)-C(44)	114.5(14)
C(48)-C(43)-Si(4)	124.8(10)

C(44)-C(43)-Si(4)	120.5(10)
C(43)-C(44)-C(47)	122.1(13)
C(46)-C(45)-C(48)	120.7(14)
C(45)-C(46)-C(47)	122.4(15)
C(46)-C(47)-C(44)	117.0(15)
C(43)-C(48)-C(45)	123.0(13)
C(54)-C(49)-C(50)	117.8(14)
C(54)-C(49)-Si(5)	123.2(10)
C(50)-C(49)-Si(5)	118.9(14)
C(51)-C(50)-C(49)	121.9(16)
C(52)-C(51)-C(50)	121.0(14)
C(51)-C(52)-C(53)	117.9(15)
C(54)-C(53)-C(52)	125.6(18)
C(53)-C(54)-C(49)	115.5(14)
C(60)-C(55)-C(56)	115.6(15)
C(60)-C(55)-Si(5)	123.2(13)
C(56)-C(55)-Si(5)	121.1(10)
C(57)-C(56)-C(55)	124.7(17)
C(58)-C(57)-C(56)	118(2)
C(59)-C(58)-C(57)	120(2)
C(58)-C(59)-C(60)	122(2)
C(55)-C(60)-C(59)	120.0(19)
C(62)-C(61)-C(66)	115.4(16)
C(62)-C(61)-Si(6)	126.5(13)
C(66)-C(61)-Si(6)	118.1(12)
C(61)-C(62)-C(63)	125.3(19)
C(62)-C(63)-C(64)	114(2)
C(65)-C(64)-C(63)	124(2)
C(64)-C(65)-C(66)	118(2)
C(65)-C(66)-C(61)	123(2)
C(68)-C(67)-C(72)	113.2(13)
C(68)-C(67)-Si(6)	123.8(11)
C(72)-C(67)-Si(6)	123.0(11)
C(69)-C(68)-C(67)	128.4(17)
C(68)-C(69)-C(70)	116.6(16)
C(71)-C(70)-C(69)	119.9(14)
C(70)-C(71)-C(72)	116.9(14)
C(67)-C(72)-C(71)	124.6(14)
C(78)-C(73)-C(74)	117.6(11)
C(78)-C(73)-Si(7)	123.7(10)
C(74)-C(73)-Si(7)	118.5(9)
C(75)-C(74)-C(73)	115.8(13)
C(76)-C(75)-C(74)	123.9(15)
C(77)-C(76)-C(75)	115.9(15)
C(76)-C(77)-C(78)	125.0(17)
C(73)-C(78)-C(77)	121.3(16)
C(84)-C(79)-C(80)	114.4(17)
C(84)-C(79)-Si(8)	125.8(14)
C(80)-C(79)-Si(8)	119.8(11)
C(81)-C(80)-C(79)	122(2)
C(82)-C(81)-C(80)	127(3)
C(81)-C(82)-C(83)	109(2)
C(84)-C(83)-C(82)	123(2)
C(79)-C(84)-C(83)	124(2)
C(90)-C(85)-C(86)	115.2(14)
C(90)-C(85)-Si(8)	122.8(11)
C(86)-C(85)-Si(8)	121.9(10)
C(87)-C(86)-C(85)	118.3(14)
C(88)-C(87)-C(86)	124.4(17)
C(87)-C(88)-C(89)	119.1(17)
C(90)-C(89)-C(88)	116.4(17)
C(89)-C(90)-C(85)	126.1(17)
C(92)-C(91)-C(96)	118.2(15)
C(92)-C(91)-Si(7)	121.1(10)
C(96)-C(91)-Si(7)	120.3(11)
C(93)-C(92)-C(91)	121.8(15)
C(92)-C(93)-C(94)	117.3(16)
C(93)-C(94)-C(95)	122.6(16)
C(96)-C(95)-C(94)	115.9(16)
C(95)-C(96)-C(91)	124.0(16)
C(98)-C(97)-N(1)	111.3(14)
C(99)-C(98)-C(97)	110.1(16)
C(100)-C(99)-C(98)	116.2(17)
N(2A)-C(100)-N(2B)	30.7(16)
N(2A)-C(100)-C(99)	127(2)
N(2B)-C(100)-C(99)	133(3)
C(101)#1-C(101)-C(102)	117.0(15)

N(3)-C(102)-C(101)	116.2(12)
N(4)-C(103)-C(104)	118.0(14)
C(103)-C(104)-C(104)#2	118.2(17)
C(106)-C(105)-N(5)	121(2)
C(105)-C(106)-C(106)#3	119(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+3,-y,-z #2 -x+2,-y+1,-z+1 #3 -x+2,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2024. 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}
Al(1)	54(2)	45(2)	34(2)	-1(1)	-7(2)	-15(2)
Al(2)	48(2)	46(2)	37(2)	2(1)	-9(2)	-19(2)
Al(3)	52(2)	45(2)	34(2)	2(1)	-6(2)	-11(2)
Al(4)	52(2)	47(2)	35(2)	1(1)	-11(2)	-15(2)
Si(1)	58(2)	48(2)	38(2)	-1(1)	-8(2)	-18(2)
Si(2)	65(2)	52(2)	37(2)	-2(1)	-12(2)	-20(2)
Si(3)	60(2)	55(2)	40(2)	2(2)	-8(2)	-21(2)
Si(4)	63(2)	49(2)	42(2)	0(1)	-8(2)	-22(2)
Si(5)	49(2)	59(2)	37(2)	1(2)	-5(1)	-13(2)
Si(6)	53(2)	64(2)	36(2)	2(2)	-8(2)	-18(2)
Si(7)	59(2)	50(2)	34(2)	0(1)	-10(1)	-18(2)
Si(8)	54(2)	53(2)	41(2)	0(2)	-12(2)	-13(2)
O(1)	52(5)	53(5)	34(4)	5(3)	-15(3)	-18(4)
O(2)	53(5)	50(5)	43(4)	4(4)	-17(4)	-7(4)
O(3)	55(6)	50(5)	45(4)	6(4)	-9(4)	-15(4)
O(4)	61(6)	49(5)	43(4)	0(4)	-11(4)	-24(4)
O(5)	86(7)	49(6)	48(4)	3(4)	-21(4)	-35(5)
O(6)	70(6)	59(6)	45(4)	10(4)	-12(4)	-29(5)
O(7)	88(7)	49(5)	33(4)	8(3)	-23(4)	-22(5)
O(8)	50(5)	61(6)	53(4)	8(4)	-15(4)	-24(4)
O(9)	60(6)	58(6)	36(4)	-1(4)	-13(4)	-21(4)
O(10)	70(6)	52(5)	37(4)	9(3)	-12(4)	-22(5)
O(11)	34(5)	64(6)	54(5)	2(4)	-4(4)	-6(4)
O(12)	66(6)	57(6)	40(4)	0(4)	-6(4)	-23(5)
O(13)	64(6)	58(6)	42(4)	-4(4)	-9(4)	-14(5)
O(14)	51(5)	72(6)	33(4)	-4(4)	-6(3)	-21(4)
O(15)	70(6)	57(6)	38(4)	4(4)	-14(4)	-17(5)
O(16)	61(6)	55(6)	51(4)	8(4)	-20(4)	-13(5)
C(1)	51(9)	63(9)	52(7)	6(6)	-7(6)	-22(7)
C(2)	81(11)	55(9)	63(8)	-7(7)	-19(7)	-34(8)
C(3)	86(14)	98(15)	80(11)	-54(10)	19(10)	-24(12)
C(4)	73(14)	72(13)	145(18)	-42(12)	32(12)	-20(11)
C(5)	87(15)	63(12)	147(17)	11(12)	-40(12)	-2(11)
C(6)	61(11)	85(12)	86(10)	25(9)	-8(8)	-21(9)
C(7)	64(9)	50(8)	48(7)	0(6)	-17(6)	-19(7)
C(8)	136(17)	108(15)	73(9)	42(9)	-51(10)	-88(13)
C(9)	106(15)	132(17)	91(12)	17(11)	-39(10)	-70(14)
C(10)	94(13)	84(12)	59(8)	8(7)	-9(8)	-68(10)
C(11)	74(12)	106(14)	67(9)	35(9)	-16(8)	-35(10)
C(12)	76(11)	68(11)	79(9)	14(8)	-18(8)	-32(9)
C(13)	74(10)	50(8)	32(6)	1(5)	-6(6)	-26(7)
C(14)	76(10)	58(10)	54(7)	16(6)	-18(7)	-23(8)
C(15)	61(10)	86(12)	59(9)	17(8)	-2(7)	-5(9)
C(16)	69(11)	91(14)	47(8)	25(9)	9(7)	-5(10)
C(17)	117(15)	89(13)	28(7)	-13(7)	-5(8)	-10(11)
C(18)	92(12)	96(12)	39(7)	-15(7)	0(7)	-40(10)
C(19)	54(9)	95(11)	35(6)	-6(6)	-8(6)	-38(8)
C(20)	83(14)	131(17)	136(15)	60(14)	-73(12)	-45(12)
C(21)	84(15)	133(19)	139(16)	53(14)	-50(13)	-47(14)
C(22)	117(19)	92(16)	210(20)	9(16)	-112(19)	-44(14)
C(23)	150(20)	133(19)	170(20)	56(16)	-117(18)	-66(16)
C(24)	91(15)	77(13)	171(17)	24(12)	-84(14)	-42(11)
C(25)	55(9)	71(10)	41(6)	4(6)	-2(6)	-28(7)
C(26)	96(12)	70(10)	48(8)	15(7)	-6(7)	-35(9)
C(27)	100(13)	126(16)	30(7)	2(8)	-8(7)	-71(12)
C(28)	115(16)	115(16)	60(10)	18(10)	1(9)	-58(14)
C(29)	100(13)	99(13)	43(7)	17(8)	-18(8)	-42(10)
C(30)	93(12)	75(11)	56(8)	18(7)	-16(8)	-49(10)
C(31)	74(10)	43(8)	61(7)	-4(6)	-17(7)	-27(7)
C(32)	59(11)	105(15)	124(13)	15(11)	-35(10)	-46(10)
C(33)	84(15)	190(20)	132(16)	39(17)	-30(13)	-87(16)
C(34)	130(20)	200(30)	69(11)	-16(14)	-19(12)	-80(20)
C(35)	81(14)	117(16)	128(15)	-10(13)	-65(13)	-28(12)
C(36)	72(11)	98(13)	48(7)	-5(7)	-9(7)	-20(9)
C(37)	67(10)	51(9)	50(7)	1(6)	-19(6)	-12(7)
C(38)	129(16)	67(11)	66(9)	2(7)	-15(9)	-61(11)
C(39)	96(16)	111(18)	170(20)	-14(14)	-15(13)	-77(14)
C(40)	111(15)	93(14)	76(11)	-3(9)	-29(10)	-58(12)
C(41)	100(15)	116(16)	82(11)	-7(11)	-45(11)	-41(12)
C(42)	103(14)	118(15)	43(7)	14(8)	-25(8)	-48(12)
C(43)	100(12)	54(9)	38(6)	-6(6)	1(7)	-32(8)

C(44)	60(10)	47(9)	80(9)	17(7)	-12(7)	-6(7)
C(45)	62(10)	61(10)	81(10)	13(7)	-33(8)	-24(8)
C(46)	75(12)	54(10)	78(10)	18(8)	-18(8)	-10(8)
C(47)	78(13)	54(10)	124(14)	11(9)	16(9)	-22(9)
C(48)	80(11)	52(8)	41(6)	3(6)	-17(6)	-18(8)
C(49)	81(12)	45(8)	49(7)	-2(6)	-15(7)	11(8)
C(50)	65(10)	82(11)	52(7)	10(7)	-16(7)	-24(8)
C(51)	80(12)	93(13)	51(8)	14(7)	-10(8)	-34(10)
C(52)	81(12)	106(14)	53(8)	19(8)	-29(8)	-36(10)
C(53)	73(13)	106(15)	151(17)	17(13)	-53(12)	-41(11)
C(54)	87(13)	82(12)	71(9)	32(8)	-30(9)	-48(10)
C(55)	51(9)	58(9)	48(7)	4(6)	-5(6)	2(7)
C(56)	56(10)	96(13)	62(8)	-15(8)	-7(7)	-6(9)
C(57)	160(20)	112(17)	77(11)	-13(11)	-44(13)	-56(16)
C(58)	118(19)	150(20)	77(12)	-60(12)	13(11)	-64(17)
C(59)	150(20)	83(15)	129(17)	-43(12)	-26(16)	-25(15)
C(60)	96(14)	109(14)	55(8)	-33(9)	-29(8)	-2(11)
C(61)	41(8)	67(10)	75(9)	-19(7)	-8(7)	-8(7)
C(62)	68(11)	69(12)	79(10)	-4(8)	-4(8)	-27(9)
C(63)	79(15)	110(18)	149(19)	-47(15)	-8(12)	-34(13)
C(64)	88(16)	109(18)	121(16)	-11(14)	4(12)	-58(14)
C(65)	130(20)	105(19)	144(19)	3(14)	-11(16)	-78(17)
C(66)	68(11)	94(14)	93(11)	4(10)	-12(8)	-40(10)
C(67)	54(9)	73(10)	44(6)	6(6)	-18(6)	-25(7)
C(68)	85(13)	80(11)	59(9)	-5(8)	-20(8)	-9(10)
C(69)	107(15)	101(14)	61(10)	-27(9)	-8(9)	6(11)
C(70)	138(18)	78(12)	43(8)	-11(7)	-21(10)	-16(11)
C(71)	61(10)	135(15)	44(7)	-20(8)	-16(7)	-18(10)
C(72)	68(10)	77(11)	53(7)	-12(7)	-1(7)	-30(8)
C(73)	61(9)	51(8)	37(6)	12(5)	-14(6)	-19(7)
C(74)	67(10)	81(11)	38(6)	-2(6)	0(6)	-23(8)
C(75)	107(14)	119(14)	25(6)	-13(7)	-7(7)	-34(12)
C(76)	130(18)	114(15)	50(9)	10(9)	-38(10)	-25(13)
C(77)	141(19)	133(17)	69(11)	15(11)	-63(12)	-9(15)
C(78)	129(16)	100(13)	43(8)	-4(8)	-23(9)	-33(12)
C(79)	70(10)	65(10)	42(7)	-7(6)	-10(6)	-11(8)
C(80)	70(12)	109(15)	76(10)	-26(9)	5(8)	-47(10)
C(81)	90(16)	210(30)	102(14)	-64(15)	24(12)	-98(18)
C(82)	71(16)	250(30)	139(19)	-60(20)	-47(14)	-60(20)
C(83)	60(15)	170(30)	150(20)	-68(18)	-30(13)	-11(15)
C(84)	58(11)	121(15)	94(11)	4(10)	-38(9)	-14(10)
C(85)	75(10)	54(9)	36(6)	-3(5)	-20(6)	-14(7)
C(86)	98(13)	69(12)	57(8)	-3(7)	-9(8)	-20(10)
C(87)	125(18)	88(16)	89(12)	0(11)	13(11)	-51(13)
C(88)	160(20)	57(12)	116(15)	28(11)	-69(15)	-51(13)
C(89)	150(20)	44(12)	123(16)	-27(10)	-47(14)	-12(12)
C(90)	101(14)	58(11)	69(9)	-6(7)	-16(8)	-8(9)
C(91)	44(8)	62(9)	53(7)	-6(6)	-7(6)	-12(7)
C(92)	71(11)	74(11)	88(10)	1(8)	-33(8)	-43(9)
C(93)	160(20)	89(14)	82(11)	-1(9)	-30(11)	-86(14)
C(94)	142(19)	88(15)	117(15)	9(11)	-1(13)	-89(14)
C(95)	98(14)	121(17)	60(9)	-2(10)	21(8)	-55(12)
C(96)	76(11)	58(10)	52(7)	6(6)	-7(7)	-24(8)
N(1)	90(11)	78(10)	89(9)	-10(7)	-25(7)	-25(8)
C(97)	83(14)	101(15)	132(14)	-15(12)	-53(12)	-36(12)
C(98)	101(14)	114(15)	67(9)	11(9)	-22(9)	-55(12)
C(99)	85(13)	115(16)	100(12)	17(11)	-23(10)	-64(12)
C(100)	103(17)	91(15)	200(20)	34(15)	-81(17)	-57(13)
N(2A)	170(30)	100(30)	90(30)	10(20)	-80(20)	-60(30)
N(2B)	40(30)	50(30)	11(19)	-32(15)	9(15)	-31(19)
N(3)	74(9)	69(8)	41(5)	-8(5)	3(5)	-14(7)
C(101)	49(8)	68(10)	51(7)	12(6)	-15(6)	-15(7)
C(102)	49(8)	55(9)	59(7)	9(6)	-25(6)	-9(6)
N(4)	148(14)	81(9)	39(6)	-1(5)	-26(7)	-58(9)
C(103)	61(10)	78(11)	63(9)	-9(7)	5(7)	-14(8)
C(104)	101(13)	89(12)	59(8)	-7(7)	-8(8)	-59(10)
N(5)	520(50)	240(30)	118(17)	107(18)	-170(30)	-270(30)
C(105)	120(20)	220(30)	150(20)	100(20)	-61(17)	-80(20)
C(106)	150(20)	150(30)	130(20)	-26(16)	33(17)	-65(19)

sh 2338

Table 1. Crystal data and structure refinement for sh2338.

Identification code	sh2338	
Empirical formula	C122 H148 Al4 N6 O23 Si8	
Formula weight	2399.10	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 17.4253(14) Å	α= 93.363(5)°.
	b = 17.9309(14) Å	β= 102.747(5)°.
	c = 24.267(3) Å	γ = 118.734(3)°.
Volume	6363.2(10) $Å^3$	
Z	2	
Density (calculated)	1.252 Mg/m^3	
Absorption coefficient	0.181 mm^{-1}	
F(000)	2540	
Crystal size	0.43 x 0.35 x 0.2 mm^3	
Theta range for data collection	1.32 to 28.93°.	
Index ranges	-23<=h<=23, -24<=k<=24, -19<=l<=33	
Reflections collected	81002	
Independent reflections	32898 [R(int) = 0.0447]	
Completeness to theta = 28.93°	97.9 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	32898 / 0 / 1483	
Goodness-of-fit on F^2	2.153	
Final R indices [I>2sigma(I)]	R1 = 0.1088, wR2 = 0.2808	
R indices (all data)	R1 = 0.1631, wR2 = 0.2953	
Largest diff. peak and hole	1.451 and -1.053 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2338. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	3565(1)	2643(1)	2326(1)	20(1)
Al(2)	4884(1)	2460(1)	3428(1)	22(1)
Al(3)	5332(1)	1427(1)	2503(1)	19(1)
Al(4)	3976(1)	1584(1)	1406(1)	17(1)
Si(1)	2189(1)	2386(1)	3084(1)	22(1)
Si(2)	3204(1)	1722(1)	3998(1)	24(1)
Si(3)	7043(1)	3632(1)	4096(1)	32(1)
Si(4)	7371(1)	2387(1)	3293(1)	27(1)
Si(5)	4447(1)	-572(1)	1907(1)	23(1)
Si(6)	2856(1)	-485(1)	1041(1)	22(1)
Si(7)	4378(1)	3082(1)	615(1)	19(1)
Si(8)	3714(1)	3915(1)	1427(1)	19(1)
O(1)	4514(2)	2868(2)	2874(1)	23(1)
O(2)	5009(2)	1594(2)	3133(1)	24(1)
O(3)	4946(2)	1805(2)	1931(1)	22(1)
O(4)	3253(2)	1778(2)	1751(1)	21(1)
O(5)	2600(2)	2349(2)	2563(1)	26(1)
O(6)	2591(3)	2104(2)	3658(1)	32(1)
O(7)	4141(3)	2021(2)	3846(1)	34(1)
O(8)	5972(3)	3278(3)	3854(1)	40(1)
O(9)	7404(3)	3160(2)	3710(1)	31(1)
O(10)	6532(2)	1985(2)	2715(1)	25(1)
O(11)	4883(2)	317(2)	2347(1)	26(1)
O(12)	3591(3)	-747(2)	1369(1)	33(1)
O(13)	3322(2)	526(2)	1015(1)	22(1)
O(14)	4306(2)	2306(2)	933(1)	23(1)
O(15)	4267(2)	3792(2)	996(1)	21(1)
O(16)	3850(2)	3566(2)	2015(1)	21(1)
C(1)	2422(4)	3503(3)	3323(2)	27(1)
C(2)	2632(4)	4122(3)	2969(2)	30(1)
C(3)	2772(4)	4950(4)	3140(2)	37(1)
C(4)	2710(4)	5171(4)	3677(2)	44(2)
C(5)	2498(5)	4572(5)	4035(2)	53(2)
C(6)	2364(4)	3758(4)	3866(2)	40(1)
C(7)	930(4)	1631(4)	2848(3)	58(2)
C(8A)	659(11)	751(10)	2459(6)	42(3)
C(9A)	-262(12)	129(12)	2190(7)	53(4)
C(10)	-704(7)	499(6)	2234(4)	79(2)
C(11A)	-630(14)	1221(13)	2409(8)	67(5)
C(12A)	256(13)	1781(13)	2668(7)	59(4)
C(8B)	397(8)	1112(8)	2411(5)	51(3)
C(9B)	-987(9)	608(8)	2713(5)	55(3)
C(11B)	-469(8)	1179(7)	3231(5)	53(3)
C(12B)	463(7)	1706(7)	3340(4)	45(2)
C(13)	3453(3)	2110(3)	4785(2)	20(1)
C(14)	4357(4)	2531(4)	5141(2)	42(1)
C(15)	4570(5)	2789(5)	5737(2)	51(2)
C(16)	3870(5)	2586(5)	5988(2)	57(2)
C(17)	2980(5)	2189(4)	5655(2)	43(2)
C(18)	2784(4)	1956(4)	5059(2)	36(1)
C(19)	2487(4)	516(4)	3846(2)	36(1)
C(20)	2866(5)	13(5)	3675(3)	65(2)
C(21)	2342(7)	-906(5)	3601(4)	92(3)
C(22)	1480(7)	-1308(5)	3680(3)	73(3)
C(23)	1118(7)	-837(5)	3804(3)	81(3)
C(24)	1606(6)	68(5)	3881(3)	67(2)
C(25)	7350(4)	3476(4)	4855(2)	32(1)
C(26)	8272(4)	3902(4)	5185(2)	39(1)
C(27)	8522(4)	3702(4)	5712(2)	40(1)
C(28)	7872(5)	3074(4)	5927(2)	42(2)
C(29)	6965(5)	2671(4)	5615(2)	43(2)
C(30)	6710(4)	2863(4)	5086(2)	35(1)
C(31)	7713(4)	4826(4)	4102(2)	37(1)
C(32)	8485(5)	5209(4)	3889(2)	47(2)
C(33)	9010(6)	6109(5)	3938(3)	66(2)
C(34)	8785(7)	6646(5)	4202(3)	76(2)
C(35)	8021(6)	6293(5)	4413(3)	67(2)
C(36)	7497(5)	5391(4)	4370(2)	46(2)
C(37)	8479(4)	2896(4)	3115(2)	34(1)
C(38)	8565(4)	2644(5)	2588(3)	50(2)
C(39)	9416(6)	2984(6)	2478(3)	79(3)

C(40)	10186(5)	3615(6)	2903(4)	80(3)
C(41)	10131(5)	3866(5)	3415(4)	67(2)
C(42)	9285(5)	3509(4)	3537(3)	50(2)
C(43)	7329(4)	1533(4)	3727(2)	37(1)
C(44)	7082(5)	699(4)	3447(3)	58(2)
C(45)	7069(6)	68(5)	3763(3)	69(2)
C(46)	7273(6)	244(5)	4358(3)	72(2)
C(47)	7533(6)	1052(5)	4646(3)	64(2)
C(48)	7569(5)	1695(5)	4329(3)	55(2)
C(49)	5356(4)	-569(3)	1612(2)	24(1)
C(50)	5206(4)	-1261(3)	1211(2)	30(1)
C(51)	5911(4)	-1238(4)	1018(2)	38(1)
C(52)	6777(4)	-518(4)	1206(2)	36(1)
C(53)	6951(4)	186(4)	1593(2)	34(1)
C(54)	6247(4)	162(3)	1792(2)	31(1)
C(55)	3996(4)	-1475(3)	2309(2)	30(1)
C(56)	3116(5)	-2155(4)	2143(3)	54(2)
C(57)	2814(6)	-2789(5)	2498(4)	82(3)
C(58)	3381(8)	-2715(5)	3000(4)	75(3)
C(59)	4267(8)	-2043(6)	3175(3)	74(3)
C(60)	4591(5)	-1419(4)	2829(2)	50(2)
C(61)	2319(3)	-1187(3)	307(2)	23(1)
C(62)	2038(3)	-919(3)	-196(2)	27(1)
C(63)	1581(4)	-1487(4)	-728(2)	34(1)
C(64)	1376(4)	-2347(4)	-762(2)	41(1)
C(65)	1639(4)	-2634(4)	-282(2)	37(1)
C(66)	2106(4)	-2055(3)	244(2)	33(1)
C(67)	1935(4)	-789(3)	1420(2)	28(1)
C(68)	1011(4)	-1328(3)	1122(2)	34(1)
C(69)	331(4)	-1490(4)	1389(3)	45(2)
C(70)	555(5)	-1107(5)	1959(3)	74(3)
C(71)	1471(6)	-561(6)	2258(3)	76(3)
C(72)	2143(5)	-426(4)	1999(2)	49(2)
C(73)	5544(3)	3706(3)	502(2)	22(1)
C(74)	6118(4)	4594(3)	690(2)	29(1)
C(75)	6993(4)	5023(4)	613(2)	35(1)
C(76)	7316(4)	4570(4)	356(2)	38(1)
C(77)	6756(4)	3687(4)	154(2)	34(1)
C(78)	5888(4)	3263(3)	226(2)	28(1)
C(79)	3497(3)	2662(3)	-107(2)	21(1)
C(80)	3579(4)	3194(3)	-514(2)	29(1)
C(81)	2922(4)	2915(4)	-1037(2)	35(1)
C(82)	2158(4)	2097(4)	-1166(2)	34(1)
C(83)	2062(4)	1551(4)	-772(2)	32(1)
C(84)	2734(4)	1831(3)	-246(2)	27(1)
C(85)	4172(3)	5109(3)	1607(2)	21(1)
C(86)	4401(4)	5652(3)	1203(2)	27(1)
C(87)	4661(4)	6511(3)	1328(2)	40(2)
C(88)	4707(4)	6879(4)	1867(2)	40(1)
C(89)	4498(4)	6361(3)	2281(2)	36(1)
C(90)	4237(4)	5491(3)	2152(2)	27(1)
C(91)	2474(3)	3363(3)	1020(2)	21(1)
C(92)	2182(4)	3409(3)	441(2)	30(1)
C(93)	1262(4)	3027(4)	148(2)	35(1)
C(94)	599(4)	2597(4)	418(2)	37(1)
C(95)	868(4)	2534(3)	996(2)	33(1)
C(96)	1783(3)	2911(3)	1289(2)	26(1)
N(1)	5802(3)	4543(3)	3085(2)	37(1)
C(97)	6218(5)	5036(4)	2650(2)	46(2)
C(98)	6316(5)	4459(5)	2196(2)	51(2)
C(99)	6915(5)	4117(4)	2449(2)	50(2)
C(100)	7158(4)	3705(4)	1993(2)	45(2)
N(2)	6337(3)	2948(3)	1582(2)	29(1)
N(3)	5016(4)	419(3)	3744(2)	51(2)
C(101)	5144(4)	632(4)	4366(2)	34(1)
C(102)	4906(4)	-143(3)	4675(2)	37(1)
N(4)	1458(3)	848(3)	1237(2)	32(1)
C(103)	1174(3)	663(3)	597(2)	28(1)
C(104)	127(3)	99(3)	336(2)	32(1)
N(5)	5066(5)	5129(4)	3834(2)	69(2)
C(105)	4824(6)	4479(6)	4222(3)	69(2)
C(106)	4677(7)	4762(8)	4772(3)	122(5)
N(6)	6513(3)	1750(3)	883(2)	36(1)
C(107)	5559(4)	1037(3)	589(2)	30(1)
C(108)	5481(4)	365(3)	136(2)	32(1)
O(17)	8553(4)	4296(4)	9473(2)	69(2)
C(109)	9202(5)	4201(5)	9274(3)	60(2)

C(110)	9705(6)	4922(6)	8985(3)	85(3)
O(18)	9065(4)	4942(4)	8502(2)	81(2)
C(111)	8400(7)	5030(6)	8696(3)	79(3)
C(112)	7919(6)	4319(6)	8998(3)	69(2)
O(19)	915(3)	4540(3)	8099(2)	71(2)
C(113)	542(6)	4836(6)	7609(4)	84(3)
C(114)	-410(6)	4224(5)	7332(3)	73(2)
O(20)	-554(5)	3407(4)	7134(2)	107(3)
C(115)	-226(10)	3092(7)	7599(5)	179(8)
C(116)	732(8)	3688(7)	7901(6)	144(6)
O(21)	2281(5)	2771(4)	7486(3)	94(2)
C(117)	3062(6)	2695(6)	7489(3)	73(2)
C(1A8)	2865(7)	1809(6)	7411(4)	54(2)
C(1B8)	2916(17)	2020(15)	7005(8)	58(7)
O(22)	2172(6)	1330(5)	6887(2)	96(2)
C(119)	1363(8)	1391(7)	6874(4)	102(3)
C(1A0)	1645(10)	2355(9)	7001(4)	66(4)
C(1B0)	1314(12)	1833(10)	7248(7)	49(4)
O(23)	498(6)	794(5)	5374(4)	130(3)
C(122)	39(13)	861(16)	4842(5)	246(12)
C(123)	746(11)	3(13)	5436(6)	214(9)

Table 3. Bond lengths [Å] and angles [°] for sh2338.

Al(1)-O(1)	1.730(3)
Al(1)-O(5)	1.746(4)
Al(1)-O(16)	1.755(3)
Al(1)-O(4)	1.802(3)
Al(2)-O(1)	1.715(3)
Al(2)-O(7)	1.736(4)
Al(2)-O(8)	1.760(4)
Al(2)-O(2)	1.799(3)
Al(3)-O(3)	1.726(3)
Al(3)-O(11)	1.732(3)
Al(3)-O(10)	1.757(4)
Al(3)-O(2)	1.799(3)
Al(4)-O(3)	1.727(3)
Al(4)-O(13)	1.741(3)
Al(4)-O(14)	1.753(3)
Al(4)-O(4)	1.806(3)
Si(1)-O(5)	1.596(3)
Si(1)-O(6)	1.637(3)
Si(1)-C(7)	1.864(7)
Si(1)-C(1)	1.869(5)
Si(2)-O(7)	1.594(4)
Si(2)-O(6)	1.634(3)
Si(2)-C(19)	1.865(6)
Si(2)-C(13)	1.872(4)
Si(3)-O(8)	1.601(4)
Si(3)-O(9)	1.634(3)
Si(3)-C(25)	1.879(5)
Si(3)-C(31)	1.879(6)
Si(4)-O(10)	1.610(3)
Si(4)-O(9)	1.638(3)
Si(4)-C(37)	1.863(6)
Si(4)-C(43)	1.890(6)
Si(5)-O(11)	1.592(3)
Si(5)-O(12)	1.633(4)
Si(5)-C(55)	1.869(5)
Si(5)-C(49)	1.877(5)
Si(6)-O(13)	1.603(3)
Si(6)-O(12)	1.634(4)
Si(6)-C(61)	1.872(4)
Si(6)-C(67)	1.894(5)
Si(7)-O(14)	1.597(3)
Si(7)-O(15)	1.642(3)
Si(7)-C(79)	1.881(5)
Si(7)-C(73)	1.883(5)
Si(8)-O(16)	1.606(3)
Si(8)-O(15)	1.641(3)
Si(8)-C(85)	1.874(5)
Si(8)-C(91)	1.874(5)
C(1)-C(2)	1.401(7)
C(1)-C(6)	1.410(6)
C(2)-C(3)	1.404(7)
C(3)-C(4)	1.381(7)
C(4)-C(5)	1.385(9)
C(5)-C(6)	1.383(8)
C(7)-C(8B)	1.212(12)
C(7)-C(12A)	1.315(19)
C(7)-C(8A)	1.586(16)
C(7)-C(12B)	1.619(12)
C(8A)-C(9A)	1.41(2)
C(9A)-C(10)	1.249(18)
C(10)-C(11A)	1.27(2)
C(10)-C(9B)	1.398(13)
C(10)-C(8B)	1.620(15)
C(11A)-C(12A)	1.34(3)
C(9B)-C(11B)	1.378(14)
C(11B)-C(12B)	1.380(15)
C(13)-C(18)	1.390(7)
C(13)-C(14)	1.405(7)
C(14)-C(15)	1.400(7)
C(15)-C(16)	1.385(9)
C(16)-C(17)	1.371(9)
C(17)-C(18)	1.399(7)
C(19)-C(24)	1.374(9)
C(19)-C(20)	1.439(8)
C(20)-C(21)	1.424(10)

C(21)-C(22)	1.385(13)
C(22)-C(23)	1.330(11)
C(23)-C(24)	1.399(10)
C(25)-C(30)	1.391(8)
C(25)-C(26)	1.409(8)
C(26)-C(27)	1.383(7)
C(27)-C(28)	1.388(9)
C(28)-C(29)	1.379(9)
C(29)-C(30)	1.383(8)
C(31)-C(36)	1.409(7)
C(31)-C(32)	1.418(9)
C(32)-C(33)	1.402(9)
C(33)-C(34)	1.376(11)
C(34)-C(35)	1.399(12)
C(35)-C(36)	1.407(10)
C(37)-C(38)	1.393(7)
C(37)-C(42)	1.407(8)
C(38)-C(39)	1.403(9)
C(39)-C(40)	1.392(11)
C(40)-C(41)	1.336(11)
C(41)-C(42)	1.406(10)
C(43)-C(48)	1.399(7)
C(43)-C(44)	1.420(8)
C(44)-C(45)	1.397(9)
C(45)-C(46)	1.387(10)
C(46)-C(47)	1.380(10)
C(47)-C(48)	1.408(9)
C(49)-C(50)	1.408(6)
C(49)-C(54)	1.413(7)
C(50)-C(51)	1.393(8)
C(51)-C(52)	1.381(8)
C(52)-C(53)	1.390(7)
C(53)-C(54)	1.397(7)
C(55)-C(56)	1.368(9)
C(55)-C(60)	1.409(8)
C(56)-C(57)	1.431(10)
C(57)-C(58)	1.343(12)
C(58)-C(59)	1.370(13)
C(59)-C(60)	1.409(9)
C(61)-C(66)	1.405(7)
C(61)-C(62)	1.410(6)
C(62)-C(63)	1.398(6)
C(63)-C(64)	1.399(8)
C(64)-C(65)	1.377(8)
C(65)-C(66)	1.395(7)
C(67)-C(68)	1.400(7)
C(67)-C(72)	1.402(7)
C(68)-C(69)	1.391(8)
C(69)-C(70)	1.390(8)
C(70)-C(71)	1.392(10)
C(71)-C(72)	1.377(9)
C(73)-C(74)	1.388(7)
C(73)-C(78)	1.419(6)
C(74)-C(75)	1.401(7)
C(75)-C(76)	1.378(7)
C(76)-C(77)	1.384(8)
C(77)-C(78)	1.386(7)
C(79)-C(84)	1.393(7)
C(79)-C(80)	1.395(6)
C(80)-C(81)	1.382(7)
C(81)-C(82)	1.380(8)
C(82)-C(83)	1.386(7)
C(83)-C(84)	1.397(7)
C(85)-C(86)	1.406(6)
C(85)-C(90)	1.407(6)
C(86)-C(87)	1.372(7)
C(87)-C(88)	1.398(7)
C(88)-C(89)	1.397(7)
C(89)-C(90)	1.392(7)
C(91)-C(92)	1.406(6)
C(91)-C(96)	1.416(7)
C(92)-C(93)	1.388(7)
C(93)-C(94)	1.376(8)
C(94)-C(95)	1.408(7)
C(95)-C(96)	1.384(7)
N(1)-C(97)	1.501(7)
C(97)-C(98)	1.560(8)

C(98)-C(99)	1.491(8)
C(99)-C(100)	1.537(8)
C(100)-N(2)	1.493(7)
N(3)-C(101)	1.474(6)
C(101)-C(102)	1.540(7)
C(102)-C(102)#1	1.542(9)
N(4)-C(103)	1.486(6)
C(103)-C(104)	1.546(7)
C(104)-C(104)#2	1.565(10)
N(5)-C(105)	1.502(10)
C(105)-C(106)	1.516(9)
C(106)-C(106)#3	1.278(16)
N(6)-C(107)	1.495(7)
C(107)-C(108)	1.516(7)
C(108)-C(108)#4	1.503(11)
O(17)-C(109)	1.400(8)
O(17)-C(112)	1.427(8)
C(109)-C(110)	1.489(11)
C(110)-O(18)	1.444(10)
O(18)-C(111)	1.413(9)
C(111)-C(112)	1.490(11)
O(19)-C(116)	1.430(11)
O(19)-C(113)	1.476(9)
C(113)-C(114)	1.442(11)
C(114)-O(20)	1.396(9)
O(20)-C(115)	1.423(11)
C(115)-C(116)	1.455(15)
O(21)-C(1A0)	1.302(12)
O(21)-C(117)	1.430(9)
O(21)-C(1B0)	1.653(18)
C(117)-C(1A8)	1.446(12)
C(117)-C(1B8)	1.52(2)
C(1A8)-O(22)	1.418(11)
C(1B8)-O(22)	1.24(2)
O(22)-C(119)	1.458(11)
C(119)-C(1B0)	1.213(17)
C(119)-C(1A0)	1.542(16)
O(23)-C(122)	1.406(12)
O(23)-C(123)	1.676(17)
C(122)-C(123)#5	1.47(2)
C(123)-C(122)#5	1.47(2)

O(1)-Al(1)-O(5)	112.79(16)
O(1)-Al(1)-O(16)	107.43(16)
O(5)-Al(1)-O(16)	111.10(16)
O(1)-Al(1)-O(4)	113.00(15)
O(5)-Al(1)-O(4)	106.67(16)
O(16)-Al(1)-O(4)	105.66(14)
O(1)-Al(2)-O(7)	114.61(18)
O(1)-Al(2)-O(8)	108.71(19)
O(7)-Al(2)-O(8)	111.10(19)
O(1)-Al(2)-O(2)	108.90(14)
O(7)-Al(2)-O(2)	106.02(17)
O(8)-Al(2)-O(2)	107.21(18)
O(3)-Al(3)-O(11)	112.20(16)
O(3)-Al(3)-O(10)	109.65(17)
O(11)-Al(3)-O(10)	111.24(17)
O(3)-Al(3)-O(2)	113.58(15)
O(11)-Al(3)-O(2)	104.06(16)
O(10)-Al(3)-O(2)	105.85(16)
O(3)-Al(4)-O(13)	115.44(16)
O(3)-Al(4)-O(14)	108.13(17)
O(13)-Al(4)-O(14)	109.33(15)
O(3)-Al(4)-O(4)	108.15(14)
O(13)-Al(4)-O(4)	106.95(16)
O(14)-Al(4)-O(4)	108.67(15)
O(5)-Si(1)-O(6)	114.53(18)
O(5)-Si(1)-C(7)	109.4(3)
O(6)-Si(1)-C(7)	106.6(2)
O(5)-Si(1)-C(1)	111.3(2)
O(6)-Si(1)-C(1)	106.22(19)
C(7)-Si(1)-C(1)	108.6(3)
O(7)-Si(2)-O(6)	114.58(18)
O(7)-Si(2)-C(19)	110.6(2)
O(6)-Si(2)-C(19)	108.1(2)
O(7)-Si(2)-C(13)	109.1(2)
O(6)-Si(2)-C(13)	106.46(19)

C(19)-Si(2)-C(13)	107.7(2)
O(8)-Si(3)-O(9)	112.99(18)
O(8)-Si(3)-C(25)	111.6(2)
O(9)-Si(3)-C(25)	107.4(2)
O(8)-Si(3)-C(31)	110.2(2)
O(9)-Si(3)-C(31)	107.2(2)
C(25)-Si(3)-C(31)	107.3(2)
O(10)-Si(4)-O(9)	112.46(18)
O(10)-Si(4)-C(37)	110.5(2)
O(9)-Si(4)-C(37)	105.6(2)
O(10)-Si(4)-C(43)	111.8(2)
O(9)-Si(4)-C(43)	108.1(2)
C(37)-Si(4)-C(43)	108.1(2)
O(11)-Si(5)-O(12)	114.08(18)
O(11)-Si(5)-C(55)	107.8(2)
O(12)-Si(5)-C(55)	106.9(2)
O(11)-Si(5)-C(49)	108.7(2)
O(12)-Si(5)-C(49)	108.58(19)
C(55)-Si(5)-C(49)	110.8(2)
O(13)-Si(6)-O(12)	112.60(19)
O(13)-Si(6)-C(61)	112.12(19)
O(12)-Si(6)-C(61)	104.85(19)
O(13)-Si(6)-C(67)	109.7(2)
O(12)-Si(6)-C(67)	109.3(2)
C(61)-Si(6)-C(67)	108.1(2)
O(14)-Si(7)-O(15)	112.65(16)
O(14)-Si(7)-C(79)	111.1(2)
O(15)-Si(7)-C(79)	108.91(18)
O(14)-Si(7)-C(73)	109.90(19)
O(15)-Si(7)-C(73)	105.53(19)
C(79)-Si(7)-C(73)	108.56(19)
O(16)-Si(8)-O(15)	114.23(17)
O(16)-Si(8)-C(85)	108.79(17)
O(15)-Si(8)-C(85)	105.81(19)
O(16)-Si(8)-C(91)	110.65(19)
O(15)-Si(8)-C(91)	108.25(18)
C(85)-Si(8)-C(91)	108.9(2)
Al(2)-O(1)-Al(1)	142.7(2)
Al(3)-O(2)-Al(2)	131.55(18)
Al(3)-O(3)-Al(4)	142.7(2)
Al(1)-O(4)-Al(4)	129.13(19)
Si(1)-O(5)-Al(1)	148.1(2)
Si(2)-O(6)-Si(1)	151.9(2)
Si(2)-O(7)-Al(2)	153.6(2)
Si(3)-O(8)-Al(2)	149.2(2)
Si(3)-O(9)-Si(4)	158.2(3)
Si(4)-O(10)-Al(3)	139.6(2)
Si(5)-O(11)-Al(3)	152.0(2)
Si(6)-O(12)-Si(5)	151.0(2)
Si(6)-O(13)-Al(4)	146.3(2)
Si(7)-O(14)-Al(4)	157.2(2)
Si(8)-O(15)-Si(7)	144.6(2)
Si(8)-O(16)-Al(1)	145.3(2)
C(2)-C(1)-C(6)	116.3(4)
C(2)-C(1)-Si(1)	122.2(3)
C(6)-C(1)-Si(1)	121.4(4)
C(1)-C(2)-C(3)	122.3(4)
C(4)-C(3)-C(2)	119.3(5)
C(3)-C(4)-C(5)	119.8(5)
C(6)-C(5)-C(4)	120.6(5)
C(5)-C(6)-C(1)	121.6(5)
C(8B)-C(7)-C(12A)	70.8(10)
C(8B)-C(7)-C(8A)	37.0(7)
C(12A)-C(7)-C(8A)	106.9(11)
C(8B)-C(7)-C(12B)	114.4(9)
C(12A)-C(7)-C(12B)	65.9(9)
C(8A)-C(7)-C(12B)	124.9(8)
C(8B)-C(7)-Si(1)	134.1(8)
C(12A)-C(7)-Si(1)	130.6(10)
C(8A)-C(7)-Si(1)	111.7(7)
C(12B)-C(7)-Si(1)	111.5(6)
C(9A)-C(8A)-C(7)	120.7(13)
C(10)-C(9A)-C(8A)	106.0(15)
C(9A)-C(10)-C(11A)	143.9(16)
C(9A)-C(10)-C(9B)	126.0(11)
C(11A)-C(10)-C(9B)	59.7(10)
C(9A)-C(10)-C(8B)	63.6(10)

C(11A)-C(10)-C(8B)	80.5(12)
C(9B)-C(10)-C(8B)	107.4(9)
C(10)-C(11A)-C(12A)	107.3(18)
C(7)-C(12A)-C(11A)	129.5(18)
C(7)-C(8B)-C(10)	130.8(10)
C(11B)-C(9B)-C(10)	128.3(12)
C(9B)-C(11B)-C(12B)	120.6(11)
C(11B)-C(12B)-C(7)	118.4(9)
C(18)-C(13)-C(14)	116.2(4)
C(18)-C(13)-Si(2)	123.8(4)
C(14)-C(13)-Si(2)	119.8(4)
C(15)-C(14)-C(13)	121.8(5)
C(16)-C(15)-C(14)	119.2(6)
C(17)-C(16)-C(15)	120.7(5)
C(16)-C(17)-C(18)	119.1(6)
C(13)-C(18)-C(17)	122.8(5)
C(24)-C(19)-C(20)	117.1(6)
C(24)-C(19)-Si(2)	124.1(5)
C(20)-C(19)-Si(2)	118.8(5)
C(21)-C(20)-C(19)	118.5(8)
C(22)-C(21)-C(20)	120.8(8)
C(23)-C(22)-C(21)	119.9(8)
C(22)-C(23)-C(24)	121.3(9)
C(19)-C(24)-C(23)	122.1(7)
C(30)-C(25)-C(26)	117.3(5)
C(30)-C(25)-Si(3)	122.1(4)
C(26)-C(25)-Si(3)	120.0(4)
C(27)-C(26)-C(25)	120.8(6)
C(26)-C(27)-C(28)	120.8(6)
C(29)-C(28)-C(27)	118.9(5)
C(28)-C(29)-C(30)	120.6(6)
C(29)-C(30)-C(25)	121.6(5)
C(36)-C(31)-C(32)	117.1(6)
C(36)-C(31)-Si(3)	119.6(5)
C(32)-C(31)-Si(3)	123.1(4)
C(33)-C(32)-C(31)	121.7(6)
C(34)-C(33)-C(32)	120.0(8)
C(33)-C(34)-C(35)	120.1(8)
C(34)-C(35)-C(36)	120.3(7)
C(35)-C(36)-C(31)	120.9(7)
C(38)-C(37)-C(42)	117.3(6)
C(38)-C(37)-Si(4)	122.6(4)
C(42)-C(37)-Si(4)	119.9(4)
C(37)-C(38)-C(39)	121.9(6)
C(40)-C(39)-C(38)	118.3(7)
C(41)-C(40)-C(39)	121.4(8)
C(40)-C(41)-C(42)	120.7(7)
C(37)-C(42)-C(41)	120.3(6)
C(48)-C(43)-C(44)	117.1(5)
C(48)-C(43)-Si(4)	122.5(5)
C(44)-C(43)-Si(4)	120.4(4)
C(45)-C(44)-C(43)	121.0(6)
C(46)-C(45)-C(44)	120.0(7)
C(47)-C(46)-C(45)	120.7(6)
C(46)-C(47)-C(48)	119.3(6)
C(43)-C(48)-C(47)	121.9(6)
C(50)-C(49)-C(54)	116.9(5)
C(50)-C(49)-Si(5)	123.8(4)
C(54)-C(49)-Si(5)	119.3(3)
C(51)-C(50)-C(49)	121.5(5)
C(52)-C(51)-C(50)	120.1(5)
C(51)-C(52)-C(53)	120.3(5)
C(52)-C(53)-C(54)	119.7(5)
C(53)-C(54)-C(49)	121.4(5)
C(56)-C(55)-C(60)	118.7(5)
C(56)-C(55)-Si(5)	123.8(4)
C(60)-C(55)-Si(5)	117.4(4)
C(55)-C(56)-C(57)	120.0(7)
C(58)-C(57)-C(56)	120.6(8)
C(57)-C(58)-C(59)	120.5(7)
C(58)-C(59)-C(60)	120.2(8)
C(59)-C(60)-C(55)	119.9(7)
C(66)-C(61)-C(62)	116.6(4)
C(66)-C(61)-Si(6)	119.6(3)
C(62)-C(61)-Si(6)	123.6(4)
C(63)-C(62)-C(61)	121.5(5)
C(62)-C(63)-C(64)	119.4(5)

C(65)-C(64)-C(63)	120.9(5)
C(64)-C(65)-C(66)	118.9(5)
C(65)-C(66)-C(61)	122.8(5)
C(68)-C(67)-C(72)	117.0(5)
C(68)-C(67)-Si(6)	121.3(4)
C(72)-C(67)-Si(6)	121.5(4)
C(69)-C(68)-C(67)	121.2(5)
C(70)-C(69)-C(68)	120.6(6)
C(69)-C(70)-C(71)	118.8(6)
C(72)-C(71)-C(70)	120.4(6)
C(71)-C(72)-C(67)	121.9(6)
C(74)-C(73)-C(78)	116.4(5)
C(74)-C(73)-Si(7)	123.6(4)
C(78)-C(73)-Si(7)	120.0(4)
C(73)-C(74)-C(75)	121.4(5)
C(76)-C(75)-C(74)	120.8(5)
C(75)-C(76)-C(77)	119.4(5)
C(76)-C(77)-C(78)	119.8(5)
C(77)-C(78)-C(73)	122.2(5)
C(84)-C(79)-C(80)	118.0(4)
C(84)-C(79)-Si(7)	121.7(3)
C(80)-C(79)-Si(7)	120.2(4)
C(81)-C(80)-C(79)	121.4(5)
C(82)-C(81)-C(80)	120.1(5)
C(81)-C(82)-C(83)	119.8(5)
C(82)-C(83)-C(84)	120.0(5)
C(79)-C(84)-C(83)	120.6(5)
C(86)-C(85)-C(90)	117.0(4)
C(86)-C(85)-Si(8)	122.7(3)
C(90)-C(85)-Si(8)	120.2(3)
C(87)-C(86)-C(85)	121.8(4)
C(86)-C(87)-C(88)	120.8(5)
C(89)-C(88)-C(87)	118.9(5)
C(90)-C(89)-C(88)	120.0(4)
C(89)-C(90)-C(85)	121.6(4)
C(92)-C(91)-C(96)	116.6(4)
C(92)-C(91)-Si(8)	121.9(4)
C(96)-C(91)-Si(8)	121.4(3)
C(93)-C(92)-C(91)	121.6(5)
C(94)-C(93)-C(92)	121.0(5)
C(93)-C(94)-C(95)	118.8(5)
C(96)-C(95)-C(94)	120.4(5)
C(95)-C(96)-C(91)	121.5(4)
N(1)-C(97)-C(98)	111.8(5)
C(99)-C(98)-C(97)	113.7(5)
C(98)-C(99)-C(100)	113.0(5)
N(2)-C(100)-C(99)	112.6(5)
N(3)-C(101)-C(102)	114.4(4)
C(101)-C(102)-C(102)#1	111.0(5)
N(4)-C(103)-C(104)	112.8(4)
C(103)-C(104)-C(104)#2	110.4(5)
N(5)-C(105)-C(106)	115.3(7)
C(106)#3-C(106)-C(105)	124.0(12)
N(6)-C(107)-C(108)	114.6(4)
C(108)#4-C(108)-C(107)	113.7(5)
C(109)-O(17)-C(112)	109.0(5)
O(17)-C(109)-C(110)	112.0(7)
O(18)-C(110)-C(109)	109.4(6)
C(111)-O(18)-C(110)	109.4(6)
O(18)-C(111)-C(112)	111.4(6)
O(17)-C(112)-C(111)	110.9(7)
C(116)-O(19)-C(113)	108.5(7)
C(114)-C(113)-O(19)	111.8(7)
O(20)-C(114)-C(113)	111.7(8)
C(114)-O(20)-C(115)	110.0(6)
O(20)-C(115)-C(116)	112.2(11)
O(19)-C(116)-C(115)	112.7(9)
C(1A0)-O(21)-C(117)	110.6(8)
C(1A0)-O(21)-C(1B0)	42.7(8)
C(117)-O(21)-C(1B0)	112.6(8)
O(21)-C(117)-C(1A8)	113.4(8)
O(21)-C(117)-C(1B8)	115.3(12)
C(1A8)-C(117)-C(1B8)	42.8(9)
O(22)-C(1A8)-C(117)	109.3(8)
O(22)-C(1B8)-C(117)	115.0(15)
C(1B8)-O(22)-C(1A8)	47.5(10)
C(1B8)-O(22)-C(119)	117.4(15)

C(1A8)-O(22)-C(119)	110.8(7)
C(1B0)-C(119)-O(22)	124.3(13)
C(1B0)-C(119)-C(1A0)	46.3(9)
O(22)-C(119)-C(1A0)	109.0(10)
O(21)-C(1A0)-C(119)	112.3(9)
C(119)-C(1B0)-O(21)	110.3(13)
C(122)-O(23)-C(123)	121.8(10)
O(23)-C(122)-C(123)#5	108.1(17)
C(122)#5-C(123)-O(23)	112.9(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x,-y,-z #3 -x+1,-y+1,-z+1
#4 -x+1,-y,-z #5 -x,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2338. 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}
Al(1)	28(1)	18(1)	12(1)	3(1)	4(1)	11(1)
Al(2)	30(1)	31(1)	10(1)	4(1)	5(1)	20(1)
Al(3)	25(1)	22(1)	13(1)	3(1)	4(1)	14(1)
Al(4)	22(1)	16(1)	12(1)	2(1)	2(1)	9(1)
Si(1)	24(1)	26(1)	19(1)	10(1)	8(1)	14(1)
Si(2)	37(1)	30(1)	15(1)	10(1)	11(1)	21(1)
Si(3)	39(1)	41(1)	17(1)	-6(1)	-3(1)	26(1)
Si(4)	32(1)	33(1)	19(1)	-1(1)	2(1)	20(1)
Si(5)	31(1)	19(1)	19(1)	5(1)	4(1)	14(1)
Si(6)	27(1)	18(1)	17(1)	1(1)	1(1)	10(1)
Si(7)	24(1)	20(1)	14(1)	6(1)	7(1)	11(1)
Si(8)	24(1)	18(1)	14(1)	5(1)	5(1)	10(1)
O(1)	32(2)	20(2)	11(1)	1(1)	-1(1)	12(2)
O(2)	38(2)	32(2)	14(1)	9(1)	10(1)	25(2)
O(3)	28(2)	27(2)	12(1)	6(1)	6(1)	14(2)
O(4)	26(2)	19(2)	13(1)	0(1)	3(1)	10(2)
O(5)	39(2)	27(2)	18(2)	7(1)	10(1)	20(2)
O(6)	46(2)	45(2)	20(2)	17(2)	15(2)	32(2)
O(7)	53(3)	47(2)	28(2)	24(2)	26(2)	38(2)
O(8)	43(2)	56(3)	21(2)	-12(2)	-5(2)	33(2)
O(9)	36(2)	40(2)	17(2)	-5(1)	-2(2)	23(2)
O(10)	29(2)	31(2)	17(2)	2(1)	6(1)	17(2)
O(11)	34(2)	22(2)	20(2)	3(1)	5(1)	15(2)
O(12)	36(2)	25(2)	32(2)	3(1)	-4(2)	16(2)
O(13)	27(2)	18(2)	18(1)	1(1)	4(1)	9(2)
O(14)	33(2)	25(2)	17(1)	10(1)	12(1)	17(2)
O(15)	24(2)	19(2)	18(1)	4(1)	6(1)	10(2)
O(16)	29(2)	19(2)	13(1)	4(1)	3(1)	10(2)
C(1)	35(3)	30(3)	21(2)	6(2)	8(2)	20(3)
C(2)	37(3)	22(3)	27(2)	0(2)	10(2)	12(2)
C(3)	41(4)	31(3)	43(3)	9(2)	17(3)	19(3)
C(4)	56(4)	42(4)	39(3)	-1(3)	8(3)	33(3)
C(5)	81(5)	75(5)	32(3)	6(3)	16(3)	61(5)
C(6)	62(4)	53(4)	27(3)	15(2)	20(3)	41(4)
C(7)	27(3)	37(4)	101(6)	40(4)	4(4)	13(3)
C(13)	22(3)	25(3)	14(2)	6(2)	6(2)	11(2)
C(14)	36(3)	52(4)	36(3)	-1(3)	4(3)	25(3)
C(15)	44(4)	65(5)	32(3)	-9(3)	-9(3)	30(4)
C(16)	83(6)	73(5)	19(3)	-1(3)	3(3)	49(5)
C(17)	55(4)	51(4)	31(3)	10(3)	21(3)	28(3)
C(18)	34(3)	43(3)	26(2)	0(2)	10(2)	17(3)
C(19)	51(4)	34(3)	18(2)	5(2)	2(2)	23(3)
C(20)	57(5)	41(4)	82(5)	-15(4)	-7(4)	26(4)
C(21)	88(7)	32(4)	121(7)	-12(4)	-27(6)	31(5)
C(22)	99(7)	35(4)	55(4)	14(3)	6(5)	17(5)
C(23)	105(7)	39(4)	83(6)	3(4)	53(5)	13(5)
C(24)	71(6)	46(4)	80(5)	-4(4)	42(4)	19(4)
C(25)	34(3)	39(3)	20(2)	-6(2)	1(2)	21(3)
C(26)	40(4)	43(3)	22(2)	1(2)	-1(2)	17(3)
C(27)	39(4)	51(4)	24(3)	2(2)	-2(2)	24(3)
C(28)	62(4)	38(3)	28(3)	1(2)	5(3)	31(3)
C(29)	58(4)	27(3)	39(3)	-1(2)	22(3)	14(3)
C(30)	32(3)	33(3)	32(3)	-7(2)	6(2)	14(3)
C(31)	50(4)	42(3)	16(2)	-4(2)	-9(2)	29(3)
C(32)	54(4)	50(4)	39(3)	9(3)	4(3)	33(4)
C(33)	68(5)	59(5)	62(4)	27(4)	15(4)	27(4)
C(34)	95(7)	47(5)	76(5)	14(4)	8(5)	35(5)
C(35)	101(7)	48(5)	55(4)	0(3)	5(4)	47(5)
C(36)	60(4)	49(4)	32(3)	0(3)	1(3)	35(4)
C(37)	35(3)	32(3)	29(3)	-1(2)	-2(2)	20(3)
C(38)	33(4)	70(5)	39(3)	9(3)	10(3)	20(3)
C(39)	52(5)	125(8)	58(5)	26(5)	28(4)	37(5)
C(40)	31(4)	90(7)	93(6)	37(5)	13(4)	10(4)
C(41)	33(4)	51(5)	86(6)	2(4)	-15(4)	13(4)
C(42)	44(4)	43(4)	47(3)	-11(3)	-13(3)	22(3)
C(43)	38(3)	44(3)	29(3)	6(2)	1(2)	26(3)
C(44)	76(5)	48(4)	42(3)	-1(3)	-8(3)	37(4)
C(45)	91(6)	47(4)	64(5)	7(3)	-3(4)	42(5)
C(46)	94(7)	72(6)	69(5)	40(4)	20(5)	55(5)
C(47)	93(6)	89(6)	39(3)	30(4)	21(4)	66(5)
C(48)	88(6)	75(5)	40(3)	25(3)	28(4)	64(5)

C(49)	35(3)	22(3)	18(2)	7(2)	4(2)	17(2)
C(50)	44(3)	22(3)	26(2)	5(2)	9(2)	18(3)
C(51)	63(4)	26(3)	34(3)	8(2)	23(3)	26(3)
C(52)	51(4)	35(3)	31(3)	8(2)	23(3)	24(3)
C(53)	39(3)	30(3)	34(3)	7(2)	16(2)	16(3)
C(54)	42(3)	32(3)	21(2)	3(2)	9(2)	21(3)
C(55)	44(3)	24(3)	35(3)	12(2)	20(2)	22(3)
C(56)	53(5)	34(4)	78(5)	24(3)	29(4)	18(3)
C(57)	81(7)	37(4)	129(8)	25(5)	71(6)	13(4)
C(58)	147(9)	48(5)	75(5)	40(4)	80(6)	60(6)
C(59)	151(9)	65(5)	47(4)	35(4)	47(5)	74(6)
C(60)	74(5)	46(4)	43(3)	26(3)	25(3)	36(4)
C(61)	29(3)	26(3)	13(2)	-3(2)	-1(2)	16(2)
C(62)	27(3)	28(3)	22(2)	5(2)	8(2)	10(2)
C(63)	28(3)	50(4)	19(2)	3(2)	4(2)	17(3)
C(64)	28(3)	49(4)	32(3)	-11(2)	8(2)	11(3)
C(65)	28(3)	28(3)	45(3)	-10(2)	9(3)	9(3)
C(66)	31(3)	25(3)	37(3)	2(2)	7(2)	12(3)
C(67)	31(3)	22(3)	25(2)	10(2)	8(2)	9(2)
C(68)	35(3)	25(3)	31(3)	2(2)	10(2)	8(3)
C(69)	32(3)	36(3)	46(3)	4(3)	17(3)	0(3)
C(70)	57(5)	83(6)	44(4)	4(4)	33(4)	0(4)
C(71)	70(6)	99(6)	24(3)	11(3)	23(3)	12(5)
C(72)	41(4)	55(4)	22(3)	6(2)	6(3)	3(3)
C(73)	25(3)	29(3)	13(2)	7(2)	5(2)	15(2)
C(74)	35(3)	32(3)	23(2)	11(2)	10(2)	18(3)
C(75)	28(3)	32(3)	35(3)	4(2)	10(2)	7(3)
C(76)	26(3)	44(4)	39(3)	11(3)	14(2)	12(3)
C(77)	41(3)	47(4)	30(3)	17(2)	19(2)	29(3)
C(78)	35(3)	27(3)	23(2)	8(2)	10(2)	16(2)
C(79)	26(3)	24(3)	15(2)	3(2)	8(2)	12(2)
C(80)	31(3)	28(3)	23(2)	5(2)	5(2)	13(2)
C(81)	44(4)	44(3)	16(2)	8(2)	5(2)	23(3)
C(82)	28(3)	51(4)	19(2)	-2(2)	1(2)	21(3)
C(83)	20(3)	34(3)	29(3)	-5(2)	8(2)	5(2)
C(84)	34(3)	31(3)	20(2)	3(2)	11(2)	19(3)
C(85)	24(3)	19(2)	16(2)	6(2)	4(2)	9(2)
C(86)	34(3)	24(3)	17(2)	5(2)	6(2)	12(2)
C(87)	67(4)	21(3)	29(3)	10(2)	12(3)	20(3)
C(88)	58(4)	19(3)	41(3)	4(2)	12(3)	18(3)
C(89)	49(4)	29(3)	29(3)	2(2)	14(3)	19(3)
C(90)	34(3)	21(3)	23(2)	5(2)	9(2)	11(2)
C(91)	24(3)	19(2)	15(2)	1(2)	3(2)	9(2)
C(92)	32(3)	40(3)	17(2)	6(2)	5(2)	20(3)
C(93)	35(3)	47(4)	18(2)	0(2)	1(2)	20(3)
C(94)	25(3)	48(4)	22(2)	-6(2)	-3(2)	13(3)
C(95)	26(3)	35(3)	30(3)	1(2)	10(2)	9(3)
C(96)	30(3)	24(3)	23(2)	4(2)	7(2)	13(2)
N(1)	42(3)	25(2)	31(2)	1(2)	0(2)	12(2)
C(97)	48(4)	35(3)	42(3)	14(3)	6(3)	13(3)
C(98)	53(4)	71(5)	36(3)	20(3)	16(3)	36(4)
C(99)	59(5)	43(4)	41(3)	5(3)	6(3)	24(4)
C(100)	51(4)	34(3)	34(3)	8(2)	9(3)	11(3)
N(2)	32(3)	30(2)	20(2)	9(2)	8(2)	11(2)
N(3)	99(5)	61(4)	37(3)	31(2)	38(3)	64(4)
C(101)	52(4)	36(3)	24(2)	16(2)	15(2)	27(3)
C(102)	56(4)	29(3)	23(2)	11(2)	10(3)	21(3)
N(4)	21(2)	31(2)	32(2)	-3(2)	6(2)	6(2)
C(103)	28(3)	20(3)	28(2)	2(2)	8(2)	5(2)
C(104)	20(3)	29(3)	34(3)	1(2)	4(2)	6(2)
N(5)	71(5)	79(5)	62(4)	-22(3)	-6(3)	55(4)
C(105)	85(6)	107(7)	44(4)	-2(4)	3(4)	79(6)
C(106)	144(10)	238(14)	53(5)	-20(6)	-8(5)	168(11)
N(6)	32(3)	34(3)	40(3)	9(2)	12(2)	13(2)
C(107)	28(3)	31(3)	33(3)	12(2)	13(2)	15(3)
C(108)	33(3)	36(3)	32(3)	14(2)	14(2)	19(3)
O(17)	81(4)	98(4)	58(3)	33(3)	39(3)	59(4)
C(109)	60(5)	70(5)	50(4)	10(3)	15(4)	34(4)
C(110)	50(5)	89(7)	61(5)	-24(4)	6(4)	1(5)
O(18)	108(5)	89(4)	56(3)	25(3)	44(3)	49(4)
C(111)	128(8)	93(7)	54(4)	21(4)	36(5)	79(7)
C(112)	83(6)	87(6)	65(5)	22(4)	34(4)	58(5)
O(19)	48(3)	59(3)	69(3)	-2(3)	-2(3)	8(3)
C(113)	59(6)	68(6)	87(6)	20(5)	3(5)	9(5)
C(114)	72(6)	53(5)	54(4)	-2(4)	4(4)	7(4)
O(20)	152(7)	69(4)	62(3)	-30(3)	-42(4)	61(4)
C(115)	213(16)	60(7)	146(10)	-25(7)	-112(10)	53(9)

C(116)	102(9)	85(8)	197(13)	-28(8)	-61(9)	58(7)
O(21)	126(6)	85(5)	119(5)	50(4)	70(5)	73(5)
C(117)	86(6)	93(7)	66(5)	22(4)	37(5)	58(6)
C(1A8)	56(7)	48(6)	62(6)	9(5)	20(5)	28(5)
C(1B8)	61(16)	53(14)	28(10)	13(9)	34(11)	-5(12)
O(22)	148(7)	98(5)	66(4)	6(3)	39(4)	77(5)
C(119)	113(9)	124(10)	91(7)	15(6)	43(6)	72(8)
C(1A0)	95(11)	97(11)	20(5)	-4(6)	-8(6)	72(10)
C(1B0)	59(12)	38(9)	44(9)	15(7)	27(8)	14(9)
O(23)	122(7)	120(7)	150(7)	15(5)	39(6)	64(6)
C(122)	260(20)	550(40)	44(7)	63(12)	9(9)	300(20)
C(123)	195(16)	350(20)	103(10)	-66(12)	-73(10)	200(17)

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sh 2049

Table 1. Crystal data and structure refinement for sh2049.

Identification code	sh2049	
Empirical formula	C126 H146 Al4 N4 O20 Si8	
Formula weight	2369.11	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 17.067(3) Å	α= 90°.
	b = 17.267(3) Å	β= 90°.
	c = 47.357(9) Å	γ = 90°.
Volume	13956(4) $Å^3$	
Z	4	
Density (calculated)	1.128 Mg/m^3	
Absorption coefficient	0.162 mm^{-1}	
F(000)	5016	
Crystal size	0.32 x 0.25 x 0.15 mm^3	
Theta range for data collection	1.68 to 20.97°.	
Index ranges	-16<=h<=16, -17<=k<=17, -47<=l<=46	
Reflections collected	60713	
Independent reflections	14542 [R(int) = 0.1180]	
Completeness to theta = 20.97°	97.5 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14542 / 0 / 1403	
Goodness-of-fit on F^2	1.817	
Final R indices [I>2sigma(I)]	R1 = 0.0838, wR2 = 0.1961	
R indices (all data)	R1 = 0.1155, wR2 = 0.2118	
Absolute structure parameter	-0.11(18)	
Largest diff. peak and hole	0.863 and -0.409 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2049. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	7044(2)	4922(1)	8926(1)	39(1)
Al(2)	5275(2)	4466(2)	9121(1)	42(1)
Al(3)	5481(2)	2892(1)	8768(1)	43(1)
Al(4)	7126(2)	3489(1)	8476(1)	40(1)
Si(1)	7420(2)	4719(1)	9586(1)	45(1)
Si(2)	5687(2)	5167(1)	9715(1)	47(1)
Si(3)	3473(2)	4591(2)	8897(1)	50(1)
Si(4)	3619(2)	2944(2)	8631(1)	57(1)
Si(5)	6201(2)	1201(1)	8797(1)	51(1)
Si(6)	7692(2)	1776(1)	8450(1)	46(1)
Si(7)	7205(2)	4781(1)	8004(1)	46(1)
Si(8)	7833(2)	5968(1)	8467(1)	46(1)
O(1)	6017(3)	5030(3)	8956(1)	42(1)
O(2)	5480(3)	3492(3)	9065(1)	45(1)
O(3)	6129(3)	3181(3)	8494(1)	45(1)
O(4)	7388(3)	4112(3)	8747(1)	43(1)
O(5)	7468(3)	4910(3)	9262(1)	50(2)
O(6)	6647(4)	5063(4)	9741(1)	58(2)
O(7)	5295(3)	4599(3)	9487(1)	49(2)
O(8)	4363(3)	4725(3)	8986(1)	51(2)
O(9)	3331(4)	3823(4)	8704(1)	65(2)
O(10)	4564(4)	2866(3)	8614(1)	54(2)
O(11)	5752(4)	1981(3)	8884(1)	53(2)
O(12)	7054(4)	1352(3)	8659(1)	55(2)
O(13)	7748(4)	2688(3)	8499(1)	48(2)
O(14)	7267(3)	3955(3)	8154(1)	45(1)
O(15)	7623(4)	5484(3)	8183(1)	56(2)
O(16)	7311(4)	5748(3)	8738(1)	53(2)
C(1)	8259(6)	5180(5)	9768(2)	52(2)
C(2)	8982(6)	5260(6)	9638(2)	63(3)
C(3)	9604(7)	5684(7)	9760(3)	84(4)
C(4)	9536(7)	6003(7)	10016(3)	76(3)
C(5)	8839(9)	5921(8)	10157(3)	102(4)
C(6)	8196(7)	5503(7)	10039(2)	77(3)
C(7)	7399(5)	3643(5)	9639(2)	48(2)
C(8)	7407(6)	3137(5)	9410(2)	55(3)
C(9)	7418(7)	2333(6)	9445(3)	70(3)
C(10)	7394(7)	2029(6)	9706(3)	77(3)
C(11)	7372(7)	2503(7)	9939(2)	76(3)
C(12)	7368(7)	3288(7)	9905(2)	69(3)
C(13)	5293(6)	4929(6)	10074(2)	57(3)
C(14)	4551(8)	4658(9)	10112(2)	89(4)
C(15)	4231(9)	4444(10)	10379(3)	109(5)
C(16)	4689(9)	4543(9)	10613(3)	94(4)
C(17)	5430(9)	4798(11)	10580(3)	118(6)
C(18)	5725(7)	4986(10)	10315(2)	102(5)
C(19)	5506(6)	6203(6)	9609(2)	60(3)
C(20)	6126(8)	6737(6)	9583(3)	91(4)
C(21)	5985(12)	7490(8)	9489(4)	117(5)
C(22)	5255(11)	7712(8)	9418(3)	94(4)
C(23)	4646(9)	7218(8)	9436(3)	85(4)
C(24)	4772(7)	6455(6)	9532(2)	75(3)
C(25)	2831(6)	4523(5)	9216(2)	51(2)
C(26)	3130(7)	4550(8)	9490(2)	88(4)
C(27)	2655(9)	4531(11)	9723(3)	119(6)
C(28)	1873(8)	4479(8)	9700(3)	89(4)
C(29)	1549(7)	4482(8)	9430(3)	92(4)
C(30)	2024(7)	4480(8)	9201(3)	85(4)
C(31)	3085(6)	5415(7)	8681(2)	58(3)
C(32)	3215(7)	6148(8)	8774(3)	90(4)
C(33)	2949(11)	6817(8)	8624(4)	118(6)
C(34)	2507(11)	6747(16)	8413(6)	167(12)
C(35)	2358(9)	5961(14)	8287(3)	122(6)
C(36)	2651(7)	5313(9)	8435(3)	87(4)
C(37)	3195(6)	2722(7)	8279(3)	75(3)
C(38)	3032(9)	1955(9)	8204(3)	110(5)
C(39)	2792(11)	1761(11)	7929(4)	138(7)
C(40)	2730(12)	2376(18)	7729(4)	151(8)
C(41)	2874(11)	3098(12)	7800(4)	122(6)
C(42)	3117(8)	3260(8)	8070(3)	87(4)
C(43)	3221(7)	2257(7)	8909(3)	80(4)

C(44)	3674(9)	1645(9)	9015(3)	98(4)
C(45)	3393(11)	1100(11)	9206(4)	118(5)
C(46)	2681(18)	1187(9)	9308(4)	142(9)
C(47)	2167(14)	1708(13)	9194(6)	204(14)
C(48)	2452(12)	2283(10)	8987(5)	168(9)
C(49)	5615(6)	623(5)	8538(2)	50(2)
C(50)	5067(7)	951(7)	8358(3)	77(3)
C(51)	4702(8)	550(8)	8141(3)	95(4)
C(52)	4861(9)	-208(8)	8109(3)	89(4)
C(53)	5413(10)	-576(7)	8282(3)	105(5)
C(54)	5770(7)	-158(6)	8492(3)	82(3)
C(55)	6350(7)	607(5)	9118(2)	64(3)
C(56)	5768(9)	539(7)	9320(3)	88(4)
C(57)	5885(14)	42(11)	9558(3)	123(6)
C(58)	6557(15)	-330(9)	9596(4)	116(6)
C(59)	7120(12)	-290(7)	9408(3)	105(5)
C(60)	7089(8)	195(7)	9178(3)	91(4)
C(61)	7416(5)	1586(5)	8075(2)	49(2)
C(62)	7052(6)	889(6)	7985(2)	67(3)
C(63)	6910(7)	737(7)	7706(3)	78(3)
C(64)	7131(7)	1256(7)	7504(2)	74(3)
C(65)	7470(7)	1946(7)	7579(2)	73(3)
C(66)	7598(7)	2077(6)	7860(2)	66(3)
C(67)	8648(6)	1295(5)	8517(2)	52(3)
C(68)	9377(7)	1667(6)	8520(2)	67(3)
C(69)	10067(8)	1291(8)	8559(3)	95(4)
C(70)	10081(10)	509(10)	8600(3)	103(5)
C(71)	9362(10)	94(8)	8596(3)	93(4)
C(72)	8677(7)	496(6)	8553(2)	71(3)
C(73)	7682(6)	4762(6)	7653(2)	59(3)
C(74)	8223(6)	5342(7)	7561(2)	75(3)
C(75)	8553(8)	5303(11)	7291(3)	100(5)
C(76)	8361(11)	4719(12)	7119(3)	115(6)
C(77)	7855(11)	4098(10)	7196(3)	127(6)
C(78)	7567(9)	4171(7)	7464(2)	95(4)
C(79)	6125(5)	4986(5)	7960(2)	47(2)
C(80)	5637(6)	4920(6)	8187(2)	65(3)
C(81)	4817(6)	5011(7)	8158(2)	73(3)
C(82)	4498(7)	5175(7)	7907(3)	83(3)
C(83)	4965(7)	5272(8)	7678(3)	89(4)
C(84)	5785(6)	5169(7)	7703(2)	71(3)
C(85)	8890(6)	5799(5)	8553(2)	52(2)
C(86)	9149(7)	5911(6)	8826(2)	67(3)
C(87)	9972(8)	5818(8)	8897(3)	88(4)
C(88)	10485(7)	5588(7)	8686(4)	90(4)
C(89)	10236(7)	5490(8)	8414(3)	80(3)
C(90)	9439(6)	5582(6)	8352(2)	65(3)
C(91)	7676(6)	7009(5)	8386(2)	54(3)
C(92)	7669(7)	7545(6)	8603(3)	77(3)
C(93)	7541(9)	8327(6)	8552(3)	107(5)
C(94)	7461(8)	8580(7)	8277(4)	98(4)
C(95)	7443(10)	8076(6)	8057(3)	101(5)
C(96)	7559(8)	7288(6)	8113(2)	82(4)
N(1)	5756(7)	6462(5)	8864(2)	91(3)
C(97)	5302(11)	6624(10)	8610(5)	177(10)
C(98)	5214(15)	7323(11)	8485(4)	174(10)
C(99)	4757(10)	7384(10)	8229(3)	125(6)
C(100)	5149(8)	7393(8)	7963(3)	92(4)
C(101)	4627(9)	7559(9)	7716(3)	110(5)
C(102)	4990(9)	7690(10)	7449(3)	109(5)
C(103)	4448(12)	7771(12)	7201(3)	147(8)
N(2)	4655(8)	8092(7)	6974(3)	114(4)
N(3)	8927(4)	3965(4)	8770(2)	55(2)
C(104)	9081(6)	3438(6)	9013(2)	65(3)
C(105)	9965(7)	3350(8)	9070(3)	84(4)
C(106)	10117(8)	2815(8)	9329(3)	90(4)
C(107)	9762(7)	3111(7)	9605(2)	71(3)
C(108)	10008(8)	2626(8)	9856(2)	80(3)
C(109)	9635(8)	2881(8)	10125(3)	92(4)
C(110)	9713(7)	2355(8)	10379(3)	87(4)
N(4)	10523(5)	2256(5)	10477(2)	66(2)
O(17)	-183(5)	3534(5)	8268(2)	96(3)
C(111)	-583(10)	3613(10)	8013(3)	118(5)
C(112)	-229(12)	2999(13)	7819(5)	159(7)
C(113)	531(11)	2814(11)	7955(4)	138(6)
C(114)	613(10)	3297(10)	8201(4)	129(5)
O(18)	9279(10)	10550(12)	7747(4)	209(7)

C(115)	9374(13)	10672(13)	7399(5)	158(7)
C(116)	8938(12)	10032(12)	7299(4)	140(6)
C(117)	8731(15)	9534(15)	7517(6)	186(9)
C(118)	9120(13)	9748(14)	7783(5)	161(7)
O(19B)	3305(19)	8827(17)	9024(7)	171(10)
C(1B9)	2390(20)	9460(20)	8738(9)	148(13)
C(1B0)	2600(20)	9076(19)	9012(7)	116(10)
C(1B1)	3730(20)	9190(20)	8804(9)	142(12)
C(1B2)	3210(20)	9500(20)	8620(8)	137(12)
O(19A)	6009(14)	6841(13)	11713(5)	127(7)
C(1A9)	4746(17)	7105(18)	11685(7)	101(8)
C(1A0)	5610(30)	6870(20)	11485(10)	156(14)
C(1A1)	5760(20)	7370(20)	11900(9)	144(13)
C(1A2)	4790(20)	7380(20)	11906(10)	146(13)
O(20A)	3010(16)	7093(16)	10344(6)	155(9)
C(1A3)	4300(20)	6894(19)	10380(7)	115(10)
C(1A4)	3210(20)	7250(20)	10643(8)	125(11)
C(1A5)	3690(20)	6840(20)	10215(8)	134(11)
C(1A6)	3880(30)	6880(30)	10741(11)	189(19)
O(20B)	6140(20)	8071(19)	10533(7)	184(11)
C(1B3)	6890(30)	8210(30)	10647(11)	173(16)
C(1B4)	7430(40)	7900(30)	10505(13)	200(20)
C(1B5)	6950(30)	7350(30)	10329(10)	167(15)
C(1B6)	6430(30)	7890(30)	10241(10)	170(15)

Table 3. Bond lengths [Å] and angles [°] for sh2049.

Al(1)-O(4)	1.736(6)
Al(1)-O(16)	1.740(6)
Al(1)-O(5)	1.752(6)
Al(1)-O(1)	1.768(6)
Al(2)-O(2)	1.738(6)
Al(2)-O(8)	1.740(7)
Al(2)-O(7)	1.750(6)
Al(2)-O(1)	1.781(6)
Al(3)-O(10)	1.727(7)
Al(3)-O(11)	1.731(6)
Al(3)-O(2)	1.748(6)
Al(3)-O(3)	1.774(6)
Al(4)-O(4)	1.736(6)
Al(4)-O(14)	1.742(6)
Al(4)-O(13)	1.747(6)
Al(4)-O(3)	1.786(7)
Si(1)-O(5)	1.568(6)
Si(1)-O(6)	1.624(7)
Si(1)-C(1)	1.853(10)
Si(1)-C(7)	1.875(9)
Si(2)-O(7)	1.603(6)
Si(2)-O(6)	1.652(7)
Si(2)-C(13)	1.873(10)
Si(2)-C(19)	1.884(11)
Si(3)-O(8)	1.594(7)
Si(3)-O(9)	1.629(7)
Si(3)-C(25)	1.869(10)
Si(3)-C(31)	1.874(11)
Si(4)-O(10)	1.620(7)
Si(4)-O(9)	1.633(7)
Si(4)-C(37)	1.855(12)
Si(4)-C(43)	1.898(13)
Si(5)-O(11)	1.602(6)
Si(5)-O(12)	1.617(7)
Si(5)-C(55)	1.852(11)
Si(5)-C(49)	1.872(10)
Si(6)-O(13)	1.595(6)
Si(6)-O(12)	1.645(7)
Si(6)-C(67)	1.859(10)
Si(6)-C(61)	1.863(10)
Si(7)-O(14)	1.595(6)
Si(7)-O(15)	1.645(6)
Si(7)-C(73)	1.852(10)
Si(7)-C(79)	1.889(10)
Si(8)-O(16)	1.607(7)
Si(8)-O(15)	1.622(6)
Si(8)-C(91)	1.858(9)
Si(8)-C(85)	1.872(11)
C(1)-C(2)	1.386(13)
C(1)-C(6)	1.404(14)
C(2)-C(3)	1.411(15)
C(3)-C(4)	1.337(16)
C(4)-C(5)	1.372(18)
C(5)-C(6)	1.426(16)
C(7)-C(8)	1.390(13)
C(7)-C(12)	1.404(14)
C(8)-C(9)	1.400(14)
C(9)-C(10)	1.340(16)
C(10)-C(11)	1.375(16)
C(11)-C(12)	1.366(15)
C(13)-C(14)	1.362(15)
C(13)-C(18)	1.362(15)
C(14)-C(15)	1.426(18)
C(15)-C(16)	1.366(19)
C(16)-C(17)	1.348(19)
C(17)-C(18)	1.393(18)
C(19)-C(24)	1.375(15)
C(19)-C(20)	1.408(16)
C(20)-C(21)	1.397(19)
C(21)-C(22)	1.35(2)
C(22)-C(23)	1.347(19)
C(23)-C(24)	1.411(16)
C(25)-C(30)	1.382(15)
C(25)-C(26)	1.394(15)
C(26)-C(27)	1.370(17)

C(27)-C(28)	1.342(17)
C(28)-C(29)	1.391(17)
C(29)-C(30)	1.357(16)
C(31)-C(32)	1.356(17)
C(31)-C(36)	1.393(16)
C(32)-C(33)	1.429(19)
C(33)-C(34)	1.26(3)
C(34)-C(35)	1.50(3)
C(35)-C(36)	1.41(2)
C(37)-C(42)	1.365(17)
C(37)-C(38)	1.401(18)
C(38)-C(39)	1.40(2)
C(39)-C(40)	1.43(3)
C(40)-C(41)	1.32(3)
C(41)-C(42)	1.37(2)
C(43)-C(48)	1.364(19)
C(43)-C(44)	1.402(19)
C(44)-C(45)	1.390(19)
C(45)-C(46)	1.32(3)
C(46)-C(47)	1.37(3)
C(47)-C(48)	1.48(3)
C(49)-C(50)	1.386(15)
C(49)-C(54)	1.392(14)
C(50)-C(51)	1.387(17)
C(51)-C(52)	1.346(17)
C(52)-C(53)	1.400(19)
C(53)-C(54)	1.372(17)
C(55)-C(56)	1.383(16)
C(55)-C(60)	1.474(17)
C(56)-C(57)	1.43(2)
C(57)-C(58)	1.33(2)
C(58)-C(59)	1.31(2)
C(59)-C(60)	1.376(18)
C(61)-C(66)	1.361(14)
C(61)-C(62)	1.421(13)
C(62)-C(63)	1.368(14)
C(63)-C(64)	1.362(16)
C(64)-C(65)	1.371(16)
C(65)-C(66)	1.367(15)
C(67)-C(72)	1.390(14)
C(67)-C(68)	1.400(15)
C(68)-C(69)	1.357(16)
C(69)-C(70)	1.37(2)
C(70)-C(71)	1.42(2)
C(71)-C(72)	1.376(16)
C(73)-C(78)	1.370(15)
C(73)-C(74)	1.429(15)
C(74)-C(75)	1.400(17)
C(75)-C(76)	1.34(2)
C(76)-C(77)	1.42(2)
C(77)-C(78)	1.366(17)
C(79)-C(80)	1.366(13)
C(79)-C(84)	1.386(13)
C(80)-C(81)	1.415(15)
C(81)-C(82)	1.337(16)
C(82)-C(83)	1.356(16)
C(83)-C(84)	1.415(15)
C(85)-C(86)	1.383(14)
C(85)-C(90)	1.387(14)
C(86)-C(87)	1.453(16)
C(87)-C(88)	1.385(18)
C(88)-C(89)	1.368(18)
C(89)-C(90)	1.400(16)
C(91)-C(92)	1.386(14)
C(91)-C(96)	1.394(15)
C(92)-C(93)	1.390(16)
C(93)-C(94)	1.378(19)
C(94)-C(95)	1.359(18)
C(95)-C(96)	1.399(15)
N(1)-C(97)	1.46(2)
C(97)-C(98)	1.35(2)
C(98)-C(99)	1.44(2)
C(99)-C(100)	1.42(2)
C(100)-C(101)	1.498(17)
C(101)-C(102)	1.43(2)
C(102)-C(103)	1.50(2)
C(103)-N(2)	1.260(17)

N(3)-C(104)	1.490(12)
C(104)-C(105)	1.541(15)
C(105)-C(106)	1.556(16)
C(106)-C(107)	1.528(17)
C(107)-C(108)	1.513(15)
C(108)-C(109)	1.494(17)
C(109)-C(110)	1.513(17)
C(110)-N(4)	1.467(14)
O(17)-C(111)	1.394(17)
O(17)-C(114)	1.454(18)
C(111)-C(112)	1.53(2)
C(112)-C(113)	1.48(2)
C(113)-C(114)	1.44(2)
O(18)-C(118)	1.42(3)
O(18)-C(115)	1.67(3)
C(115)-C(116)	1.41(3)
C(116)-C(117)	1.39(3)
C(117)-C(118)	1.47(3)
O(19B)-C(1B0)	1.28(4)
O(19B)-C(1B1)	1.41(4)
C(1B9)-C(1B2)	1.50(5)
C(1B9)-C(1B0)	1.50(5)
C(1B1)-C(1B2)	1.36(5)
O(19A)-C(1A0)	1.28(4)
O(19A)-C(1A1)	1.34(4)
C(1A9)-C(1A2)	1.15(4)
C(1A9)-C(1A0)	1.80(5)
C(1A1)-C(1A2)	1.66(5)
O(20A)-C(1A5)	1.37(4)
O(20A)-C(1A4)	1.48(4)
C(1A3)-C(1A5)	1.31(4)
C(1A3)-C(1A6)	1.85(6)
C(1A4)-C(1A6)	1.40(6)
O(20B)-C(1B3)	1.42(5)
O(20B)-C(1B6)	1.51(5)
C(1B3)-C(1B4)	1.26(6)
C(1B4)-C(1B5)	1.50(6)
C(1B5)-C(1B6)	1.34(6)

O(4)-Al(1)-O(16)	108.8(3)
O(4)-Al(1)-O(5)	107.0(3)
O(16)-Al(1)-O(5)	111.5(3)
O(4)-Al(1)-O(1)	117.4(3)
O(16)-Al(1)-O(1)	102.4(3)
O(5)-Al(1)-O(1)	109.7(3)
O(2)-Al(2)-O(8)	111.9(3)
O(2)-Al(2)-O(7)	106.0(3)
O(8)-Al(2)-O(7)	110.4(3)
O(2)-Al(2)-O(1)	108.6(3)
O(8)-Al(2)-O(1)	109.5(3)
O(7)-Al(2)-O(1)	110.5(3)
O(10)-Al(3)-O(11)	110.7(3)
O(10)-Al(3)-O(2)	110.8(3)
O(11)-Al(3)-O(2)	106.3(3)
O(10)-Al(3)-O(3)	105.4(3)
O(11)-Al(3)-O(3)	108.7(3)
O(2)-Al(3)-O(3)	114.9(3)
O(4)-Al(4)-O(14)	109.1(3)
O(4)-Al(4)-O(13)	106.7(3)
O(14)-Al(4)-O(13)	109.8(3)
O(4)-Al(4)-O(3)	113.2(3)
O(14)-Al(4)-O(3)	108.2(3)
O(13)-Al(4)-O(3)	109.9(3)
O(5)-Si(1)-O(6)	114.1(3)
O(5)-Si(1)-C(1)	109.0(4)
O(6)-Si(1)-C(1)	105.0(4)
O(5)-Si(1)-C(7)	109.9(4)
O(6)-Si(1)-C(7)	106.6(4)
C(1)-Si(1)-C(7)	112.2(4)
O(7)-Si(2)-O(6)	113.4(3)
O(7)-Si(2)-C(13)	109.0(4)
O(6)-Si(2)-C(13)	105.3(4)
O(7)-Si(2)-C(19)	109.5(4)
O(6)-Si(2)-C(19)	106.6(4)
C(13)-Si(2)-C(19)	113.0(4)
O(8)-Si(3)-O(9)	114.1(3)
O(8)-Si(3)-C(25)	110.8(4)

O(9)-Si(3)-C(25)	108.4(4)
O(8)-Si(3)-C(31)	111.7(4)
O(9)-Si(3)-C(31)	105.0(4)
C(25)-Si(3)-C(31)	106.4(4)
O(10)-Si(4)-O(9)	112.8(3)
O(10)-Si(4)-C(37)	109.0(4)
O(9)-Si(4)-C(37)	105.3(5)
O(10)-Si(4)-C(43)	109.8(5)
O(9)-Si(4)-C(43)	109.1(5)
C(37)-Si(4)-C(43)	110.8(6)
O(11)-Si(5)-O(12)	113.5(3)
O(11)-Si(5)-C(55)	108.7(4)
O(12)-Si(5)-C(55)	107.3(5)
O(11)-Si(5)-C(49)	111.2(4)
O(12)-Si(5)-C(49)	107.5(4)
C(55)-Si(5)-C(49)	108.4(4)
O(13)-Si(6)-O(12)	113.0(3)
O(13)-Si(6)-C(67)	111.2(4)
O(12)-Si(6)-C(67)	106.2(4)
O(13)-Si(6)-C(61)	109.2(4)
O(12)-Si(6)-C(61)	109.2(4)
C(67)-Si(6)-C(61)	107.9(4)
O(14)-Si(7)-O(15)	113.7(3)
O(14)-Si(7)-C(73)	110.8(4)
O(15)-Si(7)-C(73)	106.7(4)
O(14)-Si(7)-C(79)	106.3(4)
O(15)-Si(7)-C(79)	109.9(4)
C(73)-Si(7)-C(79)	109.5(4)
O(16)-Si(8)-O(15)	114.7(3)
O(16)-Si(8)-C(91)	108.3(4)
O(15)-Si(8)-C(91)	107.1(4)
O(16)-Si(8)-C(85)	108.9(4)
O(15)-Si(8)-C(85)	108.2(4)
C(91)-Si(8)-C(85)	109.6(4)
Al(1)-O(1)-Al(2)	133.1(3)
Al(2)-O(2)-Al(3)	134.1(3)
Al(3)-O(3)-Al(4)	135.6(3)
Al(4)-O(4)-Al(1)	140.6(4)
Si(1)-O(5)-Al(1)	150.5(4)
Si(1)-O(6)-Si(2)	144.2(4)
Si(2)-O(7)-Al(2)	139.1(4)
Si(3)-O(8)-Al(2)	155.7(4)
Si(3)-O(9)-Si(4)	146.1(4)
Si(4)-O(10)-Al(3)	151.5(4)
Si(5)-O(11)-Al(3)	144.1(4)
Si(5)-O(12)-Si(6)	155.7(4)
Si(6)-O(13)-Al(4)	137.3(4)
Si(7)-O(14)-Al(4)	142.5(4)
Si(8)-O(15)-Si(7)	154.7(4)
Si(8)-O(16)-Al(1)	138.3(4)
C(2)-C(1)-C(6)	115.8(9)
C(2)-C(1)-Si(1)	121.6(7)
C(6)-C(1)-Si(1)	122.5(8)
C(1)-C(2)-C(3)	122.7(10)
C(4)-C(3)-C(2)	121.2(12)
C(3)-C(4)-C(5)	118.2(11)
C(4)-C(5)-C(6)	122.1(12)
C(1)-C(6)-C(5)	119.8(11)
C(8)-C(7)-C(12)	115.3(9)
C(8)-C(7)-Si(1)	121.2(7)
C(12)-C(7)-Si(1)	123.6(7)
C(7)-C(8)-C(9)	122.0(10)
C(10)-C(9)-C(8)	119.8(11)
C(9)-C(10)-C(11)	120.5(10)
C(12)-C(11)-C(10)	119.8(10)
C(11)-C(12)-C(7)	122.5(10)
C(14)-C(13)-C(18)	114.7(10)
C(14)-C(13)-Si(2)	122.0(8)
C(18)-C(13)-Si(2)	123.3(9)
C(13)-C(14)-C(15)	124.2(11)
C(16)-C(15)-C(14)	117.9(13)
C(17)-C(16)-C(15)	119.0(12)
C(16)-C(17)-C(18)	121.2(12)
C(13)-C(18)-C(17)	122.9(13)
C(24)-C(19)-C(20)	117.0(10)
C(24)-C(19)-Si(2)	121.4(8)
C(20)-C(19)-Si(2)	121.4(8)

C(21)-C(20)-C(19)	120.5(13)
C(22)-C(21)-C(20)	120.3(14)
C(21)-C(22)-C(23)	121.2(14)
C(22)-C(23)-C(24)	119.6(13)
C(19)-C(24)-C(23)	121.3(12)
C(30)-C(25)-C(26)	114.6(10)
C(30)-C(25)-Si(3)	123.0(8)
C(26)-C(25)-Si(3)	122.3(8)
C(27)-C(26)-C(25)	122.2(12)
C(28)-C(27)-C(26)	121.5(13)
C(27)-C(28)-C(29)	118.1(12)
C(30)-C(29)-C(28)	119.9(12)
C(29)-C(30)-C(25)	123.6(11)
C(32)-C(31)-C(36)	118.4(11)
C(32)-C(31)-Si(3)	118.3(9)
C(36)-C(31)-Si(3)	123.3(10)
C(31)-C(32)-C(33)	122.8(15)
C(34)-C(33)-C(32)	120.4(19)
C(33)-C(34)-C(35)	120.2(17)
C(36)-C(35)-C(34)	117.2(15)
C(31)-C(36)-C(35)	120.3(15)
C(42)-C(37)-C(38)	116.0(12)
C(42)-C(37)-Si(4)	123.3(9)
C(38)-C(37)-Si(4)	120.2(11)
C(37)-C(38)-C(39)	121.4(16)
C(38)-C(39)-C(40)	117.4(15)
C(41)-C(40)-C(39)	121.3(15)
C(40)-C(41)-C(42)	119.3(17)
C(37)-C(42)-C(41)	124.6(14)
C(48)-C(43)-C(44)	117.3(14)
C(48)-C(43)-Si(4)	120.7(13)
C(44)-C(43)-Si(4)	121.5(9)
C(45)-C(44)-C(43)	123.6(15)
C(46)-C(45)-C(44)	118.6(19)
C(45)-C(46)-C(47)	121.5(19)
C(46)-C(47)-C(48)	119.4(18)
C(43)-C(48)-C(47)	118(2)
C(50)-C(49)-C(54)	115.3(10)
C(50)-C(49)-Si(5)	123.0(7)
C(54)-C(49)-Si(5)	121.3(9)
C(49)-C(50)-C(51)	123.7(11)
C(52)-C(51)-C(50)	118.6(13)
C(51)-C(52)-C(53)	120.7(12)
C(54)-C(53)-C(52)	119.0(12)
C(53)-C(54)-C(49)	122.7(12)
C(56)-C(55)-C(60)	116.1(11)
C(56)-C(55)-Si(5)	121.1(9)
C(60)-C(55)-Si(5)	122.8(9)
C(55)-C(56)-C(57)	119.7(15)
C(58)-C(57)-C(56)	121.2(16)
C(59)-C(58)-C(57)	121.0(16)
C(58)-C(59)-C(60)	122.7(16)
C(59)-C(60)-C(55)	118.6(13)
C(66)-C(61)-C(62)	113.6(9)
C(66)-C(61)-Si(6)	123.0(7)
C(62)-C(61)-Si(6)	123.2(8)
C(63)-C(62)-C(61)	122.1(11)
C(64)-C(63)-C(62)	120.1(11)
C(63)-C(64)-C(65)	120.5(10)
C(66)-C(65)-C(64)	117.6(11)
C(61)-C(66)-C(65)	126.1(10)
C(72)-C(67)-C(68)	115.0(9)
C(72)-C(67)-Si(6)	119.7(8)
C(68)-C(67)-Si(6)	125.2(7)
C(69)-C(68)-C(67)	123.5(11)
C(68)-C(69)-C(70)	120.6(14)
C(69)-C(70)-C(71)	118.8(12)
C(72)-C(71)-C(70)	118.8(12)
C(71)-C(72)-C(67)	123.3(12)
C(78)-C(73)-C(74)	114.6(10)
C(78)-C(73)-Si(7)	122.4(9)
C(74)-C(73)-Si(7)	123.0(8)
C(75)-C(74)-C(73)	120.3(13)
C(76)-C(75)-C(74)	119.5(14)
C(75)-C(76)-C(77)	124.2(13)
C(78)-C(77)-C(76)	112.7(14)
C(77)-C(78)-C(73)	128.6(13)

C(80)-C(79)-C(84)	117.2(9)
C(80)-C(79)-Si(7)	119.5(7)
C(84)-C(79)-Si(7)	123.2(7)
C(79)-C(80)-C(81)	121.0(10)
C(82)-C(81)-C(80)	121.0(11)
C(81)-C(82)-C(83)	119.8(12)
C(82)-C(83)-C(84)	119.9(11)
C(79)-C(84)-C(83)	121.1(10)
C(86)-C(85)-C(90)	117.7(10)
C(86)-C(85)-Si(8)	119.3(8)
C(90)-C(85)-Si(8)	123.0(8)
C(85)-C(86)-C(87)	120.6(11)
C(88)-C(87)-C(86)	118.5(12)
C(89)-C(88)-C(87)	121.1(12)
C(88)-C(89)-C(90)	119.1(11)
C(85)-C(90)-C(89)	122.8(10)
C(92)-C(91)-C(96)	117.2(9)
C(92)-C(91)-Si(8)	119.5(8)
C(96)-C(91)-Si(8)	123.3(8)
C(91)-C(92)-C(93)	121.3(11)
C(94)-C(93)-C(92)	119.3(12)
C(95)-C(94)-C(93)	121.6(11)
C(94)-C(95)-C(96)	118.3(12)
C(91)-C(96)-C(95)	122.1(11)
C(98)-C(97)-N(1)	126.3(17)
C(97)-C(98)-C(99)	119.5(17)
C(100)-C(99)-C(98)	119.3(17)
C(99)-C(100)-C(101)	114.4(14)
C(102)-C(101)-C(100)	117.7(14)
C(101)-C(102)-C(103)	116.1(14)
N(2)-C(103)-C(102)	122.3(16)
N(3)-C(104)-C(105)	111.6(8)
C(104)-C(105)-C(106)	111.1(10)
C(107)-C(106)-C(105)	114.1(10)
C(108)-C(107)-C(106)	112.1(10)
C(109)-C(108)-C(107)	112.9(10)
C(108)-C(109)-C(110)	117.7(11)
N(4)-C(110)-C(109)	113.8(10)
C(111)-O(17)-C(114)	107.2(12)
O(17)-C(111)-C(112)	105.0(14)
C(113)-C(112)-C(111)	103.5(17)
C(114)-C(113)-C(112)	108.3(17)
C(113)-C(114)-O(17)	104.4(14)
C(118)-O(18)-C(115)	105.0(18)
C(116)-C(115)-O(18)	100.3(18)
C(117)-C(116)-C(115)	112(2)
C(116)-C(117)-C(118)	111(2)
O(18)-C(118)-C(117)	103(2)
C(1B0)-O(19B)-C(1B1)	107(3)
C(1B2)-C(1B9)-C(1B0)	97(3)
O(19B)-C(1B0)-C(1B9)	114(3)
C(1B2)-C(1B1)-O(19B)	108(4)
C(1B1)-C(1B2)-C(1B9)	110(4)
C(1A0)-O(19A)-C(1A1)	111(3)
C(1A2)-C(1A9)-C(1A0)	122(4)
O(19A)-C(1A0)-C(1A9)	90(3)
O(19A)-C(1A1)-C(1A2)	110(3)
C(1A9)-C(1A2)-C(1A1)	92(3)
C(1A5)-O(20A)-C(1A4)	107(3)
C(1A5)-C(1A3)-C(1A6)	104(3)
C(1A6)-C(1A4)-O(20A)	115(4)
C(1A3)-C(1A5)-O(20A)	113(3)
C(1A4)-C(1A6)-C(1A3)	90(3)
C(1B3)-O(20B)-C(1B6)	95(4)
C(1B4)-C(1B3)-O(20B)	112(5)
C(1B3)-C(1B4)-C(1B5)	100(5)
C(1B6)-C(1B5)-C(1B4)	95(4)
C(1B5)-C(1B6)-O(20B)	94(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2049. 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}
Al(1)	51(2)	35(1)	32(1)	-2(1)	-1(1)	2(1)
Al(2)	50(2)	42(2)	36(2)	-4(1)	3(1)	0(1)
Al(3)	54(2)	36(1)	40(2)	-3(1)	2(1)	-1(1)
Al(4)	52(2)	35(1)	32(1)	-2(1)	1(1)	1(1)
Si(1)	52(2)	50(1)	35(1)	-5(1)	0(1)	1(1)
Si(2)	57(2)	47(1)	38(1)	-6(1)	1(1)	3(1)
Si(3)	49(2)	54(2)	46(2)	-4(1)	-2(1)	5(1)
Si(4)	54(2)	61(2)	56(2)	-18(1)	-2(1)	-4(1)
Si(5)	65(2)	35(1)	53(2)	-1(1)	2(1)	2(1)
Si(6)	54(2)	37(1)	46(2)	-3(1)	-1(1)	4(1)
Si(7)	61(2)	42(1)	36(1)	2(1)	-1(1)	1(1)
Si(8)	58(2)	36(1)	44(2)	3(1)	1(1)	0(1)
O(1)	47(4)	40(3)	39(3)	-1(3)	1(3)	5(3)
O(2)	53(4)	45(3)	36(3)	5(3)	-1(3)	2(3)
O(3)	53(4)	47(3)	37(3)	0(3)	-4(3)	5(3)
O(4)	54(4)	42(3)	34(3)	-1(3)	-2(3)	0(3)
O(5)	53(4)	49(3)	47(4)	-2(3)	-9(3)	-3(3)
O(6)	55(4)	67(4)	50(4)	-7(3)	-5(3)	4(3)
O(7)	54(4)	55(4)	37(3)	-5(3)	-3(3)	0(3)
O(8)	51(4)	52(4)	49(4)	-2(3)	-4(3)	-2(3)
O(9)	54(4)	75(4)	67(5)	-21(4)	-9(3)	6(3)
O(10)	60(4)	45(3)	57(4)	-11(3)	2(3)	0(3)
O(11)	72(4)	37(3)	49(4)	-2(3)	6(3)	-1(3)
O(12)	68(4)	40(3)	57(4)	3(3)	4(3)	-2(3)
O(13)	57(4)	39(3)	49(4)	-7(3)	1(3)	1(3)
O(14)	60(4)	42(3)	32(3)	-1(3)	-1(3)	-1(3)
O(15)	70(4)	49(3)	50(4)	-3(3)	-8(3)	-6(3)
O(16)	62(4)	46(3)	49(4)	2(3)	2(3)	-9(3)
C(1)	69(7)	40(5)	46(6)	-7(4)	-3(5)	3(5)
C(2)	59(7)	87(8)	43(6)	-19(5)	-6(5)	-7(6)
C(3)	55(8)	104(9)	94(10)	-13(8)	-13(7)	-6(7)
C(4)	68(9)	90(8)	70(8)	-13(7)	-23(7)	-20(7)
C(5)	103(12)	117(11)	85(9)	-46(8)	-20(9)	-21(9)
C(6)	68(8)	108(9)	54(7)	-20(7)	-4(6)	-15(7)
C(7)	48(6)	51(5)	45(6)	-5(5)	-4(4)	-2(4)
C(8)	63(7)	46(6)	56(6)	8(5)	0(5)	-11(5)
C(9)	84(9)	53(7)	74(8)	0(6)	-3(6)	3(6)
C(10)	95(9)	51(6)	86(9)	0(7)	-13(7)	-5(6)
C(11)	96(9)	70(8)	62(8)	30(6)	-21(6)	-25(7)
C(12)	82(8)	77(8)	48(7)	-2(6)	-7(5)	-3(6)
C(13)	55(7)	55(6)	61(7)	-7(5)	5(5)	5(5)
C(14)	91(10)	145(12)	31(6)	-12(7)	-1(6)	-10(9)
C(15)	105(11)	151(13)	71(10)	-16(9)	13(9)	-34(10)
C(16)	105(12)	124(11)	54(9)	13(7)	30(8)	1(9)
C(17)	93(11)	215(18)	46(8)	4(9)	-5(7)	16(12)
C(18)	75(8)	189(15)	41(7)	1(8)	-6(6)	-11(9)
C(19)	67(8)	62(7)	50(6)	-17(5)	-4(5)	12(6)
C(20)	92(10)	45(7)	135(12)	2(7)	-7(8)	-14(7)
C(21)	147(16)	55(8)	150(15)	6(8)	-12(12)	-21(9)
C(22)	132(14)	70(9)	81(9)	-10(7)	-1(9)	34(11)
C(23)	100(10)	73(9)	83(9)	3(7)	6(7)	24(9)
C(24)	84(9)	59(7)	81(8)	10(6)	11(7)	12(6)
C(25)	57(7)	48(5)	47(6)	-2(4)	-16(5)	1(5)
C(26)	65(8)	137(11)	62(8)	3(8)	20(7)	21(7)
C(27)	76(11)	209(18)	71(9)	21(10)	-17(8)	-30(10)
C(28)	95(11)	111(10)	61(9)	5(7)	15(7)	-22(8)
C(29)	57(8)	123(11)	97(11)	-21(8)	20(8)	-20(7)
C(30)	65(9)	128(11)	62(8)	-15(7)	-5(6)	-13(7)
C(31)	47(6)	75(8)	52(7)	2(5)	9(5)	14(5)
C(32)	80(9)	94(10)	96(10)	21(9)	4(7)	9(7)
C(33)	116(13)	73(9)	164(16)	62(11)	15(12)	25(9)
C(34)	72(12)	210(20)	220(30)	170(20)	36(14)	43(14)
C(35)	72(10)	199(19)	94(11)	70(13)	-2(8)	39(12)
C(36)	69(8)	125(10)	65(8)	12(8)	2(6)	14(8)
C(37)	62(8)	84(9)	78(9)	-23(7)	-4(6)	-4(6)
C(38)	129(12)	100(11)	100(11)	-47(9)	-26(9)	9(9)
C(39)	148(16)	125(13)	141(16)	-80(13)	-63(13)	-12(11)
C(40)	147(17)	230(30)	72(11)	-42(15)	-39(11)	39(17)
C(41)	152(16)	130(14)	85(12)	-22(10)	-16(10)	8(12)
C(42)	118(11)	97(9)	47(8)	-25(7)	-12(7)	2(8)
C(43)	73(9)	80(8)	86(9)	-23(7)	30(7)	-19(7)

C(44)	82(10)	119(11)	93(10)	24(9)	10(8)	-30(9)
C(45)	116(14)	134(14)	105(12)	20(11)	12(10)	-41(12)
C(46)	260(30)	61(9)	105(12)	-5(8)	48(15)	24(14)
C(47)	190(20)	130(16)	290(30)	-51(19)	210(20)	-41(16)
C(48)	143(16)	103(12)	260(20)	20(13)	132(17)	14(11)
C(49)	56(6)	43(6)	51(6)	0(4)	4(5)	-6(5)
C(50)	93(9)	63(7)	74(8)	-15(6)	-11(7)	-5(7)
C(51)	107(11)	82(10)	96(10)	-12(8)	-25(8)	7(8)
C(52)	123(11)	71(9)	74(9)	-11(7)	-9(8)	-24(8)
C(53)	159(14)	48(7)	109(11)	-16(8)	-21(10)	-14(8)
C(54)	88(9)	45(6)	112(10)	-8(7)	-15(7)	-8(6)
C(55)	90(9)	38(5)	62(7)	-7(5)	0(6)	-6(6)
C(56)	102(10)	77(8)	87(10)	16(7)	9(8)	-5(7)
C(57)	190(19)	122(13)	59(9)	29(9)	29(10)	-62(13)
C(58)	210(20)	73(9)	64(11)	17(8)	-22(13)	-14(12)
C(59)	187(17)	69(8)	59(8)	19(7)	-25(10)	22(9)
C(60)	104(11)	74(8)	97(10)	9(7)	6(8)	8(8)
C(61)	50(6)	42(5)	55(6)	-7(5)	4(5)	7(4)
C(62)	79(8)	59(7)	62(7)	-14(5)	-1(6)	-12(6)
C(63)	89(9)	87(9)	59(8)	-36(7)	-9(6)	-6(7)
C(64)	86(9)	89(9)	46(7)	-21(7)	-6(6)	6(7)
C(65)	95(9)	77(8)	49(7)	-10(6)	-1(6)	1(7)
C(66)	88(8)	50(6)	60(8)	-10(6)	-1(6)	-4(6)
C(67)	70(8)	38(6)	47(6)	-10(4)	-4(5)	12(5)
C(68)	62(8)	58(6)	82(8)	1(6)	-3(6)	13(6)
C(69)	84(10)	85(10)	118(12)	-3(8)	-4(8)	17(8)
C(70)	104(12)	126(13)	81(9)	2(9)	1(8)	80(11)
C(71)	101(11)	78(8)	100(10)	11(7)	-8(8)	25(9)
C(72)	69(8)	60(7)	84(8)	-3(6)	-2(6)	16(6)
C(73)	68(7)	58(6)	52(6)	19(5)	-3(5)	4(6)
C(74)	61(7)	95(9)	68(8)	13(7)	10(6)	10(7)
C(75)	76(9)	155(14)	69(9)	59(10)	30(7)	14(9)
C(76)	151(15)	151(15)	42(8)	3(10)	29(9)	25(12)
C(77)	200(18)	118(12)	62(10)	-11(8)	62(10)	-12(12)
C(78)	162(13)	67(7)	57(8)	8(6)	9(8)	-7(8)
C(79)	64(6)	44(5)	34(5)	0(4)	0(5)	-1(5)
C(80)	71(8)	67(7)	56(7)	13(5)	5(6)	10(6)
C(81)	54(8)	104(9)	61(8)	6(7)	5(6)	8(6)
C(82)	72(8)	102(9)	75(9)	10(7)	4(7)	-3(7)
C(83)	76(9)	127(11)	66(8)	28(8)	-15(7)	1(8)
C(84)	64(8)	92(8)	57(7)	8(6)	0(6)	2(6)
C(85)	70(7)	41(5)	44(7)	3(4)	2(5)	-7(5)
C(86)	84(9)	64(6)	55(8)	0(5)	2(6)	0(6)
C(87)	75(9)	113(10)	75(9)	-1(8)	-30(8)	1(7)
C(88)	52(8)	92(9)	128(13)	7(8)	12(9)	7(6)
C(89)	67(9)	108(9)	65(9)	13(7)	8(6)	2(7)
C(90)	61(8)	78(7)	56(7)	1(5)	0(6)	-12(6)
C(91)	60(7)	38(5)	65(7)	11(5)	-1(5)	-2(5)
C(92)	112(10)	49(6)	70(7)	-1(6)	-8(7)	-5(6)
C(93)	162(15)	42(7)	116(12)	-19(7)	-37(10)	33(7)
C(94)	107(11)	58(8)	131(13)	32(9)	-19(9)	1(7)
C(95)	181(15)	48(7)	74(9)	19(7)	9(9)	21(8)
C(96)	128(11)	57(7)	60(8)	-2(6)	10(7)	-5(7)
N(1)	137(10)	46(5)	91(8)	17(5)	34(7)	25(6)
C(97)	125(14)	105(12)	300(30)	109(16)	-90(17)	-6(10)
C(98)	280(30)	147(17)	94(12)	62(12)	-69(15)	-89(17)
C(99)	137(14)	147(14)	90(12)	45(10)	-21(10)	-73(11)
C(100)	108(11)	89(9)	79(10)	0(7)	-29(8)	-19(7)
C(101)	126(13)	118(11)	85(11)	8(8)	-52(10)	-18(9)
C(102)	139(13)	139(13)	49(9)	22(8)	-18(8)	-38(10)
C(103)	199(19)	179(17)	63(10)	54(11)	-31(11)	-80(15)
N(2)	130(10)	115(9)	97(10)	-3(8)	-36(8)	-2(8)
N(3)	51(5)	58(5)	55(5)	4(4)	-7(4)	6(4)
C(104)	74(8)	73(7)	48(6)	14(5)	5(5)	9(6)
C(105)	69(8)	112(10)	71(8)	11(7)	-7(6)	15(7)
C(106)	92(9)	98(9)	80(9)	21(7)	-14(7)	26(8)
C(107)	65(7)	97(8)	52(7)	13(6)	2(6)	7(6)
C(108)	87(9)	98(9)	55(8)	19(7)	-11(6)	2(7)
C(109)	98(10)	100(9)	79(9)	25(8)	-25(8)	26(8)
C(110)	70(9)	121(11)	69(8)	18(7)	3(6)	14(7)
N(4)	79(7)	69(6)	49(5)	16(4)	-6(4)	-8(5)

sh 2374

Table 1. Crystal data and structure refinement for sh2374.

Identification code	sh2374	
Empirical formula	C116 H120 Al4 Na4 O21 Si8	
Formula weight	2274.72	
Temperature	293(2) K	
Wavelength	0.71073 E	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.532(7) E	α= 90.53(10)°.
	b = 16.791(8) E	β= 93.05(10)°.
	c = 24.78(3) E	γ = 102.78(6)°.
Volume	5886(7) E^3	
Z	2	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	0.202 mm^{-1}	
F(000)	2384	
Crystal size	0.52 x 0.33 x 0.25 mm^3	
Theta range for data collection	1.85 to 23.90°.	
Index ranges	-16<=h<=16, -18<=k<=17, -27<=l<=27	
Reflections collected	34571	
Independent reflections	16839 [R(int) = 0.0602]	
Completeness to theta = 23.90°	92.2 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16839 / 0 / 1359	
Goodness-of-fit on F^2	1.288	
Final R indices [I>2sigma(I)]	R1 = 0.0672, wR2 = 0.1635	
R indices (all data)	R1 = 0.1046, wR2 = 0.1757	
Largest diff. peak and hole	0.659 and -0.592 $e.E^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (E^2x 10^3) for sh2374. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	3907(1)	2015(1)	2727(1)	29(1)
Al(2)	3483(1)	3550(1)	2080(1)	26(1)
Al(3)	1245(1)	2866(1)	2252(1)	34(1)
Al(4)	1726(1)	1419(1)	2973(1)	32(1)
Na(1)	4647(1)	3572(1)	3376(1)	46(1)
Na(2)	2381(1)	3215(1)	993(1)	56(1)
Si(1)	5357(1)	1782(1)	1849(1)	31(1)
Si(2)	4882(1)	3251(1)	1194(1)	29(1)
Si(3)	3251(1)	5104(1)	2696(1)	30(1)
Si(4)	1021(1)	4664(1)	2441(1)	35(1)
Si(5)	3(1)	1416(1)	1499(1)	39(1)
Si(6)	-173(1)	328(1)	2514(1)	41(1)
Si(7)	2319(1)	1020(1)	4201(1)	41(1)
Si(8)	4467(1)	1659(1)	3966(1)	41(1)
O(1)	3995(2)	3025(2)	2564(1)	32(1)
O(2)	2283(2)	3224(2)	1933(1)	33(1)
O(3)	1255(2)	2247(2)	2818(1)	39(1)
O(4)	2799(2)	1377(2)	2723(1)	37(1)
O(5)	4578(2)	1560(2)	2291(1)	35(1)
O(6)	5051(2)	2349(2)	1360(1)	36(1)
O(7)	3950(2)	3456(2)	1426(1)	30(1)
O(8)	3733(2)	4591(2)	2295(1)	31(1)
O(9)	2146(2)	5070(2)	2529(1)	41(1)
O(10)	770(2)	3688(2)	2488(1)	40(1)
O(11)	440(2)	2311(2)	1741(1)	39(1)
O(12)	-462(2)	757(2)	1953(1)	51(1)
O(13)	938(2)	526(2)	2667(1)	38(1)
O(14)	1755(2)	1317(2)	3692(1)	41(1)
O(15)	3452(2)	1452(2)	4249(1)	55(1)
O(16)	4445(2)	2138(2)	3404(1)	36(1)
C(1)	5490(3)	816(3)	1515(2)	39(1)
C(2)	5060(4)	511(4)	1012(2)	55(2)
C(3)	5143(5)	-256(5)	802(3)	80(2)
C(4)	5683(6)	-705(5)	1101(4)	96(3)
C(5)	6106(5)	-418(5)	1595(4)	85(2)
C(6)	6008(4)	317(4)	1799(2)	57(2)
C(7)	6534(3)	2332(3)	2159(2)	33(1)
C(8)	7374(3)	2324(3)	1912(2)	40(1)
C(9)	8241(3)	2787(3)	2118(2)	50(1)
C(10)	8279(4)	3276(3)	2578(2)	50(1)
C(11)	7461(4)	3304(3)	2834(2)	52(1)
C(12)	6603(3)	2839(3)	2626(2)	44(1)
C(13)	4781(3)	3229(3)	428(2)	37(1)
C(14)	4426(4)	3835(4)	151(2)	51(1)
C(15)	4410(5)	3873(4)	-411(2)	71(2)
C(16)	4753(5)	3318(5)	-712(2)	89(3)
C(17)	5123(5)	2729(5)	-453(2)	83(2)
C(18)	5138(4)	2689(4)	114(2)	58(2)
C(19)	5952(3)	4075(3)	1398(2)	31(1)
C(20)	6858(3)	3996(3)	1292(2)	45(1)
C(21)	7640(4)	4629(4)	1405(2)	55(2)
C(22)	7530(4)	5358(4)	1610(2)	52(2)
C(23)	6652(4)	5459(3)	1717(2)	47(1)
C(24)	5866(3)	4817(3)	1615(2)	43(1)
C(25)	3901(3)	6200(3)	2693(2)	36(1)
C(26)	3745(4)	6795(4)	3046(2)	62(2)
C(27)	4276(6)	7594(4)	3054(3)	86(2)
C(28)	4980(6)	7801(4)	2689(3)	92(3)
C(29)	5137(5)	7242(4)	2328(3)	78(2)
C(30)	4626(4)	6450(3)	2335(2)	46(1)
C(31)	3314(3)	4700(3)	3411(2)	34(1)
C(32)	3920(4)	5104(4)	3830(2)	52(1)
C(33)	4020(4)	4752(4)	4336(2)	65(2)
C(34)	3529(5)	3976(4)	4428(2)	67(2)
C(35)	2927(4)	3544(4)	4021(2)	57(2)
C(36)	2816(4)	3905(3)	3525(2)	47(1)
C(37)	589(3)	4970(3)	1753(2)	39(1)
C(38)	533(4)	5773(4)	1661(2)	56(2)
C(39)	207(4)	6002(5)	1153(3)	71(2)
C(40)	-73(4)	5419(5)	738(2)	70(2)
C(41)	-28(4)	4616(5)	823(2)	62(2)

C(42)	294(3)	4391(4)	1326(2)	47(1)
C(43)	460(3)	5213(4)	2960(2)	48(1)
C(44)	956(5)	5601(7)	3415(3)	133(4)
C(45)	573(7)	6048(9)	3776(4)	198(7)
C(46)	-350(7)	6119(6)	3701(4)	129(4)
C(47)	-857(5)	5752(4)	3252(3)	80(2)
C(48)	-454(4)	5296(3)	2889(2)	49(1)
C(49)	-978(3)	1472(3)	986(2)	42(1)
C(50)	-942(5)	2171(4)	685(3)	80(2)
C(51)	-1654(6)	2249(5)	308(3)	94(3)
C(52)	-2437(5)	1623(5)	231(3)	80(2)
C(53)	-2510(4)	932(5)	518(2)	72(2)
C(54)	-1778(3)	850(4)	891(2)	54(2)
C(55)	929(3)	970(3)	1177(2)	47(1)
C(56)	706(4)	306(4)	812(3)	77(2)
C(57)	1377(5)	-46(5)	604(3)	92(2)
C(58)	2330(4)	255(4)	753(3)	81(2)
C(59)	2584(4)	921(4)	1109(2)	60(2)
C(60)	1899(3)	1269(3)	1315(2)	46(1)
C(61)	-636(4)	-802(3)	2429(2)	51(2)
C(62)	-140(5)	-1342(4)	2589(3)	90(2)
C(63)	-514(7)	-2194(4)	2552(4)	106(3)
C(64)	-1397(7)	-2489(5)	2371(3)	104(3)
C(65)	-1890(9)	-1974(7)	2211(7)	256(11)
C(66)	-1530(6)	-1135(5)	2244(6)	199(7)
C(67)	-850(3)	674(3)	3059(2)	50(2)
C(68)	-819(4)	402(4)	3591(2)	66(2)
C(69)	-1350(4)	615(5)	3995(3)	78(2)
C(70)	-1936(6)	1108(5)	3879(4)	127(4)
C(71)	-1999(10)	1379(9)	3360(5)	242(9)
C(72)	-1472(7)	1149(6)	2954(4)	151(5)
C(73)	2225(3)	-104(3)	4168(2)	46(1)
C(74)	2568(6)	-499(5)	4604(2)	88(2)
C(75)	2583(7)	-1311(6)	4577(3)	121(3)
C(76)	2233(6)	-1772(5)	4123(3)	108(3)
C(77)	1850(7)	-1406(5)	3694(3)	113(3)
C(78)	1837(5)	-587(4)	3728(3)	81(2)
C(79)	1826(4)	1295(3)	4847(2)	48(1)
C(80)	2338(5)	1681(4)	5305(2)	80(2)
C(81)	1941(7)	1843(5)	5780(3)	97(3)
C(82)	992(6)	1632(4)	5816(3)	81(2)
C(83)	434(5)	1227(5)	5382(3)	90(2)
C(84)	854(5)	1085(5)	4911(2)	78(2)
C(85)	5313(3)	2354(3)	4469(2)	45(1)
C(86)	5109(5)	2507(4)	4997(2)	68(2)
C(87)	5739(6)	2990(5)	5371(3)	88(2)
C(88)	6628(6)	3329(4)	5210(3)	88(3)
C(89)	6872(5)	3206(4)	4690(4)	88(2)
C(90)	6211(4)	2706(4)	4317(3)	72(2)
C(91)	4932(3)	724(3)	3869(2)	54(2)
C(92)	4929(7)	165(7)	4264(5)	196(7)
C(93)	5368(8)	-467(8)	4225(6)	208(8)
C(94)	5773(6)	-622(4)	3780(4)	98(3)
C(95)	5782(10)	-77(6)	3380(3)	178(6)
C(96)	5367(9)	573(5)	3430(3)	143(4)
O(17)	5973(3)	4590(2)	3529(1)	61(1)
C(97)	6191(5)	5151(4)	3085(2)	74(2)
C(98)	6454(5)	6001(4)	3344(3)	78(2)
C(99)	6657(5)	5864(4)	3940(3)	80(2)
C(100)	6571(5)	4972(4)	3989(2)	75(2)
O(18)	2531(3)	4516(3)	659(2)	64(1)
C(101)	2915(5)	5158(4)	1042(2)	69(2)
C(102)	2683(5)	5910(4)	803(3)	86(2)
C(103)	2663(7)	5728(5)	194(3)	112(3)
C(104)	2416(5)	4862(6)	142(3)	91(2)
O(19)	1896(3)	2596(3)	130(2)	78(1)
C(105)	2368(7)	2073(6)	-140(4)	112(3)
C(106)	1828(11)	1730(10)	-606(6)	235(9)
C(107)	999(9)	2090(9)	-641(6)	198(6)
C(108)	1131(8)	2641(10)	-212(4)	181(6)
O(20)	419(8)	3091(7)	4247(5)	216(4)
C(109)	550(9)	3334(9)	4825(6)	171(5)
C(11A)	780(20)	4230(20)	4705(12)	202(11)
C(1A1)	306(17)	4021(16)	4066(9)	151(8)
C(11B)	-427(15)	3672(13)	4714(9)	137(7)
C(1B1)	-685(14)	3608(13)	4115(8)	122(6)
C(112)	-229(7)	3017(6)	3895(4)	112(3)

Na(3A)	2266(2)	265(2)	2218(1)	69(1)
Na(3B)	3243(10)	396(9)	2168(6)	69(1)
Na(4B)	524(3)	2165(3)	3665(2)	67(1)
Na(4A)	-106(3)	2498(3)	3065(2)	67(1)
O(21)	2471(4)	-972(3)	2014(2)	106(2)
C(113)	3389(8)	-1092(9)	1984(6)	177(5)
C(114)	3219(14)	-1770(11)	1578(7)	225(8)
C(115)	2351(14)	-2159(10)	1516(10)	305(15)
C(116)	1809(11)	-1660(9)	1783(8)	265(11)

Table 3. Bond lengths [E] and angles [°] for sh2374.

Al(1)-O(4)	1.725(3)
Al(1)-O(1)	1.726(3)
Al(1)-O(5)	1.770(4)
Al(1)-O(16)	1.802(4)
Al(1)-Na(3B)	2.978(15)
Al(1)-Na(1)	3.011(4)
Al(1)-Na(3A)	3.524(5)
Al(2)-O(2)	1.725(3)
Al(2)-O(1)	1.728(3)
Al(2)-O(8)	1.775(4)
Al(2)-O(7)	1.808(4)
Al(2)-Na(2)	3.040(4)
Al(2)-Na(1)	3.546(5)
Al(3)-O(2)	1.731(3)
Al(3)-O(3)	1.755(3)
Al(3)-O(10)	1.782(4)
Al(3)-O(11)	1.783(4)
Al(3)-Na(4A)	2.863(5)
Al(3)-Na(2)	3.598(5)
Al(4)-O(3)	1.718(4)
Al(4)-O(4)	1.725(3)
Al(4)-O(14)	1.791(4)
Al(4)-O(13)	1.805(4)
Al(4)-Na(3A)	2.938(4)
Al(4)-Na(4B)	2.967(6)
Al(4)-Na(4A)	3.551(5)
Na(1)-O(1)	2.273(4)
Na(1)-O(17)	2.288(4)
Na(1)-O(16)	2.363(4)
Na(1)-C(36)	2.878(6)
Na(1)-C(31)	2.997(5)
Na(1)-C(35)	3.028(6)
Na(1)-Si(8)	3.503(4)
Na(2)-O(18)	2.312(5)
Na(2)-O(2)	2.340(4)
Na(2)-O(19)	2.371(6)
Na(2)-O(7)	2.417(4)
Si(1)-O(5)	1.602(3)
Si(1)-O(6)	1.651(3)
Si(1)-C(1)	1.867(6)
Si(1)-C(7)	1.875(5)
Si(2)-O(7)	1.602(3)
Si(2)-O(6)	1.641(3)
Si(2)-C(19)	1.881(5)
Si(2)-C(13)	1.896(5)
Si(3)-O(8)	1.595(4)
Si(3)-O(9)	1.625(3)
Si(3)-C(25)	1.874(5)
Si(3)-C(31)	1.909(5)
Si(4)-O(10)	1.605(4)
Si(4)-O(9)	1.628(3)
Si(4)-C(43)	1.894(5)
Si(4)-C(37)	1.899(5)
Si(5)-O(11)	1.595(4)
Si(5)-O(12)	1.649(4)
Si(5)-C(49)	1.877(5)
Si(5)-C(55)	1.884(6)
Si(6)-O(13)	1.599(3)
Si(6)-O(12)	1.648(4)
Si(6)-C(61)	1.874(6)
Si(6)-C(67)	1.874(6)
Si(7)-O(14)	1.609(3)
Si(7)-O(15)	1.643(4)
Si(7)-C(73)	1.863(6)
Si(7)-C(79)	1.882(6)
Si(8)-O(16)	1.616(3)
Si(8)-O(15)	1.636(4)
Si(8)-C(91)	1.860(7)
Si(8)-C(85)	1.897(6)
O(3)-Na(4A)	2.226(6)
O(3)-Na(4B)	2.392(6)
O(4)-Na(3A)	2.204(5)
O(4)-Na(3B)	2.353(16)
O(5)-Na(3B)	2.433(15)
O(10)-Na(4A)	2.603(6)

O(13)-Na(3A)	2.397(5)
O(14)-Na(4B)	2.520(6)
C(1)-C(2)	1.403(7)
C(1)-C(6)	1.413(7)
C(2)-C(3)	1.417(9)
C(3)-C(4)	1.392(11)
C(4)-C(5)	1.374(11)
C(5)-C(6)	1.368(9)
C(7)-C(8)	1.398(6)
C(7)-C(12)	1.415(7)
C(8)-C(9)	1.395(7)
C(9)-C(10)	1.389(8)
C(10)-C(11)	1.386(7)
C(10)-Na(4A)#1	3.122(7)
C(11)-C(12)	1.386(7)
C(13)-C(18)	1.390(7)
C(13)-C(14)	1.407(7)
C(14)-C(15)	1.396(7)
C(15)-C(16)	1.380(10)
C(16)-C(17)	1.374(11)
C(17)-C(18)	1.408(8)
C(19)-C(24)	1.385(7)
C(19)-C(20)	1.390(7)
C(20)-C(21)	1.388(7)
C(21)-C(22)	1.366(8)
C(22)-C(23)	1.364(8)
C(23)-C(24)	1.397(7)
C(25)-C(26)	1.386(8)
C(25)-C(30)	1.408(6)
C(26)-C(27)	1.391(8)
C(27)-C(28)	1.391(9)
C(28)-C(29)	1.354(9)
C(29)-C(30)	1.373(7)
C(31)-C(32)	1.391(7)
C(31)-C(36)	1.409(7)
C(32)-C(33)	1.407(7)
C(33)-C(34)	1.368(8)
C(34)-C(35)	1.385(8)
C(35)-C(36)	1.393(7)
C(37)-C(38)	1.389(7)
C(37)-C(42)	1.413(7)
C(38)-C(39)	1.408(7)
C(39)-C(40)	1.393(10)
C(40)-C(41)	1.381(9)
C(41)-C(42)	1.391(7)
C(43)-C(48)	1.369(7)
C(43)-C(44)	1.381(8)
C(44)-C(45)	1.378(12)
C(45)-C(46)	1.376(13)
C(46)-C(47)	1.364(10)
C(47)-C(48)	1.407(9)
C(49)-C(54)	1.388(7)
C(49)-C(50)	1.389(8)
C(50)-C(51)	1.385(8)
C(51)-C(52)	1.371(10)
C(52)-C(53)	1.352(10)
C(53)-C(54)	1.403(8)
C(55)-C(56)	1.399(9)
C(55)-C(60)	1.411(7)
C(56)-C(57)	1.368(9)
C(57)-C(58)	1.393(9)
C(58)-C(59)	1.390(9)
C(59)-C(60)	1.377(8)
C(59)-Na(3B)	2.954(15)
C(59)-Na(3A)	2.989(7)
C(60)-Na(3A)	2.911(6)
C(61)-C(62)	1.327(9)
C(61)-C(66)	1.349(9)
C(62)-C(63)	1.414(10)
C(63)-C(64)	1.321(11)
C(64)-C(65)	1.292(14)
C(65)-C(66)	1.390(13)
C(67)-C(72)	1.347(9)
C(67)-C(68)	1.401(7)
C(67)-Na(4A)	3.013(7)
C(68)-C(69)	1.387(9)
C(69)-C(70)	1.335(10)

C(70)-C(71)	1.374(13)
C(71)-C(72)	1.399(13)
C(71)-Na(4A)	3.096(14)
C(72)-Na(4A)	2.662(13)
C(73)-C(78)	1.371(8)
C(73)-C(74)	1.399(8)
C(74)-C(75)	1.370(10)
C(75)-C(76)	1.367(11)
C(76)-C(77)	1.386(10)
C(77)-C(78)	1.382(10)
C(79)-C(80)	1.395(8)
C(79)-C(84)	1.397(8)
C(80)-C(81)	1.388(9)
C(81)-C(82)	1.354(10)
C(82)-C(83)	1.389(10)
C(83)-C(84)	1.387(9)
C(85)-C(90)	1.382(7)
C(85)-C(86)	1.389(8)
C(86)-C(87)	1.387(9)
C(87)-C(88)	1.374(10)
C(88)-C(89)	1.379(11)
C(89)-C(90)	1.418(9)
C(91)-C(96)	1.337(10)
C(91)-C(92)	1.363(8)
C(92)-C(93)	1.358(14)
C(93)-C(94)	1.329(14)
C(94)-C(95)	1.355(11)
C(95)-C(96)	1.367(12)
O(17)-C(100)	1.449(7)
O(17)-C(97)	1.456(6)
C(97)-C(98)	1.520(9)
C(98)-C(99)	1.521(9)
C(99)-C(100)	1.481(9)
O(18)-C(101)	1.425(8)
O(18)-C(104)	1.430(7)
C(101)-C(102)	1.496(9)
C(102)-C(103)	1.533(10)
C(103)-C(104)	1.421(11)
O(19)-C(108)	1.378(9)
O(19)-C(105)	1.411(10)
C(105)-C(106)	1.405(12)
C(106)-C(107)	1.462(15)
C(107)-C(108)	1.381(14)
O(20)-C(112)	1.234(12)
O(20)-C(109)	1.475(14)
O(20)-C(1A1)	1.67(2)
O(20)-Na(4B)	2.147(13)
C(109)-C(11A)	1.50(3)
C(109)-C(11B)	1.65(2)
C(11A)-C(1A1)	1.70(3)
C(1A1)-C(112)	1.73(3)
C(11B)-C(1B1)	1.51(2)
C(1B1)-C(112)	1.43(2)
C(112)-Na(4B)	2.077(11)
C(112)-Na(4A)	2.259(11)
Na(3A)-O(21)	2.220(6)
Na(3B)-O(21)	2.341(16)
Na(3B)-C(113)	2.59(2)
Na(4A)-C(10)#2	3.122(7)
O(21)-C(113)	1.399(11)
O(21)-C(116)	1.423(13)
C(113)-C(114)	1.481(16)
C(114)-C(115)	1.287(18)
C(115)-C(116)	1.448(18)

O(4)-Al(1)-O(1)	118.57(16)
O(4)-Al(1)-O(5)	106.75(18)
O(1)-Al(1)-O(5)	109.82(16)
O(4)-Al(1)-O(16)	110.32(17)
O(1)-Al(1)-O(16)	100.19(17)
O(5)-Al(1)-O(16)	111.12(17)
O(4)-Al(1)-Na(3B)	52.1(3)
O(1)-Al(1)-Na(3B)	136.6(3)
O(5)-Al(1)-Na(3B)	54.8(3)
O(16)-Al(1)-Na(3B)	123.1(3)
O(4)-Al(1)-Na(1)	128.19(14)
O(1)-Al(1)-Na(1)	48.58(12)

O(5)-Al(1)-Na(1)	125.01(13)
O(16)-Al(1)-Na(1)	51.67(13)
Na(3B)-Al(1)-Na(1)	174.8(3)
O(4)-Al(1)-Na(3A)	29.92(13)
O(1)-Al(1)-Na(3A)	129.05(13)
O(5)-Al(1)-Na(3A)	76.94(13)
O(16)-Al(1)-Na(3A)	125.12(14)
Na(3B)-Al(1)-Na(3A)	23.0(3)
Na(1)-Al(1)-Na(3A)	158.05(8)
O(2)-Al(2)-O(1)	117.43(16)
O(2)-Al(2)-O(8)	109.13(17)
O(1)-Al(2)-O(8)	107.15(17)
O(2)-Al(2)-O(7)	101.71(17)
O(1)-Al(2)-O(7)	111.17(17)
O(8)-Al(2)-O(7)	110.12(16)
O(2)-Al(2)-Na(2)	49.99(13)
O(1)-Al(2)-Na(2)	138.77(14)
O(8)-Al(2)-Na(2)	114.04(14)
O(7)-Al(2)-Na(2)	52.64(11)
O(2)-Al(2)-Na(1)	125.72(13)
O(1)-Al(2)-Na(1)	32.01(12)
O(8)-Al(2)-Na(1)	75.49(13)
O(7)-Al(2)-Na(1)	128.24(12)
Na(2)-Al(2)-Na(1)	170.08(7)
O(2)-Al(3)-O(3)	119.51(17)
O(2)-Al(3)-O(10)	111.07(16)
O(3)-Al(3)-O(10)	103.83(17)
O(2)-Al(3)-O(11)	105.11(17)
O(3)-Al(3)-O(11)	108.73(17)
O(10)-Al(3)-O(11)	108.23(17)
O(2)-Al(3)-Na(4A)	162.14(15)
O(3)-Al(3)-Na(4A)	51.01(15)
O(10)-Al(3)-Na(4A)	63.22(15)
O(11)-Al(3)-Na(4A)	92.70(15)
O(2)-Al(3)-Na(2)	32.84(12)
O(3)-Al(3)-Na(2)	138.69(14)
O(10)-Al(3)-Na(2)	114.87(13)
O(11)-Al(3)-Na(2)	73.12(13)
Na(4A)-Al(3)-Na(2)	164.61(11)
O(3)-Al(4)-O(4)	118.25(16)
O(3)-Al(4)-O(14)	107.95(19)
O(4)-Al(4)-O(14)	111.13(18)
O(3)-Al(4)-O(13)	107.51(17)
O(4)-Al(4)-O(13)	102.84(18)
O(14)-Al(4)-O(13)	108.71(17)
O(3)-Al(4)-Na(3A)	127.64(14)
O(4)-Al(4)-Na(3A)	48.25(14)
O(14)-Al(4)-Na(3A)	124.25(15)
O(13)-Al(4)-Na(3A)	54.61(13)
O(3)-Al(4)-Na(4B)	53.72(15)
O(4)-Al(4)-Na(4B)	152.26(16)
O(14)-Al(4)-Na(4B)	57.83(17)
O(13)-Al(4)-Na(4B)	104.86(16)
Na(3A)-Al(4)-Na(4B)	159.47(12)
O(3)-Al(4)-Na(4A)	29.60(12)
O(4)-Al(4)-Na(4A)	147.84(14)
O(14)-Al(4)-Na(4A)	89.25(17)
O(13)-Al(4)-Na(4A)	93.09(14)
Na(3A)-Al(4)-Na(4A)	137.71(11)
Na(4B)-Al(4)-Na(4A)	31.56(12)
O(1)-Na(1)-O(17)	127.23(16)
O(1)-Na(1)-O(16)	71.43(14)
O(17)-Na(1)-O(16)	130.50(16)
O(1)-Na(1)-C(36)	84.86(16)
O(17)-Na(1)-C(36)	119.63(18)
O(16)-Na(1)-C(36)	106.23(15)
O(1)-Na(1)-C(31)	92.05(15)
O(17)-Na(1)-C(31)	94.31(16)
O(16)-Na(1)-C(31)	133.65(14)
C(36)-Na(1)-C(31)	27.66(13)
O(1)-Na(1)-Al(1)	34.71(10)
O(17)-Na(1)-Al(1)	141.72(14)
O(16)-Na(1)-Al(1)	36.75(9)
C(36)-Na(1)-Al(1)	95.24(14)
C(31)-Na(1)-Al(1)	114.97(12)
O(1)-Na(1)-C(35)	102.59(17)
O(17)-Na(1)-C(35)	119.99(19)

O(16)-Na(1)-C(35)	92.48(16)
C(36)-Na(1)-C(35)	27.14(14)
C(31)-Na(1)-C(35)	48.08(14)
Al(1)-Na(1)-C(35)	98.21(15)
O(1)-Na(1)-Si(8)	93.42(13)
O(17)-Na(1)-Si(8)	120.99(13)
O(16)-Na(1)-Si(8)	22.95(8)
C(36)-Na(1)-Si(8)	102.64(13)
C(31)-Na(1)-Si(8)	128.86(11)
Al(1)-Na(1)-Si(8)	58.83(8)
C(35)-Na(1)-Si(8)	81.19(13)
O(1)-Na(1)-Al(2)	23.76(9)
O(17)-Na(1)-Al(2)	115.33(14)
O(16)-Na(1)-Al(2)	94.52(13)
C(36)-Na(1)-Al(2)	72.45(13)
C(31)-Na(1)-Al(2)	71.61(12)
Al(1)-Na(1)-Al(2)	57.85(9)
C(35)-Na(1)-Al(2)	96.57(14)
Si(8)-Na(1)-Al(2)	115.51(10)
O(18)-Na(2)-O(2)	110.95(18)
O(18)-Na(2)-O(19)	92.46(18)
O(2)-Na(2)-O(19)	150.55(16)
O(18)-Na(2)-O(7)	95.69(15)
O(2)-Na(2)-O(7)	70.34(14)
O(19)-Na(2)-O(7)	126.59(19)
O(18)-Na(2)-Al(2)	101.96(15)
O(2)-Na(2)-Al(2)	34.38(9)
O(19)-Na(2)-Al(2)	158.20(17)
O(7)-Na(2)-Al(2)	36.49(9)
O(18)-Na(2)-Al(3)	115.43(15)
O(2)-Na(2)-Al(3)	23.66(8)
O(19)-Na(2)-Al(3)	129.45(14)
O(7)-Na(2)-Al(3)	93.32(12)
Al(2)-Na(2)-Al(3)	57.95(7)
O(5)-Si(1)-O(6)	113.08(18)
O(5)-Si(1)-C(1)	108.61(19)
O(6)-Si(1)-C(1)	105.9(2)
O(5)-Si(1)-C(7)	112.06(19)
O(6)-Si(1)-C(7)	107.88(19)
C(1)-Si(1)-C(7)	109.1(2)
O(7)-Si(2)-O(6)	113.83(16)
O(7)-Si(2)-C(19)	110.6(2)
O(6)-Si(2)-C(19)	110.88(19)
O(7)-Si(2)-C(13)	109.8(2)
O(6)-Si(2)-C(13)	105.0(2)
C(19)-Si(2)-C(13)	106.2(2)
O(8)-Si(3)-O(9)	113.55(19)
O(8)-Si(3)-C(25)	108.6(2)
O(9)-Si(3)-C(25)	107.7(2)
O(8)-Si(3)-C(31)	110.0(2)
O(9)-Si(3)-C(31)	107.5(2)
C(25)-Si(3)-C(31)	109.4(2)
O(10)-Si(4)-O(9)	113.47(18)
O(10)-Si(4)-C(43)	114.0(2)
O(9)-Si(4)-C(43)	104.0(2)
O(10)-Si(4)-C(37)	110.2(2)
O(9)-Si(4)-C(37)	108.3(2)
C(43)-Si(4)-C(37)	106.3(2)
O(11)-Si(5)-O(12)	113.8(2)
O(11)-Si(5)-C(49)	108.6(2)
O(12)-Si(5)-C(49)	106.5(2)
O(11)-Si(5)-C(55)	111.3(2)
O(12)-Si(5)-C(55)	106.2(2)
C(49)-Si(5)-C(55)	110.2(2)
O(13)-Si(6)-O(12)	113.81(18)
O(13)-Si(6)-C(61)	110.1(2)
O(12)-Si(6)-C(61)	107.7(2)
O(13)-Si(6)-C(67)	111.9(2)
O(12)-Si(6)-C(67)	106.6(2)
C(61)-Si(6)-C(67)	106.4(2)
O(14)-Si(7)-O(15)	113.72(18)
O(14)-Si(7)-C(73)	111.3(2)
O(15)-Si(7)-C(73)	106.7(2)
O(14)-Si(7)-C(79)	109.6(2)
O(15)-Si(7)-C(79)	106.1(2)
C(73)-Si(7)-C(79)	109.2(2)
O(16)-Si(8)-O(15)	113.77(19)

O(16)-Si(8)-C(91)	110.4(2)
O(15)-Si(8)-C(91)	111.4(2)
O(16)-Si(8)-C(85)	108.0(2)
O(15)-Si(8)-C(85)	105.4(2)
C(91)-Si(8)-C(85)	107.4(2)
O(16)-Si(8)-Na(1)	34.76(14)
O(15)-Si(8)-Na(1)	106.30(16)
C(91)-Si(8)-Na(1)	138.30(18)
C(85)-Si(8)-Na(1)	78.19(16)
Al(1)-O(1)-Al(2)	136.3(2)
Al(1)-O(1)-Na(1)	96.71(15)
Al(2)-O(1)-Na(1)	124.23(19)
Al(2)-O(2)-Al(3)	140.43(18)
Al(2)-O(2)-Na(2)	95.63(17)
Al(3)-O(2)-Na(2)	123.51(18)
Al(4)-O(3)-Al(3)	134.8(2)
Al(4)-O(3)-Na(4A)	127.99(19)
Al(3)-O(3)-Na(4A)	91.20(19)
Al(4)-O(3)-Na(4B)	90.89(19)
Al(3)-O(3)-Na(4B)	134.2(2)
Na(4A)-O(3)-Na(4B)	47.33(19)
Al(4)-O(4)-Al(1)	136.0(2)
Al(4)-O(4)-Na(3A)	96.03(17)
Al(1)-O(4)-Na(3A)	127.1(2)
Al(4)-O(4)-Na(3B)	131.3(4)
Al(1)-O(4)-Na(3B)	92.5(4)
Na(3A)-O(4)-Na(3B)	35.6(3)
Si(1)-O(5)-Al(1)	141.8(2)
Si(1)-O(5)-Na(3B)	121.9(4)
Al(1)-O(5)-Na(3B)	88.8(4)
Si(2)-O(6)-Si(1)	146.0(2)
Si(2)-O(7)-Al(2)	137.50(19)
Si(2)-O(7)-Na(2)	127.97(17)
Al(2)-O(7)-Na(2)	90.87(15)
Si(3)-O(8)-Al(2)	133.85(18)
Si(3)-O(9)-Si(4)	156.9(2)
Si(4)-O(10)-Al(3)	136.09(19)
Si(4)-O(10)-Na(4A)	143.1(2)
Al(3)-O(10)-Na(4A)	79.10(17)
Si(5)-O(11)-Al(3)	143.3(2)
Si(6)-O(12)-Si(5)	141.2(2)
Si(6)-O(13)-Al(4)	131.6(2)
Si(6)-O(13)-Na(3A)	133.2(2)
Al(4)-O(13)-Na(3A)	87.52(15)
Si(7)-O(14)-Al(4)	144.0(2)
Si(7)-O(14)-Na(4B)	130.1(2)
Al(4)-O(14)-Na(4B)	85.19(19)
Si(8)-O(15)-Si(7)	148.5(2)
Si(8)-O(16)-Al(1)	141.5(2)
Si(8)-O(16)-Na(1)	122.3(2)
Al(1)-O(16)-Na(1)	91.57(16)
C(2)-C(1)-C(6)	116.4(5)
C(2)-C(1)-Si(1)	124.9(4)
C(6)-C(1)-Si(1)	118.5(4)
C(1)-C(2)-C(3)	121.6(6)
C(4)-C(3)-C(2)	118.7(7)
C(5)-C(4)-C(3)	120.6(7)
C(6)-C(5)-C(4)	120.3(7)
C(5)-C(6)-C(1)	122.4(6)
C(8)-C(7)-C(12)	116.8(4)
C(8)-C(7)-Si(1)	121.5(4)
C(12)-C(7)-Si(1)	121.3(3)
C(9)-C(8)-C(7)	121.6(5)
C(10)-C(9)-C(8)	119.7(5)
C(11)-C(10)-C(9)	120.5(5)
C(11)-C(10)-Na(4A)#1	124.5(4)
C(9)-C(10)-Na(4A)#1	88.4(4)
C(10)-C(11)-C(12)	119.3(5)
C(11)-C(12)-C(7)	122.1(5)
C(18)-C(13)-C(14)	116.7(4)
C(18)-C(13)-Si(2)	123.1(4)
C(14)-C(13)-Si(2)	119.8(4)
C(15)-C(14)-C(13)	121.2(6)
C(16)-C(15)-C(14)	120.6(6)
C(17)-C(16)-C(15)	119.5(6)
C(16)-C(17)-C(18)	119.9(7)
C(13)-C(18)-C(17)	121.9(6)

C(24)-C(19)-C(20)	116.9(4)
C(24)-C(19)-Si(2)	121.4(3)
C(20)-C(19)-Si(2)	121.4(4)
C(21)-C(20)-C(19)	121.4(6)
C(22)-C(21)-C(20)	120.2(5)
C(23)-C(22)-C(21)	120.0(5)
C(22)-C(23)-C(24)	119.8(6)
C(19)-C(24)-C(23)	121.6(5)
C(26)-C(25)-C(30)	116.2(5)
C(26)-C(25)-Si(3)	123.7(4)
C(30)-C(25)-Si(3)	119.9(4)
C(25)-C(26)-C(27)	122.4(6)
C(28)-C(27)-C(26)	118.5(6)
C(29)-C(28)-C(27)	120.9(6)
C(28)-C(29)-C(30)	120.0(6)
C(29)-C(30)-C(25)	122.0(5)
C(32)-C(31)-C(36)	115.5(4)
C(32)-C(31)-Si(3)	124.0(4)
C(36)-C(31)-Si(3)	120.1(4)
C(32)-C(31)-Na(1)	85.5(3)
C(36)-C(31)-Na(1)	71.4(3)
Si(3)-C(31)-Na(1)	105.0(2)
C(31)-C(32)-C(33)	122.5(5)
C(34)-C(33)-C(32)	120.0(5)
C(33)-C(34)-C(35)	119.6(5)
C(34)-C(35)-C(36)	120.0(5)
C(34)-C(35)-Na(1)	88.0(4)
C(36)-C(35)-Na(1)	70.4(3)
C(35)-C(36)-C(31)	122.4(5)
C(35)-C(36)-Na(1)	82.5(3)
C(31)-C(36)-Na(1)	80.9(3)
C(38)-C(37)-C(42)	118.0(5)
C(38)-C(37)-Si(4)	120.4(4)
C(42)-C(37)-Si(4)	121.6(4)
C(37)-C(38)-C(39)	120.6(6)
C(40)-C(39)-C(38)	120.1(6)
C(41)-C(40)-C(39)	120.1(5)
C(40)-C(41)-C(42)	119.7(6)
C(41)-C(42)-C(37)	121.4(6)
C(48)-C(43)-C(44)	115.4(6)
C(48)-C(43)-Si(4)	121.8(4)
C(44)-C(43)-Si(4)	122.8(4)
C(45)-C(44)-C(43)	123.2(8)
C(46)-C(45)-C(44)	120.7(8)
C(47)-C(46)-C(45)	117.6(7)
C(46)-C(47)-C(48)	120.9(7)
C(43)-C(48)-C(47)	122.3(6)
C(54)-C(49)-C(50)	116.1(5)
C(54)-C(49)-Si(5)	123.6(4)
C(50)-C(49)-Si(5)	120.3(4)
C(51)-C(50)-C(49)	122.6(6)
C(52)-C(51)-C(50)	119.4(7)
C(53)-C(52)-C(51)	120.3(6)
C(52)-C(53)-C(54)	120.0(6)
C(49)-C(54)-C(53)	121.6(6)
C(56)-C(55)-C(60)	115.8(5)
C(56)-C(55)-Si(5)	122.9(4)
C(60)-C(55)-Si(5)	121.1(4)
C(57)-C(56)-C(55)	122.8(6)
C(56)-C(57)-C(58)	120.1(7)
C(59)-C(58)-C(57)	119.0(6)
C(60)-C(59)-C(58)	120.1(5)
C(60)-C(59)-Na(3B)	94.9(5)
C(58)-C(59)-Na(3B)	110.0(6)
C(60)-C(59)-Na(3A)	73.3(3)
C(58)-C(59)-Na(3A)	106.4(5)
Na(3B)-C(59)-Na(3A)	27.2(3)
C(59)-C(60)-C(55)	122.1(5)
C(59)-C(60)-Na(3A)	79.7(3)
C(55)-C(60)-Na(3A)	103.4(3)
C(62)-C(61)-C(66)	114.4(6)
C(62)-C(61)-Si(6)	122.8(4)
C(66)-C(61)-Si(6)	122.6(5)
C(61)-C(62)-C(63)	122.5(7)
C(64)-C(63)-C(62)	120.8(8)
C(65)-C(64)-C(63)	117.6(8)
C(64)-C(65)-C(66)	122.1(10)

C(61)-C(66)-C(65)	122.5(9)
C(72)-C(67)-C(68)	115.0(6)
C(72)-C(67)-Si(6)	121.8(5)
C(68)-C(67)-Si(6)	123.0(4)
C(72)-C(67)-Na(4A)	62.0(5)
C(68)-C(67)-Na(4A)	108.9(4)
Si(6)-C(67)-Na(4A)	101.7(2)
C(69)-C(68)-C(67)	124.1(6)
C(70)-C(69)-C(68)	119.1(6)
C(69)-C(70)-C(71)	118.6(7)
C(70)-C(71)-C(72)	121.7(8)
C(70)-C(71)-Na(4A)	110.9(10)
C(72)-C(71)-Na(4A)	59.0(7)
C(67)-C(72)-C(71)	121.3(7)
C(67)-C(72)-Na(4A)	91.4(6)
C(71)-C(72)-Na(4A)	94.2(10)
C(78)-C(73)-C(74)	116.4(6)
C(78)-C(73)-Si(7)	123.3(4)
C(74)-C(73)-Si(7)	120.2(5)
C(75)-C(74)-C(73)	121.8(7)
C(76)-C(75)-C(74)	120.6(7)
C(75)-C(76)-C(77)	118.9(8)
C(78)-C(77)-C(76)	119.8(8)
C(73)-C(78)-C(77)	122.3(6)
C(80)-C(79)-C(84)	112.9(5)
C(80)-C(79)-Si(7)	126.9(5)
C(84)-C(79)-Si(7)	120.2(4)
C(81)-C(80)-C(79)	124.5(7)
C(82)-C(81)-C(80)	120.0(7)
C(81)-C(82)-C(83)	119.0(6)
C(84)-C(83)-C(82)	119.5(7)
C(83)-C(84)-C(79)	124.2(6)
C(90)-C(85)-C(86)	116.7(5)
C(90)-C(85)-Si(8)	118.8(4)
C(86)-C(85)-Si(8)	124.4(4)
C(87)-C(86)-C(85)	124.5(6)
C(88)-C(87)-C(86)	117.5(7)
C(87)-C(88)-C(89)	120.9(6)
C(88)-C(89)-C(90)	120.2(7)
C(85)-C(90)-C(89)	120.3(7)
C(96)-C(91)-C(92)	114.0(8)
C(96)-C(91)-Si(8)	123.5(5)
C(92)-C(91)-Si(8)	122.3(7)
C(93)-C(92)-C(91)	122.9(10)
C(94)-C(93)-C(92)	122.3(9)
C(93)-C(94)-C(95)	115.8(9)
C(94)-C(95)-C(96)	121.4(10)
C(91)-C(96)-C(95)	123.5(7)
C(100)-O(17)-C(97)	105.7(4)
C(100)-O(17)-Na(1)	137.6(3)
C(97)-O(17)-Na(1)	114.9(3)
O(17)-C(97)-C(98)	105.7(5)
C(97)-C(98)-C(99)	105.0(5)
C(100)-C(99)-C(98)	105.6(6)
O(17)-C(100)-C(99)	106.4(5)
C(101)-O(18)-C(104)	108.9(5)
C(101)-O(18)-Na(2)	114.7(3)
C(104)-O(18)-Na(2)	136.2(5)
O(18)-C(101)-C(102)	105.4(5)
C(101)-C(102)-C(103)	102.4(6)
C(104)-C(103)-C(102)	105.1(5)
C(103)-C(104)-O(18)	109.2(6)
C(108)-O(19)-C(105)	105.1(7)
C(108)-O(19)-Na(2)	130.2(6)
C(105)-O(19)-Na(2)	124.8(4)
C(106)-C(105)-O(19)	109.9(8)
C(105)-C(106)-C(107)	106.4(10)
C(108)-C(107)-C(106)	104.9(9)
O(19)-C(108)-C(107)	113.0(10)
C(112)-O(20)-C(109)	135.7(12)
C(112)-O(20)-C(1A1)	71.4(11)
C(109)-O(20)-C(1A1)	92.1(12)
C(112)-O(20)-Na(4B)	69.9(8)
C(109)-O(20)-Na(4B)	144.8(10)
C(1A1)-O(20)-Na(4B)	122.2(11)
O(20)-C(109)-C(11A)	93.0(15)
O(20)-C(109)-C(11B)	84.8(11)

C(11A)-C(109)-C(11B)	69.6(15)
C(109)-C(11A)-C(1A1)	90(2)
O(20)-C(1A1)-C(11A)	79.6(16)
O(20)-C(1A1)-C(112)	42.5(7)
C(11A)-C(1A1)-C(112)	117.7(18)
C(1B1)-C(11B)-C(109)	108.2(16)
C(112)-C(1B1)-C(11B)	107.0(16)
O(20)-C(112)-C(1B1)	97.1(12)
O(20)-C(112)-C(1A1)	66.1(10)
C(1B1)-C(112)-C(1A1)	54.3(11)
O(20)-C(112)-Na(4B)	76.2(8)
C(1B1)-C(112)-Na(4B)	173.1(11)
C(1A1)-C(112)-Na(4B)	122.9(10)
O(20)-C(112)-Na(4A)	121.5(9)
C(1B1)-C(112)-Na(4A)	136.2(10)
C(1A1)-C(112)-Na(4A)	120.8(9)
Na(4B)-C(112)-Na(4A)	50.6(3)
O(4)-Na(3A)-O(21)	145.0(2)
O(4)-Na(3A)-O(13)	73.58(15)
O(21)-Na(3A)-O(13)	124.4(2)
O(4)-Na(3A)-C(60)	89.88(18)
O(21)-Na(3A)-C(60)	116.6(2)
O(13)-Na(3A)-C(60)	91.32(17)
O(4)-Na(3A)-Al(4)	35.72(10)
O(21)-Na(3A)-Al(4)	150.9(2)
O(13)-Na(3A)-Al(4)	37.87(10)
C(60)-Na(3A)-Al(4)	90.07(16)
O(4)-Na(3A)-C(59)	101.24(19)
O(21)-Na(3A)-C(59)	95.3(2)
O(13)-Na(3A)-C(59)	117.88(19)
C(60)-Na(3A)-C(59)	26.95(16)
Al(4)-Na(3A)-C(59)	113.52(17)
O(4)-Na(3A)-Al(1)	22.98(9)
O(21)-Na(3A)-Al(1)	130.2(2)
O(13)-Na(3A)-Al(1)	96.34(14)
C(60)-Na(3A)-Al(1)	86.22(15)
Al(4)-Na(3A)-Al(1)	58.51(9)
C(59)-Na(3A)-Al(1)	87.99(17)
O(21)-Na(3B)-O(4)	128.1(6)
O(21)-Na(3B)-O(5)	156.9(7)
O(4)-Na(3B)-O(5)	71.8(4)
O(21)-Na(3B)-C(113)	32.4(3)
O(4)-Na(3B)-C(113)	150.4(7)
O(5)-Na(3B)-C(113)	124.5(7)
O(21)-Na(3B)-C(59)	93.7(5)
O(4)-Na(3B)-C(59)	98.7(5)
O(5)-Na(3B)-C(59)	94.5(5)
C(113)-Na(3B)-C(59)	103.8(6)
O(21)-Na(3B)-Al(1)	160.0(6)
O(4)-Na(3B)-Al(1)	35.4(2)
O(5)-Na(3B)-Al(1)	36.5(2)
C(113)-Na(3B)-Al(1)	151.2(6)
C(59)-Na(3B)-Al(1)	99.9(5)
C(112)-Na(4B)-O(20)	33.9(3)
C(112)-Na(4B)-O(3)	121.5(3)
O(20)-Na(4B)-O(3)	131.5(4)
C(112)-Na(4B)-O(14)	159.7(4)
O(20)-Na(4B)-O(14)	125.8(4)
O(3)-Na(4B)-O(14)	70.54(19)
C(112)-Na(4B)-Al(4)	156.7(3)
O(20)-Na(4B)-Al(4)	148.6(4)
O(3)-Na(4B)-Al(4)	35.38(12)
O(14)-Na(4B)-Al(4)	36.98(11)
O(3)-Na(4A)-C(112)	120.9(3)
O(3)-Na(4A)-O(10)	69.92(16)
C(112)-Na(4A)-O(10)	107.5(3)
O(3)-Na(4A)-C(72)	110.2(3)
C(112)-Na(4A)-C(72)	105.8(4)
O(10)-Na(4A)-C(72)	139.9(3)
O(3)-Na(4A)-Al(3)	37.79(11)
C(112)-Na(4A)-Al(3)	134.6(3)
O(10)-Na(4A)-Al(3)	37.68(11)
C(72)-Na(4A)-Al(3)	119.1(3)
O(3)-Na(4A)-C(67)	87.0(2)
C(112)-Na(4A)-C(67)	109.2(3)
O(10)-Na(4A)-C(67)	142.9(2)
C(72)-Na(4A)-C(67)	26.55(18)

Al(3)-Na(4A)-C(67)	108.1(2)
O(3)-Na(4A)-C(71)	133.0(3)
C(112)-Na(4A)-C(71)	80.5(4)
O(10)-Na(4A)-C(71)	148.3(3)
C(72)-Na(4A)-C(71)	26.8(3)
Al(3)-Na(4A)-C(71)	144.9(3)
C(67)-Na(4A)-C(71)	46.1(2)
O(3)-Na(4A)-C(10)#2	138.4(2)
C(112)-Na(4A)-C(10)#2	91.5(3)
O(10)-Na(4A)-C(10)#2	76.09(17)
C(72)-Na(4A)-C(10)#2	81.4(2)
Al(3)-Na(4A)-C(10)#2	101.08(18)
C(67)-Na(4A)-C(10)#2	107.5(2)
C(71)-Na(4A)-C(10)#2	73.0(2)
O(3)-Na(4A)-Al(4)	22.41(10)
C(112)-Na(4A)-Al(4)	114.8(3)
O(10)-Na(4A)-Al(4)	92.33(15)
C(72)-Na(4A)-Al(4)	93.5(2)
Al(3)-Na(4A)-Al(4)	58.82(11)
C(67)-Na(4A)-Al(4)	67.90(14)
C(71)-Na(4A)-Al(4)	112.5(2)
C(10)#2-Na(4A)-Al(4)	153.52(19)
C(113)-O(21)-C(116)	109.8(10)
C(113)-O(21)-Na(3A)	119.2(7)
C(116)-O(21)-Na(3A)	129.4(8)
C(113)-O(21)-Na(3B)	83.7(8)
C(116)-O(21)-Na(3B)	158.9(10)
Na(3A)-O(21)-Na(3B)	35.6(4)
O(21)-C(113)-C(114)	100.2(11)
O(21)-C(113)-Na(3B)	63.8(7)
C(114)-C(113)-Na(3B)	144.9(12)
C(115)-C(114)-C(113)	114.2(15)
C(114)-C(115)-C(116)	105.8(13)
O(21)-C(116)-C(115)	106.7(12)

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

Table 4. Anisotropic displacement parameters (E^2x 10^3) for sh2374. 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}
Al(1)	27(1)	34(1)	27(1)	14(1)	4(1)	6(1)
Al(2)	27(1)	26(1)	24(1)	9(1)	3(1)	5(1)
Al(3)	25(1)	37(1)	37(1)	16(1)	-2(1)	1(1)
Al(4)	30(1)	35(1)	28(1)	14(1)	3(1)	2(1)
Na(1)	50(1)	45(1)	41(1)	4(1)	-3(1)	7(1)
Na(2)	54(1)	69(2)	38(1)	15(1)	-12(1)	2(1)
Si(1)	31(1)	29(1)	33(1)	7(1)	5(1)	7(1)
Si(2)	32(1)	32(1)	23(1)	8(1)	5(1)	5(1)
Si(3)	32(1)	34(1)	25(1)	7(1)	3(1)	7(1)
Si(4)	31(1)	51(1)	26(1)	8(1)	4(1)	15(1)
Si(5)	31(1)	41(1)	40(1)	14(1)	-1(1)	0(1)
Si(6)	31(1)	40(1)	47(1)	19(1)	2(1)	-3(1)
Si(7)	42(1)	49(1)	27(1)	20(1)	5(1)	2(1)
Si(8)	39(1)	48(1)	34(1)	24(1)	-4(1)	2(1)
O(1)	34(2)	33(2)	28(2)	14(1)	0(1)	7(1)
O(2)	28(2)	34(2)	36(2)	12(1)	1(1)	4(1)
O(3)	33(2)	42(2)	40(2)	19(2)	7(1)	6(2)
O(4)	34(2)	37(2)	37(2)	13(1)	3(1)	2(1)
O(5)	34(2)	33(2)	41(2)	9(1)	7(1)	7(1)
O(6)	39(2)	35(2)	34(2)	8(1)	5(1)	10(2)
O(7)	29(2)	34(2)	26(2)	9(1)	1(1)	3(1)
O(8)	30(2)	30(2)	30(2)	7(1)	3(1)	4(1)
O(9)	28(2)	57(2)	41(2)	14(2)	6(1)	11(2)
O(10)	34(2)	51(2)	37(2)	15(2)	8(1)	15(2)
O(11)	31(2)	42(2)	42(2)	8(2)	-4(1)	2(2)
O(12)	38(2)	56(2)	50(2)	27(2)	-5(2)	-7(2)
O(13)	33(2)	38(2)	40(2)	12(2)	2(1)	3(2)
O(14)	44(2)	47(2)	29(2)	17(1)	1(1)	0(2)
O(15)	46(2)	77(3)	31(2)	24(2)	0(2)	-7(2)
O(16)	35(2)	42(2)	30(2)	19(1)	2(1)	7(1)
C(1)	36(3)	31(3)	51(3)	6(2)	12(2)	5(2)
C(2)	62(4)	48(4)	54(3)	-5(3)	17(3)	5(3)
C(3)	67(4)	68(6)	95(5)	-36(4)	18(4)	-7(4)
C(4)	83(6)	43(5)	165(9)	-21(5)	36(6)	16(4)
C(5)	89(5)	40(5)	133(7)	10(4)	16(5)	26(4)
C(6)	63(4)	35(4)	75(4)	9(3)	8(3)	16(3)
C(7)	35(3)	31(3)	36(3)	8(2)	5(2)	11(2)
C(8)	39(3)	43(3)	42(3)	8(2)	8(2)	15(2)
C(9)	31(3)	54(4)	66(4)	17(3)	8(2)	13(3)
C(10)	38(3)	42(4)	68(4)	7(3)	-4(3)	2(2)
C(11)	40(3)	56(4)	58(3)	-4(3)	0(3)	8(3)
C(12)	31(3)	53(4)	48(3)	2(3)	8(2)	5(2)
C(13)	44(3)	37(3)	27(2)	5(2)	7(2)	3(2)
C(14)	61(3)	60(4)	33(3)	13(3)	8(2)	17(3)
C(15)	90(5)	91(5)	29(3)	19(3)	0(3)	16(4)
C(16)	104(6)	118(7)	22(3)	3(4)	5(3)	-25(5)
C(17)	112(6)	81(5)	42(4)	-19(3)	30(4)	-11(4)
C(18)	74(4)	54(4)	44(3)	-2(3)	17(3)	9(3)
C(19)	38(3)	30(3)	28(2)	12(2)	8(2)	11(2)
C(20)	42(3)	45(4)	51(3)	13(2)	12(2)	10(3)
C(21)	33(3)	60(4)	70(4)	18(3)	15(3)	3(3)
C(22)	38(3)	53(4)	56(3)	10(3)	7(2)	-7(3)
C(23)	53(3)	43(4)	38(3)	-3(2)	3(2)	-6(3)
C(24)	35(3)	53(4)	36(3)	9(2)	3(2)	2(2)
C(25)	52(3)	32(3)	24(2)	2(2)	1(2)	9(2)
C(26)	93(5)	50(4)	47(3)	9(3)	20(3)	18(3)
C(27)	161(7)	36(4)	62(4)	-6(3)	29(4)	19(4)
C(28)	145(7)	40(4)	76(5)	4(4)	27(5)	-18(4)
C(29)	111(5)	46(4)	63(4)	6(3)	26(4)	-16(4)
C(30)	63(3)	34(3)	39(3)	1(2)	9(2)	4(3)
C(31)	37(3)	37(3)	31(2)	8(2)	3(2)	15(2)
C(32)	63(4)	53(4)	36(3)	9(2)	-7(3)	9(3)
C(33)	89(5)	67(5)	35(3)	7(3)	-20(3)	15(4)
C(34)	95(5)	79(5)	33(3)	21(3)	5(3)	33(4)
C(35)	79(4)	49(4)	44(3)	22(3)	16(3)	11(3)
C(36)	51(3)	52(4)	38(3)	12(2)	8(2)	8(3)
C(37)	34(3)	55(4)	30(3)	10(2)	8(2)	17(2)
C(38)	57(4)	69(5)	46(3)	19(3)	3(3)	22(3)
C(39)	72(4)	88(5)	61(4)	38(4)	9(3)	35(4)
C(40)	58(4)	119(7)	40(3)	33(4)	5(3)	30(4)
C(41)	51(3)	102(6)	34(3)	10(3)	-1(2)	17(3)

C(42)	43(3)	66(4)	34(3)	7(3)	3(2)	19(3)
C(43)	34(3)	69(4)	42(3)	1(3)	12(2)	15(3)
C(44)	67(5)	262(13)	63(5)	-83(6)	5(4)	25(6)
C(45)	81(7)	357(19)	121(8)	-155(10)	33(6)	-28(8)
C(46)	102(7)	153(9)	124(7)	-79(7)	56(6)	2(6)
C(47)	71(5)	81(6)	101(5)	14(4)	48(4)	32(4)
C(48)	47(3)	46(4)	55(3)	4(3)	15(3)	13(3)
C(49)	34(3)	48(4)	42(3)	6(2)	0(2)	9(2)
C(50)	85(5)	67(5)	77(4)	23(4)	-31(4)	3(4)
C(51)	116(6)	86(6)	80(5)	17(4)	-43(5)	32(5)
C(52)	68(5)	113(7)	67(4)	-13(4)	-31(3)	45(5)
C(53)	35(3)	117(7)	58(4)	-20(4)	-10(3)	6(3)
C(54)	41(3)	65(4)	51(3)	0(3)	1(3)	2(3)
C(55)	35(3)	46(4)	56(3)	15(3)	-1(2)	0(2)
C(56)	48(4)	63(5)	117(6)	-20(4)	-4(4)	10(3)
C(57)	61(4)	71(6)	141(7)	-43(5)	-10(4)	11(4)
C(58)	49(4)	80(6)	120(6)	-24(4)	9(4)	24(4)
C(59)	32(3)	66(5)	81(4)	-6(3)	-1(3)	9(3)
C(60)	37(3)	50(4)	49(3)	7(2)	4(2)	3(3)
C(61)	44(3)	39(4)	63(3)	17(3)	-4(3)	-3(3)
C(62)	74(5)	45(5)	140(7)	-2(4)	-8(4)	-4(4)
C(63)	119(7)	36(5)	161(8)	3(5)	25(6)	11(5)
C(64)	126(8)	49(5)	115(6)	10(4)	12(5)	-27(5)
C(65)	160(11)	73(8)	470(30)	78(12)	-154(14)	-75(8)
C(66)	76(6)	64(6)	430(20)	53(9)	-107(9)	-26(5)
C(67)	36(3)	46(4)	70(4)	31(3)	18(2)	11(2)
C(68)	55(4)	97(5)	54(4)	14(3)	-1(3)	32(3)
C(69)	63(4)	109(7)	64(4)	13(4)	13(3)	24(4)
C(70)	147(8)	111(8)	160(8)	76(6)	115(7)	83(6)
C(71)	305(16)	292(17)	241(13)	219(13)	219(13)	253(14)
C(72)	180(9)	182(10)	155(8)	138(8)	124(7)	145(8)
C(73)	44(3)	59(4)	39(3)	18(3)	9(2)	18(3)
C(74)	163(7)	76(6)	48(4)	5(3)	-5(4)	78(5)
C(75)	212(10)	101(8)	76(5)	8(5)	-27(6)	100(7)
C(76)	168(8)	61(5)	106(6)	-2(5)	-37(6)	61(5)
C(77)	181(9)	70(6)	91(6)	1(4)	-49(6)	44(6)
C(78)	123(6)	53(5)	68(4)	17(4)	-20(4)	25(4)
C(79)	64(4)	45(3)	31(3)	22(2)	6(2)	6(3)
C(80)	79(5)	95(6)	49(4)	-2(3)	7(3)	-17(4)
C(81)	127(7)	98(6)	52(4)	-9(4)	13(4)	-6(5)
C(82)	127(7)	70(5)	51(4)	6(3)	32(4)	24(5)
C(83)	90(5)	116(7)	66(5)	15(4)	37(4)	21(5)
C(84)	70(4)	116(6)	45(3)	5(3)	12(3)	12(4)
C(85)	47(3)	42(3)	43(3)	24(2)	-10(2)	2(2)
C(86)	80(4)	60(4)	54(4)	6(3)	-18(3)	1(3)
C(87)	103(6)	78(6)	72(5)	-2(4)	-27(4)	8(5)
C(88)	104(6)	49(5)	97(6)	6(4)	-58(5)	2(4)
C(89)	56(4)	66(5)	127(7)	28(5)	-30(4)	-8(3)
C(90)	52(4)	88(5)	66(4)	21(3)	-13(3)	-6(3)
C(91)	38(3)	44(4)	73(4)	33(3)	-14(3)	-4(2)
C(92)	194(10)	217(12)	254(13)	207(11)	152(10)	167(10)
C(93)	193(12)	201(14)	296(17)	206(13)	141(12)	147(10)
C(94)	128(7)	29(4)	134(7)	-3(4)	-65(6)	32(4)
C(95)	420(20)	112(8)	55(5)	-1(5)	-11(7)	173(11)
C(96)	335(15)	84(7)	45(4)	14(4)	3(6)	122(8)
O(17)	69(3)	60(3)	46(2)	10(2)	-5(2)	2(2)
C(97)	69(4)	99(6)	47(3)	22(3)	-1(3)	4(4)
C(98)	66(4)	71(5)	92(5)	27(4)	6(4)	5(4)
C(99)	92(5)	61(5)	78(5)	4(4)	-16(4)	0(4)
C(100)	79(4)	89(6)	50(4)	13(3)	-17(3)	8(4)
O(18)	68(3)	72(3)	52(2)	21(2)	-1(2)	18(2)
C(101)	86(5)	79(5)	47(3)	14(3)	4(3)	26(4)
C(102)	80(5)	71(5)	112(6)	20(4)	34(4)	22(4)
C(103)	144(8)	103(7)	72(5)	52(5)	-7(5)	-5(6)
C(104)	93(5)	132(8)	57(4)	22(4)	-12(4)	49(5)
O(19)	86(3)	77(4)	61(3)	6(2)	-19(2)	3(3)
C(105)	121(7)	91(7)	121(7)	-13(5)	-39(6)	25(6)
C(106)	239(15)	266(18)	227(14)	-164(13)	-150(13)	160(14)
C(107)	165(11)	197(14)	220(14)	-91(11)	-137(10)	57(10)
C(108)	138(9)	315(19)	106(7)	-66(9)	-68(7)	105(10)
O(21)	122(5)	64(4)	137(5)	-25(3)	-8(4)	36(3)
C(113)	129(10)	160(13)	263(16)	-4(12)	-4(10)	81(9)
C(114)	280(20)	162(16)	233(16)	-80(13)	89(15)	32(14)
C(115)	236(19)	150(15)	490(30)	-183(18)	170(20)	-64(13)
C(116)	231(16)	132(12)	410(30)	-123(15)	172(17)	-29(12)

sh 2339

Table 1. Crystal data and structure refinement for sh2339.

Identification code	sh2339	
Empirical formula	C121 H118 Al4 Ge O20 Si8	
Formula weight	2297.38	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.5120(14) Å	α= 100.100(6)°.
	b = 16.493(2) Å	β= 91.758(4)°.
	c = 28.091(3) Å	γ = 115.977(4)°.
Volume	5906.7(11) $Å^3$	
Z	2	
Density (calculated)	1.292 Mg/m^3	
Absorption coefficient	0.436 mm^{-1}	
F(000)	2400	
Crystal size	0.53 x 0.35 x 0.22 mm^3	
Theta range for data collection	1.40 to 29.09°.	
Index ranges	-19<=h<=19, -22<=k<=22, -38<=l<=38	
Reflections collected	136214	
Independent reflections	31358 [R(int) = 0.0436]	
Completeness to theta = 29.09°	99.0 %	
Absorption correction	Numerical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	31358 / 0 / 1372	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0567, wR2 = 0.1386	
R indices (all data)	R1 = 0.0920, wR2 = 0.1630	
Largest diff. peak and hole	1.728 and -0.914 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2339. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ge(1)	2865(1)	7887(1)	3116(1)	16(1)
Al(1)	4934(1)	8734(1)	2488(1)	13(1)
Al(2)	4445(1)	7311(1)	3135(1)	13(1)
Al(3)	2630(1)	5976(1)	2343(1)	13(1)
Al(4)	2620(1)	7686(1)	2054(1)	14(1)
Si(1)	7068(1)	8496(1)	2493(1)	14(1)
Si(2)	6738(1)	7607(1)	3386(1)	14(1)
Si(3)	2763(1)	6383(1)	3853(1)	14(1)
Si(4)	1554(1)	4602(1)	3047(1)	15(1)
Si(5)	1980(1)	5116(1)	1207(1)	16(1)
Si(6)	861(1)	6316(1)	1178(1)	16(1)
Si(7)	2607(1)	9623(1)	2541(1)	16(1)
Si(8)	5022(1)	10748(1)	2662(1)	18(1)
O(1)	4280(1)	8240(1)	2971(1)	14(1)
O(2)	3940(1)	6390(1)	2615(1)	15(1)
O(3)	2446(1)	6993(1)	2500(1)	14(1)
O(4)	3962(1)	8101(1)	1964(1)	15(1)
O(5)	5941(2)	8461(1)	2440(1)	17(1)
O(6)	7125(2)	7850(1)	2866(1)	17(1)
O(7)	5587(2)	7509(1)	3413(1)	17(1)
O(8)	3364(1)	7030(1)	3466(1)	15(1)
O(9)	2127(2)	5319(1)	3571(1)	18(1)
O(10)	1805(2)	5108(1)	2597(1)	18(1)
O(11)	2613(2)	5751(1)	1724(1)	17(1)
O(12)	1153(2)	5460(1)	1029(1)	19(1)
O(13)	1773(2)	7181(1)	1542(1)	19(1)
O(14)	2625(2)	8629(1)	2443(1)	18(1)
O(15)	3781(2)	10456(1)	2619(1)	21(1)
O(16)	5262(2)	9879(1)	2575(1)	19(1)
C(1)	7344(2)	8037(2)	1890(1)	17(1)
C(2)	7016(3)	8233(2)	1470(1)	27(1)
C(3)	7284(3)	7977(3)	1018(1)	36(1)
C(4)	7875(3)	7510(3)	974(1)	35(1)
C(5)	8198(3)	7293(2)	1383(1)	34(1)
C(6)	7944(2)	7564(2)	1836(1)	24(1)
C(7)	8099(2)	9696(2)	2718(1)	18(1)
C(8)	7942(2)	10473(2)	2727(1)	26(1)
C(9)	8748(3)	11358(2)	2882(2)	34(1)
C(10)	9724(3)	11482(2)	3035(1)	30(1)
C(11)	9896(3)	10725(2)	3036(1)	33(1)
C(12)	9092(2)	9843(2)	2880(1)	28(1)
C(13)	7590(2)	8556(2)	3898(1)	17(1)
C(14)	7735(3)	9458(2)	3908(1)	25(1)
C(15)	8321(3)	10176(2)	4300(1)	29(1)
C(16)	8760(2)	10005(2)	4690(1)	28(1)
C(17)	8629(3)	9124(2)	4692(1)	28(1)
C(18)	8057(2)	8411(2)	4296(1)	22(1)
C(19)	6717(2)	6487(2)	3440(1)	17(1)
C(20)	5940(2)	5888(2)	3673(1)	24(1)
C(21)	5906(3)	5046(2)	3724(1)	29(1)
C(22)	6647(3)	4797(2)	3546(1)	29(1)
C(23)	7425(3)	5387(2)	3316(1)	29(1)
C(24)	7453(2)	6221(2)	3264(1)	23(1)
C(25)	3756(2)	6454(2)	4320(1)	17(1)
C(26)	3575(2)	5686(2)	4522(1)	22(1)
C(27)	4317(3)	5709(2)	4859(1)	27(1)
C(28)	5249(3)	6496(2)	4996(1)	28(1)
C(29)	5441(2)	7272(2)	4808(1)	25(1)
C(30)	4691(2)	7246(2)	4470(1)	21(1)
C(31)	1871(2)	6834(2)	4099(1)	18(1)
C(32)	835(2)	6462(2)	3895(1)	26(1)
C(33)	208(3)	6864(2)	4056(1)	30(1)
C(34)	590(3)	7643(2)	4422(1)	31(1)
C(35)	1608(3)	8028(3)	4630(1)	32(1)
C(36)	2238(3)	7627(2)	4472(1)	26(1)
C(37)	136(2)	4112(2)	3082(1)	17(1)
C(38)	-566(2)	3976(2)	2689(1)	26(1)
C(39)	-1624(3)	3604(2)	2723(2)	34(1)
C(40)	-1992(3)	3376(2)	3151(2)	34(1)
C(41)	-1312(3)	3518(2)	3547(2)	37(1)
C(42)	-257(3)	3884(2)	3514(1)	29(1)

C(43)	2037(2)	3714(2)	2981(1)	17(1)
C(44)	1904(2)	3154(2)	2525(1)	22(1)
C(45)	2214(3)	2459(2)	2459(1)	26(1)
C(46)	2676(3)	2316(2)	2853(1)	28(1)
C(47)	2827(3)	2864(3)	3310(1)	35(1)
C(48)	2507(3)	3550(2)	3373(1)	27(1)
C(49)	1247(2)	3889(2)	1268(1)	20(1)
C(50)	306(2)	3589(2)	1465(1)	22(1)
C(51)	-208(3)	2699(2)	1545(1)	30(1)
C(52)	199(3)	2079(2)	1423(1)	31(1)
C(53)	1125(3)	2354(2)	1223(1)	31(1)
C(54)	1643(2)	3254(2)	1148(1)	24(1)
C(55)	2875(2)	5238(2)	733(1)	20(1)
C(56)	3916(2)	5883(2)	823(1)	27(1)
C(57)	4560(3)	6011(3)	457(2)	40(1)
C(58)	4158(3)	5493(3)	-10(1)	41(1)
C(59)	3134(3)	4858(3)	-113(1)	39(1)
C(60)	2495(3)	4730(2)	257(1)	30(1)
C(61)	662(2)	6695(2)	612(1)	19(1)
C(62)	754(2)	6272(2)	152(1)	23(1)
C(63)	647(3)	6606(2)	-259(1)	27(1)
C(64)	450(3)	7362(2)	-214(1)	28(1)
C(65)	363(3)	7790(2)	239(1)	29(1)
C(66)	466(3)	7458(2)	650(1)	26(1)
C(67)	-343(2)	5860(2)	1476(1)	22(1)
C(68)	-1290(3)	5232(2)	1203(2)	34(1)
C(69)	-2178(3)	4842(3)	1432(2)	44(1)
C(70)	-2134(3)	5072(3)	1929(2)	49(1)
C(71)	-1215(3)	5693(3)	2204(2)	48(1)
C(72)	-322(3)	6091(3)	1982(1)	35(1)
C(73)	1980(2)	9697(2)	3105(1)	20(1)
C(74)	1022(3)	8971(2)	3147(1)	26(1)
C(75)	518(3)	9017(3)	3557(1)	32(1)
C(76)	966(3)	9778(3)	3936(1)	39(1)
C(77)	1923(3)	10489(3)	3910(1)	38(1)
C(78)	2426(3)	10450(2)	3498(1)	27(1)
C(79)	1906(3)	9745(2)	2011(1)	23(1)
C(80)	874(3)	9554(3)	1988(1)	36(1)
C(81)	365(3)	9655(3)	1590(2)	43(1)
C(82)	884(3)	9961(3)	1211(1)	41(1)
C(83)	1905(5)	10168(5)	1225(2)	73(2)
C(84)	2426(4)	10074(4)	1623(2)	62(2)
C(85)	5565(2)	11444(2)	3292(1)	20(1)
C(86)	6251(3)	11293(2)	3585(1)	27(1)
C(87)	6611(3)	11792(3)	4060(1)	37(1)
C(88)	6300(3)	12451(2)	4254(1)	37(1)
C(89)	5639(3)	12622(2)	3968(1)	33(1)
C(90)	5275(3)	12126(2)	3495(1)	27(1)
C(91)	5578(3)	11399(2)	2176(1)	29(1)
C(92)	6348(3)	11272(3)	1933(1)	44(1)
C(93)	6762(3)	11714(3)	1553(2)	50(1)
C(94)	6454(5)	12309(3)	1434(2)	69(2)
C(95A)	5856(5)	12551(4)	1705(2)	42(1)
C(96A)	5416(5)	12100(4)	2078(2)	33(1)
C(95B)	5090(16)	12044(11)	1475(5)	51(4)
C(96B)	4774(12)	11653(10)	1884(5)	34(3)
C(97)	1307(4)	4011(3)	5024(2)	47(1)
C(98)	456(4)	3553(3)	4680(2)	46(1)
C(99)	287(3)	2751(3)	4372(2)	42(1)
C(100)	966(3)	2375(3)	4400(1)	39(1)
C(101)	1824(3)	2810(3)	4749(2)	44(1)
C(102)	1997(4)	3629(3)	5062(2)	51(1)
C(103)	1491(5)	4916(4)	5350(2)	70(2)
O(17)	4308(2)	8400(2)	1077(1)	40(1)
C(104)	3605(3)	7833(3)	657(1)	35(1)
C(105)	3253(3)	8389(3)	400(2)	55(1)
C(106)	5175(3)	9144(3)	943(2)	51(1)
C(107)	4806(4)	9696(3)	686(2)	49(1)
O(18)	4118(2)	9123(2)	260(1)	43(1)
O(19)	4872(2)	5435(2)	2313(1)	35(1)
C(108)	4718(3)	4567(2)	2414(1)	31(1)
C(109)	4387(3)	3868(3)	1947(2)	40(1)
C(110)	5617(3)	5729(2)	1976(1)	34(1)
C(111)	5294(3)	5008(3)	1517(2)	41(1)
O(20)	5143(2)	4145(2)	1615(1)	43(1)
C(112)	4413(4)	208(4)	5223(2)	58(1)
C(113)	4863(8)	282(7)	5647(4)	60(2)

C(114)	5789(6)	45(5)	5676(3)	35(2)
C(115)	4003(9)	132(8)	4770(4)	66(3)
C(116)	4653(7)	31(6)	4755(3)	43(2)
C(117)	3257(5)	831(5)	97(2)	77(2)
C(118)	2440(6)	39(5)	-158(3)	94(2)
C(119)	1533(6)	27(5)	-230(3)	90(2)
C(120)	1437(6)	783(5)	-71(3)	91(2)
C(121)	2151(6)	1576(5)	160(3)	93(2)
C(1A2)	2920(9)	1764(7)	267(4)	57(2)
C(1A3)	3587(9)	2606(8)	488(4)	64(3)
C(1B2)	3409(9)	1481(8)	246(4)	60(2)
C(1B3)	4232(10)	2224(9)	491(5)	82(4)

Table 3. Bond lengths [Å] and angles [°] for sh2339.

Ge(1)-O(3)	1.9469(19)
Ge(1)-O(1)	1.9513(19)
Ge(1)-O(8)	2.1970(19)
Ge(1)-Al(2)	2.8435(9)
Ge(1)-Al(4)	2.9362(9)
Al(1)-O(16)	1.703(2)
Al(1)-O(5)	1.710(2)
Al(1)-O(1)	1.787(2)
Al(1)-O(4)	1.814(2)
Al(2)-O(7)	1.679(2)
Al(2)-O(8)	1.772(2)
Al(2)-O(2)	1.778(2)
Al(2)-O(1)	1.784(2)
Al(3)-O(10)	1.704(2)
Al(3)-O(11)	1.710(2)
Al(3)-O(3)	1.794(2)
Al(3)-O(2)	1.805(2)
Al(4)-O(13)	1.688(2)
Al(4)-O(14)	1.734(2)
Al(4)-O(3)	1.792(2)
Al(4)-O(4)	1.802(2)
Si(1)-O(5)	1.612(2)
Si(1)-O(6)	1.645(2)
Si(1)-C(1)	1.860(3)
Si(1)-C(7)	1.862(3)
Si(2)-O(7)	1.612(2)
Si(2)-O(6)	1.635(2)
Si(2)-C(13)	1.858(3)
Si(2)-C(19)	1.865(3)
Si(3)-O(9)	1.615(2)
Si(3)-O(8)	1.655(2)
Si(3)-C(31)	1.851(3)
Si(3)-C(25)	1.868(3)
Si(4)-O(10)	1.601(2)
Si(4)-O(9)	1.646(2)
Si(4)-C(43)	1.866(3)
Si(4)-C(37)	1.866(3)
Si(5)-O(11)	1.609(2)
Si(5)-O(12)	1.634(2)
Si(5)-C(55)	1.864(3)
Si(5)-C(49)	1.872(3)
Si(6)-O(13)	1.607(2)
Si(6)-O(12)	1.635(2)
Si(6)-C(61)	1.865(3)
Si(6)-C(67)	1.866(3)
Si(7)-O(14)	1.627(2)
Si(7)-O(15)	1.631(2)
Si(7)-C(73)	1.865(3)
Si(7)-C(79)	1.866(3)
Si(8)-O(16)	1.598(2)
Si(8)-O(15)	1.642(2)
Si(8)-C(85)	1.865(3)
Si(8)-C(91)	1.869(3)
C(1)-C(6)	1.397(4)
C(1)-C(2)	1.397(4)
C(2)-C(3)	1.389(5)
C(3)-C(4)	1.377(5)
C(4)-C(5)	1.387(5)
C(5)-C(6)	1.388(4)
C(7)-C(8)	1.392(4)
C(7)-C(12)	1.399(4)
C(8)-C(9)	1.392(5)
C(9)-C(10)	1.383(5)
C(10)-C(11)	1.377(5)
C(11)-C(12)	1.388(5)
C(13)-C(18)	1.398(4)
C(13)-C(14)	1.404(4)
C(14)-C(15)	1.393(4)
C(15)-C(16)	1.380(5)
C(16)-C(17)	1.382(5)
C(17)-C(18)	1.391(4)
C(19)-C(24)	1.394(4)
C(19)-C(20)	1.405(4)
C(20)-C(21)	1.399(4)
C(21)-C(22)	1.388(5)

C(22)-C(23)	1.394(5)
C(23)-C(24)	1.392(4)
C(25)-C(30)	1.395(4)
C(25)-C(26)	1.402(4)
C(26)-C(27)	1.394(4)
C(27)-C(28)	1.385(5)
C(28)-C(29)	1.388(5)
C(29)-C(30)	1.403(4)
C(31)-C(36)	1.403(4)
C(31)-C(32)	1.406(4)
C(32)-C(33)	1.386(4)
C(33)-C(34)	1.375(5)
C(34)-C(35)	1.387(5)
C(35)-C(36)	1.386(4)
C(37)-C(38)	1.396(4)
C(37)-C(42)	1.398(4)
C(38)-C(39)	1.395(5)
C(39)-C(40)	1.378(6)
C(40)-C(41)	1.380(6)
C(41)-C(42)	1.390(5)
C(43)-C(44)	1.395(4)
C(43)-C(48)	1.404(4)
C(44)-C(45)	1.390(4)
C(45)-C(46)	1.383(5)
C(46)-C(47)	1.383(5)
C(47)-C(48)	1.387(5)
C(49)-C(54)	1.398(4)
C(49)-C(50)	1.403(4)
C(50)-C(51)	1.388(4)
C(51)-C(52)	1.389(5)
C(52)-C(53)	1.389(5)
C(53)-C(54)	1.397(5)
C(55)-C(60)	1.397(4)
C(55)-C(56)	1.398(4)
C(56)-C(57)	1.390(5)
C(57)-C(58)	1.384(6)
C(58)-C(59)	1.376(6)
C(59)-C(60)	1.395(5)
C(61)-C(66)	1.395(4)
C(61)-C(62)	1.396(4)
C(62)-C(63)	1.396(4)
C(63)-C(64)	1.383(5)
C(64)-C(65)	1.381(5)
C(65)-C(66)	1.392(4)
C(67)-C(68)	1.400(5)
C(67)-C(72)	1.400(5)
C(68)-C(69)	1.400(5)
C(69)-C(70)	1.373(7)
C(70)-C(71)	1.373(7)
C(71)-C(72)	1.395(5)
C(73)-C(78)	1.396(4)
C(73)-C(74)	1.407(4)
C(74)-C(75)	1.391(4)
C(75)-C(76)	1.381(6)
C(76)-C(77)	1.385(6)
C(77)-C(78)	1.394(5)
C(79)-C(80)	1.386(5)
C(79)-C(84)	1.395(5)
C(80)-C(81)	1.396(5)
C(81)-C(82)	1.362(6)
C(82)-C(83)	1.365(7)
C(83)-C(84)	1.400(6)
C(85)-C(86)	1.402(5)
C(85)-C(90)	1.404(4)
C(86)-C(87)	1.389(5)
C(87)-C(88)	1.387(6)
C(88)-C(89)	1.383(6)
C(89)-C(90)	1.382(5)
C(91)-C(96A)	1.346(6)
C(91)-C(92)	1.401(5)
C(91)-C(96B)	1.644(13)
C(92)-C(93)	1.400(5)
C(93)-C(94)	1.328(7)
C(94)-C(95A)	1.315(7)
C(94)-C(95B)	1.84(2)
C(95A)-C(96A)	1.399(7)
C(95B)-C(96B)	1.407(18)

C(97)-C(98)	1.372(7)
C(97)-C(102)	1.408(7)
C(97)-C(103)	1.515(6)
C(98)-C(99)	1.364(6)
C(99)-C(100)	1.381(6)
C(100)-C(101)	1.387(6)
C(101)-C(102)	1.391(6)
O(17)-C(104)	1.418(4)
O(17)-C(106)	1.438(4)
C(104)-C(105)	1.498(6)
C(105)-O(18)	1.435(5)
C(106)-C(107)	1.507(6)
C(107)-O(18)	1.423(5)
O(19)-C(108)	1.430(4)
O(19)-C(110)	1.438(4)
C(108)-C(109)	1.494(5)
C(109)-O(20)	1.433(5)
C(110)-C(111)	1.493(5)
C(111)-O(20)	1.422(5)
C(112)-C(113)	1.300(11)
C(112)-C(115)	1.349(12)
C(112)-C(116)	1.383(10)
C(112)-C(116)#1	1.570(10)
C(113)-C(116)#1	1.482(13)
C(113)-C(114)	1.559(13)
C(114)-C(115)#1	1.311(13)
C(114)-C(116)#1	1.314(11)
C(115)-C(116)	1.027(13)
C(115)-C(114)#1	1.311(13)
C(116)-C(114)#1	1.314(11)
C(116)-C(113)#1	1.482(13)
C(116)-C(112)#1	1.570(10)
C(116)-C(116)#1	1.723(17)
C(117)-C(1B2)	1.001(11)
C(117)-C(118)	1.375(9)
C(117)-C(1A2)	1.802(12)
C(118)-C(119)	1.316(9)
C(119)-C(120)	1.317(9)
C(120)-C(121)	1.297(9)
C(121)-C(1A2)	1.037(11)
C(121)-C(1B2)	1.911(13)
C(1A2)-C(1A3)	1.318(14)
C(1B2)-C(1B3)	1.331(16)

O(3)-Ge(1)-O(1)	86.21(8)
O(3)-Ge(1)-O(8)	91.10(7)
O(1)-Ge(1)-O(8)	75.15(7)
O(3)-Ge(1)-Al(2)	79.71(6)
O(1)-Ge(1)-Al(2)	38.28(6)
O(8)-Ge(1)-Al(2)	38.53(5)
O(3)-Ge(1)-Al(4)	36.41(6)
O(1)-Ge(1)-Al(4)	78.47(6)
O(8)-Ge(1)-Al(4)	122.21(5)
Al(2)-Ge(1)-Al(4)	95.22(2)
O(16)-Al(1)-O(5)	115.37(10)
O(16)-Al(1)-O(1)	111.90(10)
O(5)-Al(1)-O(1)	106.08(10)
O(16)-Al(1)-O(4)	109.92(10)
O(5)-Al(1)-O(4)	110.44(10)
O(1)-Al(1)-O(4)	102.30(9)
O(7)-Al(2)-O(8)	119.49(10)
O(7)-Al(2)-O(2)	114.99(10)
O(8)-Al(2)-O(2)	101.34(10)
O(7)-Al(2)-O(1)	119.82(10)
O(8)-Al(2)-O(1)	91.05(9)
O(2)-Al(2)-O(1)	106.38(10)
O(7)-Al(2)-Ge(1)	146.10(8)
O(8)-Al(2)-Ge(1)	50.58(6)
O(2)-Al(2)-Ge(1)	98.87(7)
O(1)-Al(2)-Ge(1)	42.66(6)
O(10)-Al(3)-O(11)	117.46(10)
O(10)-Al(3)-O(3)	111.70(10)
O(11)-Al(3)-O(3)	106.79(10)
O(10)-Al(3)-O(2)	110.25(10)
O(11)-Al(3)-O(2)	107.96(10)
O(3)-Al(3)-O(2)	101.40(9)
O(13)-Al(4)-O(14)	119.54(11)

O(13)-Al(4)-O(3)	115.81(10)
O(14)-Al(4)-O(3)	96.40(10)
O(13)-Al(4)-O(4)	115.54(10)
O(14)-Al(4)-O(4)	102.08(10)
O(3)-Al(4)-O(4)	104.69(9)
O(13)-Al(4)-Ge(1)	144.77(8)
O(14)-Al(4)-Ge(1)	58.67(7)
O(3)-Al(4)-Ge(1)	40.16(6)
O(4)-Al(4)-Ge(1)	98.05(7)
O(5)-Si(1)-O(6)	111.11(11)
O(5)-Si(1)-C(1)	109.78(12)
O(6)-Si(1)-C(1)	107.22(12)
O(5)-Si(1)-C(7)	111.53(12)
O(6)-Si(1)-C(7)	108.89(12)
C(1)-Si(1)-C(7)	108.17(13)
O(7)-Si(2)-O(6)	110.07(10)
O(7)-Si(2)-C(13)	107.19(12)
O(6)-Si(2)-C(13)	110.27(12)
O(7)-Si(2)-C(19)	108.54(12)
O(6)-Si(2)-C(19)	109.23(12)
C(13)-Si(2)-C(19)	111.52(13)
O(9)-Si(3)-O(8)	109.89(10)
O(9)-Si(3)-C(31)	110.58(12)
O(8)-Si(3)-C(31)	105.39(11)
O(9)-Si(3)-C(25)	107.87(12)
O(8)-Si(3)-C(25)	108.35(12)
C(31)-Si(3)-C(25)	114.67(13)
O(10)-Si(4)-O(9)	112.35(11)
O(10)-Si(4)-C(43)	110.07(12)
O(9)-Si(4)-C(43)	106.32(12)
O(10)-Si(4)-C(37)	108.32(12)
O(9)-Si(4)-C(37)	106.70(12)
C(43)-Si(4)-C(37)	113.10(12)
O(11)-Si(5)-O(12)	109.93(11)
O(11)-Si(5)-C(55)	110.18(12)
O(12)-Si(5)-C(55)	106.71(12)
O(11)-Si(5)-C(49)	109.78(12)
O(12)-Si(5)-C(49)	108.30(12)
C(55)-Si(5)-C(49)	111.88(14)
O(13)-Si(6)-O(12)	111.54(11)
O(13)-Si(6)-C(61)	108.20(12)
O(12)-Si(6)-C(61)	108.44(12)
O(13)-Si(6)-C(67)	110.62(13)
O(12)-Si(6)-C(67)	106.20(12)
C(61)-Si(6)-C(67)	111.84(13)
O(14)-Si(7)-O(15)	110.22(11)
O(14)-Si(7)-C(73)	106.50(12)
O(15)-Si(7)-C(73)	110.01(13)
O(14)-Si(7)-C(79)	111.39(13)
O(15)-Si(7)-C(79)	106.93(13)
C(73)-Si(7)-C(79)	111.82(14)
O(16)-Si(8)-O(15)	113.05(11)
O(16)-Si(8)-C(85)	109.70(13)
O(15)-Si(8)-C(85)	105.97(12)
O(16)-Si(8)-C(91)	106.63(13)
O(15)-Si(8)-C(91)	108.07(15)
C(85)-Si(8)-C(91)	113.56(14)
Al(2)-O(1)-Al(1)	118.68(11)
Al(2)-O(1)-Ge(1)	99.06(9)
Al(1)-O(1)-Ge(1)	131.14(11)
Al(2)-O(2)-Al(3)	119.53(11)
Al(4)-O(3)-Al(3)	117.96(11)
Al(4)-O(3)-Ge(1)	103.43(9)
Al(3)-O(3)-Ge(1)	128.70(10)
Al(4)-O(4)-Al(1)	118.69(11)
Si(1)-O(5)-Al(1)	163.52(14)
Si(2)-O(6)-Si(1)	138.89(13)
Si(2)-O(7)-Al(2)	150.32(14)
Si(3)-O(8)-Al(2)	141.73(12)
Si(3)-O(8)-Ge(1)	127.27(10)
Al(2)-O(8)-Ge(1)	90.89(8)
Si(3)-O(9)-Si(4)	146.34(14)
Si(4)-O(10)-Al(3)	149.31(14)
Si(5)-O(11)-Al(3)	147.12(13)
Si(5)-O(12)-Si(6)	139.72(13)
Si(6)-O(13)-Al(4)	153.54(14)
Si(7)-O(14)-Al(4)	151.32(13)

Si(7)-O(15)-Si(8)	147.06(14)
Si(8)-O(16)-Al(1)	154.08(14)
C(6)-C(1)-C(2)	117.4(3)
C(6)-C(1)-Si(1)	123.0(2)
C(2)-C(1)-Si(1)	119.4(2)
C(3)-C(2)-C(1)	121.5(3)
C(4)-C(3)-C(2)	120.0(3)
C(3)-C(4)-C(5)	119.8(3)
C(4)-C(5)-C(6)	120.0(3)
C(5)-C(6)-C(1)	121.3(3)
C(8)-C(7)-C(12)	117.2(3)
C(8)-C(7)-Si(1)	123.3(2)
C(12)-C(7)-Si(1)	119.5(2)
C(9)-C(8)-C(7)	121.2(3)
C(10)-C(9)-C(8)	120.3(3)
C(11)-C(10)-C(9)	119.7(3)
C(10)-C(11)-C(12)	119.9(3)
C(11)-C(12)-C(7)	121.7(3)
C(18)-C(13)-C(14)	117.3(3)
C(18)-C(13)-Si(2)	123.1(2)
C(14)-C(13)-Si(2)	119.6(2)
C(15)-C(14)-C(13)	121.0(3)
C(16)-C(15)-C(14)	120.1(3)
C(15)-C(16)-C(17)	120.3(3)
C(16)-C(17)-C(18)	119.5(3)
C(17)-C(18)-C(13)	121.8(3)
C(24)-C(19)-C(20)	118.1(3)
C(24)-C(19)-Si(2)	122.7(2)
C(20)-C(19)-Si(2)	119.2(2)
C(21)-C(20)-C(19)	120.8(3)
C(22)-C(21)-C(20)	120.1(3)
C(21)-C(22)-C(23)	119.8(3)
C(24)-C(23)-C(22)	120.0(3)
C(23)-C(24)-C(19)	121.3(3)
C(30)-C(25)-C(26)	118.3(3)
C(30)-C(25)-Si(3)	122.1(2)
C(26)-C(25)-Si(3)	119.6(2)
C(27)-C(26)-C(25)	120.8(3)
C(28)-C(27)-C(26)	120.1(3)
C(27)-C(28)-C(29)	120.3(3)
C(28)-C(29)-C(30)	119.5(3)
C(25)-C(30)-C(29)	121.1(3)
C(36)-C(31)-C(32)	117.1(3)
C(36)-C(31)-Si(3)	120.3(2)
C(32)-C(31)-Si(3)	122.4(2)
C(33)-C(32)-C(31)	121.3(3)
C(34)-C(33)-C(32)	120.4(3)
C(33)-C(34)-C(35)	119.7(3)
C(36)-C(35)-C(34)	120.2(3)
C(35)-C(36)-C(31)	121.3(3)
C(38)-C(37)-C(42)	117.6(3)
C(38)-C(37)-Si(4)	122.2(2)
C(42)-C(37)-Si(4)	120.2(2)
C(39)-C(38)-C(37)	121.3(3)
C(40)-C(39)-C(38)	120.0(3)
C(39)-C(40)-C(41)	119.8(3)
C(40)-C(41)-C(42)	120.4(3)
C(41)-C(42)-C(37)	121.0(3)
C(44)-C(43)-C(48)	117.1(3)
C(44)-C(43)-Si(4)	119.5(2)
C(48)-C(43)-Si(4)	123.4(2)
C(45)-C(44)-C(43)	121.8(3)
C(46)-C(45)-C(44)	119.8(3)
C(47)-C(46)-C(45)	119.9(3)
C(46)-C(47)-C(48)	120.0(3)
C(47)-C(48)-C(43)	121.5(3)
C(54)-C(49)-C(50)	117.5(3)
C(54)-C(49)-Si(5)	121.6(2)
C(50)-C(49)-Si(5)	120.7(2)
C(51)-C(50)-C(49)	121.3(3)
C(50)-C(51)-C(52)	120.2(3)
C(51)-C(52)-C(53)	119.7(3)
C(52)-C(53)-C(54)	119.8(3)
C(53)-C(54)-C(49)	121.5(3)
C(60)-C(55)-C(56)	117.4(3)
C(60)-C(55)-Si(5)	120.1(2)
C(56)-C(55)-Si(5)	122.3(2)

C(57)-C(56)-C(55)	121.8(3)
C(58)-C(57)-C(56)	119.2(3)
C(59)-C(58)-C(57)	120.6(3)
C(58)-C(59)-C(60)	119.8(3)
C(59)-C(60)-C(55)	121.2(3)
C(66)-C(61)-C(62)	118.4(3)
C(66)-C(61)-Si(6)	119.0(2)
C(62)-C(61)-Si(6)	122.5(2)
C(63)-C(62)-C(61)	120.5(3)
C(64)-C(63)-C(62)	120.2(3)
C(65)-C(64)-C(63)	119.9(3)
C(64)-C(65)-C(66)	120.1(3)
C(65)-C(66)-C(61)	120.8(3)
C(68)-C(67)-C(72)	117.8(3)
C(68)-C(67)-Si(6)	120.8(3)
C(72)-C(67)-Si(6)	121.3(2)
C(67)-C(68)-C(69)	120.6(4)
C(70)-C(69)-C(68)	120.4(4)
C(69)-C(70)-C(71)	119.9(4)
C(70)-C(71)-C(72)	120.6(4)
C(71)-C(72)-C(67)	120.7(4)
C(78)-C(73)-C(74)	117.6(3)
C(78)-C(73)-Si(7)	122.6(2)
C(74)-C(73)-Si(7)	119.8(2)
C(75)-C(74)-C(73)	121.2(3)
C(76)-C(75)-C(74)	120.0(3)
C(75)-C(76)-C(77)	119.9(3)
C(76)-C(77)-C(78)	120.3(4)
C(77)-C(78)-C(73)	120.9(3)
C(80)-C(79)-C(84)	116.9(3)
C(80)-C(79)-Si(7)	122.7(2)
C(84)-C(79)-Si(7)	120.4(3)
C(79)-C(80)-C(81)	121.8(3)
C(82)-C(81)-C(80)	120.2(4)
C(81)-C(82)-C(83)	119.5(3)
C(82)-C(83)-C(84)	120.9(4)
C(79)-C(84)-C(83)	120.7(4)
C(86)-C(85)-C(90)	117.5(3)
C(86)-C(85)-Si(8)	121.8(2)
C(90)-C(85)-Si(8)	120.7(2)
C(87)-C(86)-C(85)	120.8(3)
C(88)-C(87)-C(86)	120.4(4)
C(89)-C(88)-C(87)	119.6(3)
C(90)-C(89)-C(88)	120.2(3)
C(89)-C(90)-C(85)	121.4(3)
C(96A)-C(91)-C(92)	114.1(4)
C(96A)-C(91)-C(96B)	36.0(5)
C(92)-C(91)-C(96B)	119.1(5)
C(96A)-C(91)-Si(8)	125.3(3)
C(92)-C(91)-Si(8)	119.8(3)
C(96B)-C(91)-Si(8)	114.2(5)
C(93)-C(92)-C(91)	122.1(4)
C(94)-C(93)-C(92)	119.2(5)
C(95A)-C(94)-C(93)	119.8(5)
C(95A)-C(94)-C(95B)	38.0(6)
C(93)-C(94)-C(95B)	117.1(5)
C(94)-C(95A)-C(96A)	121.3(5)
C(91)-C(96A)-C(95A)	122.0(5)
C(96B)-C(95B)-C(94)	109.1(11)
C(95B)-C(96B)-C(91)	117.6(12)
C(98)-C(97)-C(102)	118.9(4)
C(98)-C(97)-C(103)	119.7(5)
C(102)-C(97)-C(103)	121.4(5)
C(99)-C(98)-C(97)	121.0(4)
C(98)-C(99)-C(100)	120.8(4)
C(99)-C(100)-C(101)	119.8(4)
C(100)-C(101)-C(102)	119.3(4)
C(101)-C(102)-C(97)	120.2(4)
C(104)-O(17)-C(106)	110.0(3)
O(17)-C(104)-C(105)	110.5(3)
O(18)-C(105)-C(104)	110.6(3)
O(17)-C(106)-C(107)	109.9(4)
O(18)-C(107)-C(106)	110.3(3)
C(107)-O(18)-C(105)	108.8(3)
C(108)-O(19)-C(110)	111.6(2)
O(19)-C(108)-C(109)	108.9(3)
O(20)-C(109)-C(108)	111.0(3)

O(19)-C(110)-C(111)	110.2(3)
O(20)-C(111)-C(110)	111.1(3)
C(111)-O(20)-C(109)	109.8(3)
C(113)-C(112)-C(115)	176.1(8)
C(113)-C(112)-C(116)	132.0(7)
C(115)-C(112)-C(116)	44.1(6)
C(113)-C(112)-C(116)#1	61.3(6)
C(115)-C(112)-C(116)#1	115.0(7)
C(116)-C(112)-C(116)#1	71.0(6)
C(112)-C(113)-C(116)#1	68.4(6)
C(112)-C(113)-C(114)	119.5(8)
C(116)#1-C(113)-C(114)	51.1(6)
C(115)#1-C(114)-C(116)#1	46.1(6)
C(115)#1-C(114)-C(113)	107.3(8)
C(116)#1-C(114)-C(113)	61.4(6)
C(116)-C(115)-C(114)#1	67.1(9)
C(116)-C(115)-C(112)	69.7(9)
C(114)#1-C(115)-C(112)	136.8(10)
C(115)-C(116)-C(114)#1	66.8(9)
C(115)-C(116)-C(112)	66.2(8)
C(114)#1-C(116)-C(112)	133.0(8)
C(115)-C(116)-C(113)#1	133.9(11)
C(114)#1-C(116)-C(113)#1	67.5(7)
C(112)-C(116)-C(113)#1	158.7(8)
C(115)-C(116)-C(112)#1	172.9(11)
C(114)#1-C(116)-C(112)#1	117.8(7)
C(112)-C(116)-C(112)#1	109.0(6)
C(113)#1-C(116)-C(112)#1	50.3(5)
C(115)-C(116)-C(116)#1	125.5(12)
C(114)#1-C(116)-C(116)#1	166.4(10)
C(112)-C(116)-C(116)#1	59.6(5)
C(113)#1-C(116)-C(116)#1	99.5(8)
C(112)#1-C(116)-C(116)#1	49.4(5)
C(1B2)-C(117)-C(118)	138.3(10)
C(1B2)-C(117)-C(1A2)	26.0(8)
C(118)-C(117)-C(1A2)	112.4(6)
C(119)-C(118)-C(117)	119.2(8)
C(118)-C(119)-C(120)	119.3(8)
C(121)-C(120)-C(119)	127.3(8)
C(1A2)-C(121)-C(120)	128.7(10)
C(1A2)-C(121)-C(1B2)	20.2(7)
C(120)-C(121)-C(1B2)	108.5(7)
C(121)-C(1A2)-C(1A3)	123.3(12)
C(121)-C(1A2)-C(117)	113.1(10)
C(1A3)-C(1A2)-C(117)	123.6(9)
C(117)-C(1B2)-C(1B3)	135.1(13)
C(117)-C(1B2)-C(121)	107.2(10)
C(1B3)-C(1B2)-C(121)	117.6(10)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2339. 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}
Ge(1)	15(1)	16(1)	15(1)	3(1)	4(1)	7(1)
Al(1)	13(1)	13(1)	14(1)	4(1)	2(1)	5(1)
Al(2)	13(1)	14(1)	13(1)	4(1)	1(1)	6(1)
Al(3)	14(1)	12(1)	13(1)	4(1)	0(1)	5(1)
Al(4)	13(1)	14(1)	14(1)	5(1)	1(1)	6(1)
Si(1)	13(1)	15(1)	15(1)	4(1)	2(1)	6(1)
Si(2)	13(1)	16(1)	14(1)	4(1)	0(1)	7(1)
Si(3)	14(1)	14(1)	12(1)	4(1)	2(1)	5(1)
Si(4)	15(1)	13(1)	16(1)	5(1)	1(1)	4(1)
Si(5)	17(1)	17(1)	14(1)	4(1)	0(1)	7(1)
Si(6)	15(1)	17(1)	16(1)	5(1)	0(1)	7(1)
Si(7)	20(1)	18(1)	16(1)	5(1)	3(1)	12(1)
Si(8)	20(1)	12(1)	21(1)	5(1)	5(1)	6(1)
O(1)	14(1)	13(1)	15(1)	4(1)	3(1)	6(1)
O(2)	14(1)	16(1)	16(1)	2(1)	-1(1)	7(1)
O(3)	14(1)	13(1)	15(1)	5(1)	1(1)	5(1)
O(4)	15(1)	19(1)	13(1)	5(1)	2(1)	7(1)
O(5)	15(1)	18(1)	19(1)	4(1)	1(1)	8(1)
O(6)	17(1)	20(1)	17(1)	7(1)	4(1)	10(1)
O(7)	14(1)	21(1)	16(1)	5(1)	0(1)	7(1)
O(8)	15(1)	16(1)	14(1)	5(1)	3(1)	7(1)
O(9)	18(1)	15(1)	18(1)	5(1)	1(1)	5(1)
O(10)	19(1)	15(1)	17(1)	5(1)	0(1)	4(1)
O(11)	19(1)	18(1)	15(1)	5(1)	0(1)	7(1)
O(12)	19(1)	20(1)	18(1)	2(1)	-1(1)	10(1)
O(13)	18(1)	18(1)	18(1)	4(1)	-2(1)	7(1)
O(14)	21(1)	18(1)	18(1)	5(1)	5(1)	10(1)
O(15)	23(1)	17(1)	26(1)	6(1)	4(1)	11(1)
O(16)	17(1)	14(1)	25(1)	5(1)	4(1)	6(1)
C(1)	16(1)	16(1)	18(1)	6(1)	4(1)	4(1)
C(2)	31(2)	39(2)	19(2)	8(1)	5(1)	22(2)
C(3)	38(2)	53(2)	17(2)	8(2)	3(1)	21(2)
C(4)	40(2)	36(2)	25(2)	2(1)	14(2)	16(2)
C(5)	41(2)	30(2)	40(2)	8(2)	21(2)	22(2)
C(6)	28(2)	24(2)	27(2)	11(1)	9(1)	15(1)
C(7)	16(1)	18(1)	17(1)	4(1)	3(1)	5(1)
C(8)	18(1)	23(2)	37(2)	5(1)	0(1)	8(1)
C(9)	31(2)	18(2)	51(2)	4(2)	1(2)	10(1)
C(10)	22(2)	19(2)	37(2)	3(1)	2(1)	-2(1)
C(11)	17(1)	30(2)	44(2)	6(2)	-6(1)	4(1)
C(12)	21(2)	22(2)	41(2)	8(1)	1(1)	8(1)
C(13)	13(1)	20(1)	16(1)	4(1)	3(1)	6(1)
C(14)	33(2)	24(2)	19(2)	4(1)	2(1)	14(1)
C(15)	37(2)	18(2)	29(2)	0(1)	5(1)	10(1)
C(16)	22(2)	28(2)	25(2)	-7(1)	-4(1)	7(1)
C(17)	25(2)	36(2)	24(2)	0(1)	-5(1)	16(1)
C(18)	20(1)	23(2)	24(2)	3(1)	-2(1)	11(1)
C(19)	18(1)	17(1)	16(1)	4(1)	-1(1)	7(1)
C(20)	26(2)	23(2)	26(2)	9(1)	8(1)	13(1)
C(21)	33(2)	23(2)	34(2)	16(1)	12(1)	11(1)
C(22)	41(2)	20(2)	34(2)	13(1)	9(2)	17(1)
C(23)	35(2)	29(2)	34(2)	12(1)	10(1)	22(2)
C(24)	24(2)	23(2)	28(2)	11(1)	9(1)	12(1)
C(25)	20(1)	21(1)	13(1)	4(1)	3(1)	11(1)
C(26)	23(1)	22(2)	20(1)	5(1)	0(1)	10(1)
C(27)	36(2)	32(2)	22(2)	10(1)	3(1)	21(2)
C(28)	26(2)	43(2)	19(2)	6(1)	-1(1)	20(2)
C(29)	19(1)	33(2)	19(2)	4(1)	-1(1)	8(1)
C(30)	21(1)	24(2)	18(1)	6(1)	4(1)	9(1)
C(31)	20(1)	19(1)	17(1)	10(1)	7(1)	8(1)
C(32)	22(2)	24(2)	29(2)	2(1)	2(1)	9(1)
C(33)	20(2)	34(2)	40(2)	8(2)	4(1)	14(1)
C(34)	31(2)	33(2)	38(2)	10(2)	13(1)	22(2)
C(35)	36(2)	34(2)	28(2)	-2(1)	4(1)	21(2)
C(36)	25(2)	29(2)	23(2)	0(1)	2(1)	14(1)
C(37)	16(1)	11(1)	23(1)	3(1)	1(1)	5(1)
C(38)	21(2)	28(2)	28(2)	6(1)	0(1)	11(1)
C(39)	21(2)	29(2)	51(2)	6(2)	-6(2)	11(1)
C(40)	18(2)	20(2)	64(3)	10(2)	13(2)	7(1)
C(41)	31(2)	28(2)	48(2)	12(2)	22(2)	7(2)
C(42)	27(2)	25(2)	28(2)	10(1)	5(1)	4(1)

C(43)	15(1)	14(1)	21(1)	6(1)	3(1)	5(1)
C(44)	25(2)	23(2)	19(1)	5(1)	1(1)	11(1)
C(45)	30(2)	23(2)	25(2)	4(1)	4(1)	13(1)
C(46)	30(2)	22(2)	36(2)	6(1)	3(1)	16(1)
C(47)	46(2)	33(2)	32(2)	7(2)	-6(2)	26(2)
C(48)	37(2)	26(2)	20(2)	2(1)	-5(1)	16(1)
C(49)	23(1)	18(1)	16(1)	3(1)	-4(1)	7(1)
C(50)	23(1)	23(2)	18(1)	3(1)	-2(1)	9(1)
C(51)	27(2)	27(2)	25(2)	8(1)	-1(1)	2(1)
C(52)	40(2)	17(2)	24(2)	4(1)	-7(1)	3(1)
C(53)	43(2)	21(2)	27(2)	4(1)	-4(1)	15(2)
C(54)	26(2)	23(2)	22(2)	5(1)	-1(1)	11(1)
C(55)	25(1)	23(2)	16(1)	5(1)	3(1)	14(1)
C(56)	24(2)	32(2)	24(2)	5(1)	2(1)	11(1)
C(57)	27(2)	45(2)	46(2)	13(2)	13(2)	14(2)
C(58)	47(2)	47(2)	37(2)	14(2)	25(2)	26(2)
C(59)	55(2)	41(2)	21(2)	3(2)	13(2)	23(2)
C(60)	34(2)	32(2)	21(2)	4(1)	5(1)	12(2)
C(61)	14(1)	21(1)	18(1)	6(1)	-2(1)	5(1)
C(62)	26(2)	19(2)	20(2)	3(1)	-5(1)	7(1)
C(63)	32(2)	25(2)	16(1)	1(1)	-7(1)	7(1)
C(64)	30(2)	26(2)	24(2)	9(1)	-8(1)	7(1)
C(65)	34(2)	31(2)	28(2)	10(1)	-1(1)	18(2)
C(66)	30(2)	32(2)	21(2)	7(1)	2(1)	19(1)
C(67)	20(1)	20(1)	31(2)	12(1)	6(1)	12(1)
C(68)	21(2)	24(2)	54(2)	7(2)	6(2)	8(1)
C(69)	19(2)	30(2)	84(3)	21(2)	11(2)	9(1)
C(70)	33(2)	55(3)	82(3)	44(2)	32(2)	28(2)
C(71)	46(2)	74(3)	45(2)	34(2)	26(2)	38(2)
C(72)	28(2)	54(2)	32(2)	16(2)	10(1)	24(2)
C(73)	26(2)	25(2)	18(1)	9(1)	5(1)	18(1)
C(74)	30(2)	29(2)	25(2)	11(1)	9(1)	18(1)
C(75)	34(2)	42(2)	33(2)	22(2)	16(2)	22(2)
C(76)	51(2)	55(2)	29(2)	18(2)	22(2)	36(2)
C(77)	54(2)	45(2)	23(2)	4(2)	8(2)	31(2)
C(78)	35(2)	32(2)	20(2)	6(1)	6(1)	20(2)
C(79)	32(2)	25(2)	18(1)	6(1)	2(1)	18(1)
C(80)	25(2)	48(2)	35(2)	23(2)	0(1)	11(2)
C(81)	32(2)	47(2)	46(2)	18(2)	-11(2)	13(2)
C(82)	62(3)	40(2)	28(2)	6(2)	-12(2)	31(2)
C(83)	87(4)	147(6)	34(2)	54(3)	28(2)	83(4)
C(84)	61(3)	133(5)	36(2)	48(3)	26(2)	70(3)
C(85)	18(1)	16(1)	22(2)	6(1)	5(1)	3(1)
C(86)	27(2)	25(2)	26(2)	8(1)	4(1)	8(1)
C(87)	36(2)	35(2)	28(2)	9(2)	-1(2)	5(2)
C(88)	43(2)	27(2)	22(2)	3(1)	8(2)	-2(2)
C(89)	41(2)	21(2)	30(2)	3(1)	14(2)	6(1)
C(90)	29(2)	19(2)	28(2)	4(1)	9(1)	7(1)
C(91)	43(2)	16(2)	25(2)	7(1)	11(1)	9(1)
C(92)	25(2)	70(3)	31(2)	22(2)	3(2)	14(2)
C(93)	33(2)	60(3)	35(2)	13(2)	8(2)	1(2)
C(94)	113(5)	40(3)	60(3)	24(2)	56(3)	32(3)
C(95A)	55(4)	41(3)	53(4)	35(3)	23(3)	32(3)
C(96A)	39(3)	31(3)	39(3)	17(2)	14(2)	22(2)
C(95B)	96(13)	54(9)	30(7)	23(7)	9(8)	52(10)
C(96B)	59(9)	39(7)	32(6)	21(6)	14(6)	40(7)
C(97)	71(3)	29(2)	36(2)	14(2)	25(2)	15(2)
C(98)	60(3)	46(2)	44(2)	23(2)	17(2)	28(2)
C(99)	49(2)	47(2)	34(2)	20(2)	6(2)	22(2)
C(100)	46(2)	34(2)	36(2)	10(2)	6(2)	17(2)
C(101)	42(2)	40(2)	47(2)	15(2)	4(2)	14(2)
C(102)	50(3)	38(2)	39(2)	15(2)	0(2)	-5(2)
C(103)	97(4)	47(3)	53(3)	5(2)	16(3)	23(3)
O(17)	34(1)	47(2)	20(1)	16(1)	1(1)	-3(1)
C(104)	38(2)	35(2)	25(2)	10(1)	0(1)	8(2)
C(105)	28(2)	56(3)	70(3)	35(2)	-9(2)	3(2)
C(106)	31(2)	60(3)	34(2)	24(2)	-7(2)	-8(2)
C(107)	54(3)	35(2)	40(2)	12(2)	8(2)	4(2)
O(18)	35(1)	44(2)	45(2)	25(1)	-5(1)	8(1)
O(19)	34(1)	27(1)	49(2)	7(1)	17(1)	19(1)
C(108)	29(2)	30(2)	37(2)	10(2)	10(1)	16(1)
C(109)	41(2)	25(2)	52(2)	8(2)	15(2)	12(2)
C(110)	29(2)	21(2)	52(2)	9(2)	14(2)	11(1)
C(111)	48(2)	38(2)	41(2)	15(2)	13(2)	20(2)
O(20)	60(2)	27(1)	44(2)	5(1)	22(1)	21(1)

sh 2151

Table 1. Crystal data and structure refinement for sh2151.

Identification code	sh2151	
Empirical formula	C141 H153 Al4 N4 O17 Si8	
Formula weight	2508.31	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 14.142(3) Å	α= 90°.
	b = 35.355(7) Å	β= 94.36(3)°.
	c = 28.754(6) Å	γ = 90°.
Volume	14335(5) $Å^3$	
Z	4	
Density (calculated)	1.162 Mg/m^3	
Absorption coefficient	0.160 mm^{-1}	
F(000)	5308	
Crystal size	0.6 x 0.45 x 0.4 mm^3	
Theta range for data collection	1.85 to 24.08°.	
Index ranges	-15<=h<=15, -39<=k<=40, -32<=l<=32	
Reflections collected	90418	
Independent reflections	21303 [R(int) = 0.0951]	
Completeness to theta = 24.08°	93.8 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	21303 / 0 / 1338	
Goodness-of-fit on F^2	0.934	
Final R indices [I>2sigma(I)]	R1 = 0.0665, wR2 = 0.1507	
R indices (all data)	R1 = 0.1363, wR2 = 0.1730	
Largest diff. peak and hole	0.704 and -0.450 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2151. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	1949(1)	9172(1)	3289(1)	32(1)
Al(2)	1887(1)	9001(1)	2178(1)	32(1)
Al(3)	1810(1)	8097(1)	2411(1)	32(1)
Al(4)	2071(1)	8278(1)	3517(1)	32(1)
Si(1)	202(1)	9768(1)	3093(1)	36(1)
Si(2)	566(1)	9720(1)	2030(1)	36(1)
Si(3)	3443(1)	8826(1)	1436(1)	38(1)
Si(4)	2949(1)	7956(1)	1528(1)	38(1)
Si(5)	176(1)	7487(1)	2593(1)	38(1)
Si(6)	866(1)	7552(1)	3671(1)	37(1)
Si(7)	3837(1)	8440(1)	4288(1)	38(1)
Si(8)	3359(1)	9312(1)	4184(1)	36(1)
O(1)	2375(3)	9150(1)	2730(1)	37(1)
O(2)	1428(2)	8544(1)	2201(1)	35(1)
O(3)	2370(3)	8117(1)	2970(1)	35(1)
O(4)	1582(3)	8730(1)	3480(1)	35(1)
O(5)	955(2)	9457(1)	3279(1)	41(1)
O(6)	78(2)	9785(1)	2521(1)	44(1)
O(7)	977(2)	9300(1)	1975(1)	39(1)
O(8)	2795(3)	9015(1)	1803(1)	43(1)
O(9)	3434(3)	8366(1)	1442(1)	44(1)
O(10)	2623(2)	7905(1)	2047(1)	41(1)
O(11)	793(2)	7818(1)	2392(1)	41(1)
O(12)	304(2)	7459(1)	3163(1)	45(1)
O(13)	1228(2)	7978(1)	3731(1)	38(1)
O(14)	3109(2)	8274(1)	3885(1)	41(1)
O(15)	3859(2)	8900(1)	4289(1)	41(1)
O(16)	2874(2)	9348(1)	3662(1)	38(1)
C(1)	-976(4)	9638(1)	3291(2)	37(1)
C(2)	-1682(4)	9458(2)	3001(2)	57(2)
C(3)	-2531(5)	9344(2)	3163(3)	75(2)
C(4)	-2711(5)	9411(2)	3621(3)	76(2)
C(5)	-2041(5)	9587(2)	3916(2)	69(2)
C(6)	-1188(4)	9700(2)	3755(2)	53(2)
C(7)	572(4)	10238(1)	3331(2)	44(1)
C(8)	1516(5)	10315(2)	3456(2)	59(2)
C(9)	1845(6)	10663(2)	3631(3)	87(2)
C(10)	1180(7)	10943(2)	3692(3)	105(3)
C(11)	246(6)	10882(2)	3572(3)	94(3)
C(12)	-68(5)	10534(2)	3395(2)	68(2)
C(13)	-388(4)	9808(1)	1560(2)	46(1)
C(14)	-343(5)	9689(2)	1107(2)	79(2)
C(15)	-1050(8)	9754(2)	750(3)	112(3)
C(16)	-1830(8)	9956(3)	856(4)	120(4)
C(17)	-1911(6)	10092(3)	1297(4)	127(4)
C(18)	-1182(5)	10014(2)	1641(2)	93(2)
C(19)	1532(4)	10076(1)	1998(2)	42(1)
C(20)	2341(5)	10008(2)	1764(2)	61(2)
C(21)	3049(5)	10278(2)	1730(3)	82(2)
C(22)	2969(6)	10620(2)	1939(3)	84(2)
C(23)	2191(6)	10700(2)	2174(3)	77(2)
C(24)	1474(5)	10432(2)	2202(2)	60(2)
C(25)	3063(4)	8978(1)	829(2)	46(1)
C(26)	2321(5)	9230(2)	728(2)	64(2)
C(27)	2021(6)	9326(2)	263(3)	89(2)
C(28)	2464(7)	9173(2)	-101(2)	90(2)
C(29)	3189(6)	8926(2)	-11(2)	70(2)
C(30)	3490(4)	8829(2)	443(2)	56(2)
C(31)	502(4)	7021(1)	2343(2)	44(1)
C(32)	1419(5)	6946(2)	2242(2)	67(2)
C(33)	1708(6)	6596(2)	2083(3)	86(2)
C(34)	1064(8)	6309(2)	2019(3)	91(3)
C(35)	150(7)	6373(2)	2098(3)	89(2)
C(36)	-142(5)	6728(2)	2264(2)	70(2)
C(37)	4703(4)	8968(1)	1591(2)	41(1)
C(38)	5005(5)	9341(2)	1520(2)	62(2)
C(39)	5918(6)	9453(2)	1645(3)	82(2)
C(40)	6566(5)	9204(2)	1852(2)	78(2)
C(41)	6294(5)	8847(2)	1935(2)	71(2)
C(42)	5387(4)	8726(2)	1802(2)	54(2)
C(43)	3890(4)	7608(1)	1433(2)	41(1)

C(44)	4665(4)	7690(2)	1178(2)	52(2)
C(45)	5368(5)	7426(2)	1110(2)	66(2)
C(46)	5312(5)	7070(2)	1288(3)	75(2)
C(47)	4570(6)	6973(2)	1542(3)	84(2)
C(48)	3864(5)	7238(2)	1612(2)	67(2)
C(49)	1916(4)	7891(1)	1092(2)	44(1)
C(50)	1138(4)	7670(2)	1192(2)	58(2)
C(51)	369(5)	7617(2)	870(3)	76(2)
C(52)	338(6)	7778(2)	433(3)	83(2)
C(53)	1085(6)	7999(2)	322(2)	75(2)
C(54)	1857(5)	8052(2)	640(2)	58(2)
C(55)	-1107(4)	7584(1)	2439(2)	41(1)
C(56)	-1719(5)	7700(2)	2769(2)	66(2)
C(57)	-2652(5)	7787(2)	2641(3)	90(2)
C(58)	-3019(6)	7751(2)	2183(3)	84(2)
C(59)	-2441(5)	7637(2)	1855(2)	74(2)
C(60)	-1506(5)	7558(2)	1976(2)	59(2)
C(61)	-19(4)	7462(1)	4107(2)	39(1)
C(62)	-766(5)	7205(2)	4031(2)	65(2)
C(63)	-1399(5)	7140(2)	4372(3)	85(2)
C(64)	-1309(6)	7320(2)	4787(3)	80(2)
C(65)	-598(5)	7581(2)	4873(2)	75(2)
C(66)	31(4)	7644(2)	4541(2)	60(2)
C(67)	1894(4)	7220(1)	3750(2)	44(1)
C(68)	2690(5)	7303(2)	4045(2)	56(2)
C(69)	3441(5)	7050(2)	4121(2)	69(2)
C(70)	3421(6)	6709(2)	3899(2)	73(2)
C(71)	2665(6)	6619(2)	3600(3)	86(2)
C(72)	1899(5)	6867(2)	3527(2)	66(2)
C(73)	3521(4)	8280(1)	4875(2)	42(1)
C(74)	2628(5)	8136(2)	4941(2)	57(2)
C(75)	2352(6)	8054(2)	5381(2)	79(2)
C(76)	2968(7)	8110(2)	5769(2)	79(2)
C(77)	3851(6)	8248(2)	5723(2)	77(2)
C(78)	4124(5)	8329(2)	5275(2)	64(2)
C(79)	5062(4)	8276(1)	4184(2)	45(1)
C(80)	5706(5)	8501(2)	3968(2)	69(2)
C(81)	6567(6)	8364(2)	3859(3)	100(3)
C(82)	6838(6)	7997(2)	3972(3)	92(2)
C(83)	6225(6)	7774(2)	4176(3)	92(2)
C(84)	5343(5)	7907(2)	4279(2)	71(2)
C(85)	4326(4)	9665(1)	4266(2)	42(1)
C(86)	5187(4)	9590(2)	4518(2)	54(2)
C(87)	5894(5)	9854(2)	4595(2)	70(2)
C(88)	5774(6)	10203(3)	4414(2)	82(2)
C(89)	4944(6)	10298(2)	4164(3)	86(2)
C(90)	4216(5)	10035(2)	4093(2)	64(2)
C(91)	2451(4)	9392(1)	4614(2)	40(1)
C(92)	2359(4)	9169(2)	5007(2)	56(2)
C(93)	1671(5)	9236(2)	5317(2)	66(2)
C(94)	1075(5)	9534(2)	5250(2)	79(2)
C(95)	1163(6)	9769(2)	4872(3)	103(3)
C(96)	1841(5)	9701(2)	4561(2)	81(2)
N(1)	3959(4)	9486(2)	2653(2)	92(2)
C(97)	3944(7)	9880(3)	2813(3)	121(3)
C(98)	4708(8)	9267(3)	2878(4)	140(4)
N(2)	-181(4)	8461(1)	1751(2)	63(1)
C(99)	-152(6)	8602(2)	1272(2)	86(2)
C(100)	-905(6)	8633(2)	2018(3)	99(2)
N(3)	4013(4)	7834(2)	3098(2)	81(2)
C(101)	4032(7)	7440(3)	2982(3)	129(3)
C(102)	4669(8)	8054(3)	2849(4)	147(4)
N(4)	-37(4)	8805(1)	3791(2)	62(1)
C(103)	-736(7)	8537(2)	3588(3)	113(3)
C(104)	50(7)	8796(2)	4296(3)	115(3)
C(105)	4069(9)	10074(3)	51(4)	140(4)
C(106)	4534(7)	9786(3)	270(3)	110(3)
C(107)	4593(8)	10296(3)	-236(3)	118(3)
C(108)	1138(8)	10571(3)	713(3)	122(3)
C(109)	314(8)	10728(3)	530(3)	124(3)
C(110)	323(8)	11004(3)	191(3)	124(3)
C(112)	1203(7)	11111(3)	65(3)	112(3)
C(113)	1992(8)	10965(3)	255(3)	127(3)
C(114)	1975(8)	10697(3)	577(3)	126(3)
C(115)	1471(8)	6321(3)	727(4)	127(3)
C(116)	1809(8)	6683(3)	772(4)	137(4)
C(117)	2447(9)	6814(4)	474(4)	155(4)

C(118)	2665(11)	6598(4)	126(5)	190(5)
C(119)	2345(10)	6217(4)	83(5)	177(5)
C(120)	1727(8)	6113(3)	368(3)	121(3)
C(121)	4575(7)	9436(3)	-1124(3)	122(3)
C(122)	4269(9)	9410(4)	-1596(4)	160(4)
C(123)	4352(8)	9040(3)	-1816(4)	140(4)
C(124)	4766(7)	8761(3)	-1566(3)	109(3)
C(125)	5132(8)	8826(3)	-1130(4)	133(3)
C(126)	5029(7)	9174(3)	-912(3)	109(3)
C(127)	-2845(7)	7991(2)	210(3)	106(3)
C(128)	-2547(7)	8087(2)	651(3)	103(3)
C(129)	-2984(6)	8369(2)	868(3)	99(2)
C(130)	-3717(6)	8565(2)	644(3)	98(2)
C(131)	-4038(7)	8461(2)	193(3)	106(3)
C(132)	-3571(7)	8169(2)	-11(3)	108(3)
C(133)	2592(8)	8920(3)	6693(4)	137(4)
C(134)	2264(8)	8930(3)	7130(4)	138(4)
C(135)	2340(8)	9245(3)	7374(4)	145(4)
C(136)	2743(9)	9550(3)	7207(4)	149(4)
C(137)	3082(8)	9534(3)	6770(4)	130(3)
C(138)	2983(8)	9229(3)	6533(4)	130(3)
O(17)	394(10)	8761(4)	-1757(5)	260(5)
C(139)	1341(13)	8746(4)	-1439(6)	222(7)
C(140)	1840(13)	8384(5)	-1626(6)	230(7)
C(141)	1316(10)	8216(4)	-2059(5)	176(5)
C(142)	437(10)	8468(4)	-2136(5)	182(5)

Table 3. Bond lengths [Å] and angles [°] for sh2151.

Al(1)-O(5)	1.727(3)
Al(1)-O(16)	1.742(3)
Al(1)-O(4)	1.748(3)
Al(1)-O(1)	1.762(4)
Al(2)-O(7)	1.732(3)
Al(2)-O(8)	1.738(4)
Al(2)-O(2)	1.747(3)
Al(2)-O(1)	1.763(3)
Al(3)-O(3)	1.740(4)
Al(3)-O(11)	1.741(3)
Al(3)-O(10)	1.749(3)
Al(3)-O(2)	1.760(3)
Al(4)-O(13)	1.741(3)
Al(4)-O(14)	1.743(4)
Al(4)-O(4)	1.743(3)
Al(4)-O(3)	1.755(4)
Si(1)-O(5)	1.597(3)
Si(1)-O(6)	1.641(3)
Si(1)-C(1)	1.857(5)
Si(1)-C(7)	1.859(5)
Si(2)-O(7)	1.607(3)
Si(2)-O(6)	1.634(4)
Si(2)-C(13)	1.861(6)
Si(2)-C(19)	1.864(5)
Si(3)-O(8)	1.596(3)
Si(3)-O(9)	1.627(3)
Si(3)-C(25)	1.865(6)
Si(3)-C(37)	1.872(6)
Si(4)-O(10)	1.604(3)
Si(4)-O(9)	1.630(3)
Si(4)-C(43)	1.848(5)
Si(4)-C(49)	1.866(6)
Si(5)-O(11)	1.595(3)
Si(5)-O(12)	1.639(3)
Si(5)-C(55)	1.866(5)
Si(5)-C(31)	1.870(5)
Si(6)-O(13)	1.599(3)
Si(6)-O(12)	1.642(4)
Si(6)-C(61)	1.864(5)
Si(6)-C(67)	1.867(6)
Si(7)-O(14)	1.601(4)
Si(7)-O(15)	1.628(3)
Si(7)-C(73)	1.866(5)
Si(7)-C(79)	1.873(6)
Si(8)-O(16)	1.608(3)
Si(8)-O(15)	1.637(3)
Si(8)-C(85)	1.852(5)
Si(8)-C(91)	1.870(5)
C(1)-C(2)	1.404(7)
C(1)-C(6)	1.408(7)
C(2)-C(3)	1.379(8)
C(3)-C(4)	1.381(9)
C(4)-C(5)	1.373(9)
C(5)-C(6)	1.384(8)
C(7)-C(8)	1.382(8)
C(7)-C(12)	1.404(8)
C(8)-C(9)	1.394(8)
C(9)-C(10)	1.386(10)
C(10)-C(11)	1.357(10)
C(11)-C(12)	1.393(8)
C(13)-C(18)	1.372(9)
C(13)-C(14)	1.375(8)
C(14)-C(15)	1.397(10)
C(15)-C(16)	1.367(14)
C(16)-C(17)	1.368(13)
C(17)-C(18)	1.402(11)
C(19)-C(20)	1.390(8)
C(19)-C(24)	1.394(7)
C(20)-C(21)	1.393(9)
C(21)-C(22)	1.357(10)
C(22)-C(23)	1.365(10)
C(23)-C(24)	1.395(9)
C(25)-C(26)	1.390(8)
C(25)-C(30)	1.406(7)
C(26)-C(27)	1.414(9)

C(27)-C(28)	1.374(11)
C(28)-C(29)	1.356(10)
C(29)-C(30)	1.384(8)
C(31)-C(32)	1.376(8)
C(31)-C(36)	1.387(8)
C(32)-C(33)	1.391(8)
C(33)-C(34)	1.367(11)
C(34)-C(35)	1.348(11)
C(35)-C(36)	1.415(9)
C(37)-C(42)	1.394(7)
C(37)-C(38)	1.407(7)
C(38)-C(39)	1.372(9)
C(39)-C(40)	1.374(10)
C(40)-C(41)	1.348(9)
C(41)-C(42)	1.380(8)
C(43)-C(44)	1.394(7)
C(43)-C(48)	1.407(7)
C(44)-C(45)	1.389(8)
C(45)-C(46)	1.362(9)
C(46)-C(47)	1.369(9)
C(47)-C(48)	1.394(9)
C(49)-C(50)	1.398(8)
C(49)-C(54)	1.414(7)
C(50)-C(51)	1.388(9)
C(51)-C(52)	1.377(9)
C(52)-C(53)	1.371(10)
C(53)-C(54)	1.382(9)
C(55)-C(56)	1.394(8)
C(55)-C(60)	1.409(7)
C(56)-C(57)	1.376(9)
C(57)-C(58)	1.384(10)
C(58)-C(59)	1.358(9)
C(59)-C(60)	1.369(9)
C(61)-C(62)	1.398(7)
C(61)-C(66)	1.401(7)
C(62)-C(63)	1.395(9)
C(63)-C(64)	1.351(9)
C(64)-C(65)	1.373(10)
C(65)-C(66)	1.373(8)
C(67)-C(68)	1.390(8)
C(67)-C(72)	1.404(7)
C(68)-C(69)	1.392(8)
C(69)-C(70)	1.363(8)
C(70)-C(71)	1.359(10)
C(71)-C(72)	1.398(9)
C(73)-C(74)	1.389(8)
C(73)-C(78)	1.390(8)
C(74)-C(75)	1.382(8)
C(75)-C(76)	1.377(10)
C(76)-C(77)	1.356(10)
C(77)-C(78)	1.402(9)
C(79)-C(84)	1.385(7)
C(79)-C(80)	1.390(8)
C(80)-C(81)	1.368(9)
C(81)-C(82)	1.383(10)
C(82)-C(83)	1.339(10)
C(83)-C(84)	1.386(9)
C(85)-C(86)	1.394(8)
C(85)-C(90)	1.404(7)
C(86)-C(87)	1.373(8)
C(87)-C(88)	1.346(10)
C(88)-C(89)	1.370(11)
C(89)-C(90)	1.393(9)
C(91)-C(92)	1.392(7)
C(91)-C(96)	1.392(8)
C(92)-C(93)	1.389(8)
C(93)-C(94)	1.355(9)
C(94)-C(95)	1.382(9)
C(95)-C(96)	1.381(9)
N(1)-C(98)	1.427(11)
N(1)-C(97)	1.468(10)
N(1)-H(1)	1.57(8)
N(2)-C(100)	1.459(9)
N(2)-C(99)	1.468(8)
N(2)-H(2)	1.53(7)
N(3)-C(101)	1.435(10)
N(3)-C(102)	1.443(11)

N(3)-H(3)	1.74(8)
N(4)-C(104)	1.450(9)
N(4)-C(103)	1.459(9)
N(4)-H(4)	1.69(6)
C(105)-C(106)	1.343(12)
C(105)-C(107)	1.393(13)
C(106)-C(107)#1	1.279(12)
C(107)-C(106)#1	1.279(12)
C(108)-C(114)	1.350(13)
C(108)-C(109)	1.362(12)
C(109)-C(110)	1.379(12)
C(110)-C(112)	1.375(12)
C(112)-C(113)	1.309(12)
C(113)-C(114)	1.327(12)
C(115)-C(120)	1.340(12)
C(115)-C(116)	1.367(12)
C(116)-C(117)	1.372(14)
C(117)-C(118)	1.311(15)
C(118)-C(119)	1.425(16)
C(119)-C(120)	1.295(15)
C(121)-C(126)	1.258(11)
C(121)-C(122)	1.394(13)
C(122)-C(123)	1.464(14)
C(123)-C(124)	1.329(12)
C(124)-C(125)	1.339(12)
C(125)-C(126)	1.394(12)
C(127)-C(132)	1.324(11)
C(127)-C(128)	1.349(11)
C(128)-C(129)	1.352(10)
C(129)-C(130)	1.367(10)
C(130)-C(131)	1.390(10)
C(131)-C(132)	1.379(11)
C(133)-C(138)	1.323(12)
C(133)-C(134)	1.371(13)
C(134)-C(135)	1.318(13)
C(135)-C(136)	1.329(14)
C(136)-C(137)	1.378(13)
C(137)-C(138)	1.279(12)
O(17)-C(142)	1.505(15)
O(17)-C(139)	1.565(18)
C(139)-C(140)	1.577(19)
C(140)-C(141)	1.522(17)
C(141)-C(142)	1.533(16)

O(5)-Al(1)-O(16)	111.97(17)
O(5)-Al(1)-O(4)	105.37(19)
O(16)-Al(1)-O(4)	110.70(17)
O(5)-Al(1)-O(1)	110.12(17)
O(16)-Al(1)-O(1)	106.53(18)
O(4)-Al(1)-O(1)	112.25(17)
O(7)-Al(2)-O(8)	109.86(17)
O(7)-Al(2)-O(2)	108.02(18)
O(8)-Al(2)-O(2)	110.10(17)
O(7)-Al(2)-O(1)	110.50(16)
O(8)-Al(2)-O(1)	107.00(18)
O(2)-Al(2)-O(1)	111.37(17)
O(3)-Al(3)-O(11)	111.57(17)
O(3)-Al(3)-O(10)	107.14(19)
O(11)-Al(3)-O(10)	109.94(17)
O(3)-Al(3)-O(2)	112.84(16)
O(11)-Al(3)-O(2)	105.43(18)
O(10)-Al(3)-O(2)	109.94(16)
O(13)-Al(4)-O(14)	110.46(17)
O(13)-Al(4)-O(4)	107.50(18)
O(14)-Al(4)-O(4)	110.85(17)
O(13)-Al(4)-O(3)	109.75(17)
O(14)-Al(4)-O(3)	106.93(19)
O(4)-Al(4)-O(3)	111.37(17)
O(5)-Si(1)-O(6)	112.19(18)
O(5)-Si(1)-C(1)	108.5(2)
O(6)-Si(1)-C(1)	106.7(2)
O(5)-Si(1)-C(7)	109.3(2)
O(6)-Si(1)-C(7)	110.1(2)
C(1)-Si(1)-C(7)	110.0(2)
O(7)-Si(2)-O(6)	113.10(17)
O(7)-Si(2)-C(13)	109.3(2)
O(6)-Si(2)-C(13)	105.9(2)

O(7)-Si(2)-C(19)	110.2(2)
O(6)-Si(2)-C(19)	107.9(2)
C(13)-Si(2)-C(19)	110.3(2)
O(8)-Si(3)-O(9)	113.88(18)
O(8)-Si(3)-C(25)	111.1(2)
O(9)-Si(3)-C(25)	107.2(2)
O(8)-Si(3)-C(37)	108.3(2)
O(9)-Si(3)-C(37)	105.8(2)
C(25)-Si(3)-C(37)	110.4(2)
O(10)-Si(4)-O(9)	113.16(18)
O(10)-Si(4)-C(43)	108.9(2)
O(9)-Si(4)-C(43)	104.7(2)
O(10)-Si(4)-C(49)	110.3(2)
O(9)-Si(4)-C(49)	108.9(2)
C(43)-Si(4)-C(49)	110.8(2)
O(11)-Si(5)-O(12)	112.73(18)
O(11)-Si(5)-C(55)	109.2(2)
O(12)-Si(5)-C(55)	106.3(2)
O(11)-Si(5)-C(31)	110.5(2)
O(12)-Si(5)-C(31)	108.6(2)
C(55)-Si(5)-C(31)	109.5(2)
O(13)-Si(6)-O(12)	114.48(18)
O(13)-Si(6)-C(61)	108.3(2)
O(12)-Si(6)-C(61)	105.1(2)
O(13)-Si(6)-C(67)	109.8(2)
O(12)-Si(6)-C(67)	107.5(2)
C(61)-Si(6)-C(67)	111.6(2)
O(14)-Si(7)-O(15)	112.19(18)
O(14)-Si(7)-C(73)	111.0(2)
O(15)-Si(7)-C(73)	107.8(2)
O(14)-Si(7)-C(79)	108.8(2)
O(15)-Si(7)-C(79)	107.0(2)
C(73)-Si(7)-C(79)	109.8(2)
O(16)-Si(8)-O(15)	112.95(18)
O(16)-Si(8)-C(85)	108.9(2)
O(15)-Si(8)-C(85)	105.7(2)
O(16)-Si(8)-C(91)	109.9(2)
O(15)-Si(8)-C(91)	108.8(2)
C(85)-Si(8)-C(91)	110.5(2)
Al(1)-O(1)-Al(2)	134.2(2)
Al(2)-O(2)-Al(3)	137.6(2)
Al(3)-O(3)-Al(4)	135.9(3)
Al(4)-O(4)-Al(1)	135.5(3)
Si(1)-O(5)-Al(1)	158.4(2)
Si(2)-O(6)-Si(1)	147.3(2)
Si(2)-O(7)-Al(2)	142.8(2)
Si(3)-O(8)-Al(2)	152.5(2)
Si(3)-O(9)-Si(4)	153.5(2)
Si(4)-O(10)-Al(3)	139.6(2)
Si(5)-O(11)-Al(3)	151.4(2)
Si(5)-O(12)-Si(6)	152.5(2)
Si(6)-O(13)-Al(4)	139.3(2)
Si(7)-O(14)-Al(4)	154.4(2)
Si(7)-O(15)-Si(8)	151.9(2)
Si(8)-O(16)-Al(1)	142.5(2)
C(2)-C(1)-C(6)	116.0(5)
C(2)-C(1)-Si(1)	123.0(4)
C(6)-C(1)-Si(1)	120.9(4)
C(3)-C(2)-C(1)	122.1(6)
C(2)-C(3)-C(4)	120.0(6)
C(5)-C(4)-C(3)	120.0(7)
C(4)-C(5)-C(6)	120.1(6)
C(5)-C(6)-C(1)	121.8(6)
C(8)-C(7)-C(12)	116.1(5)
C(8)-C(7)-Si(1)	120.8(4)
C(12)-C(7)-Si(1)	123.2(4)
C(7)-C(8)-C(9)	123.8(6)
C(10)-C(9)-C(8)	117.7(7)
C(11)-C(10)-C(9)	120.8(6)
C(10)-C(11)-C(12)	120.6(7)
C(11)-C(12)-C(7)	121.0(6)
C(18)-C(13)-C(14)	114.9(6)
C(18)-C(13)-Si(2)	121.5(5)
C(14)-C(13)-Si(2)	123.6(5)
C(13)-C(14)-C(15)	124.3(8)
C(16)-C(15)-C(14)	117.8(8)
C(15)-C(16)-C(17)	121.0(8)

C(16)-C(17)-C(18)	118.5(9)
C(13)-C(18)-C(17)	123.4(8)
C(20)-C(19)-C(24)	115.8(5)
C(20)-C(19)-Si(2)	122.7(4)
C(24)-C(19)-Si(2)	121.4(4)
C(19)-C(20)-C(21)	122.6(6)
C(22)-C(21)-C(20)	119.6(7)
C(21)-C(22)-C(23)	120.2(6)
C(22)-C(23)-C(24)	120.2(7)
C(19)-C(24)-C(23)	121.6(6)
C(26)-C(25)-C(30)	116.0(5)
C(26)-C(25)-Si(3)	122.6(4)
C(30)-C(25)-Si(3)	121.4(4)
C(25)-C(26)-C(27)	121.3(6)
C(28)-C(27)-C(26)	120.4(7)
C(29)-C(28)-C(27)	119.3(7)
C(28)-C(29)-C(30)	120.9(6)
C(29)-C(30)-C(25)	122.2(6)
C(32)-C(31)-C(36)	116.0(5)
C(32)-C(31)-Si(5)	121.0(4)
C(36)-C(31)-Si(5)	123.0(5)
C(31)-C(32)-C(33)	123.1(6)
C(34)-C(33)-C(32)	119.6(7)
C(35)-C(34)-C(33)	119.5(7)
C(34)-C(35)-C(36)	120.8(7)
C(31)-C(36)-C(35)	120.9(7)
C(42)-C(37)-C(38)	115.5(5)
C(42)-C(37)-Si(3)	123.8(4)
C(38)-C(37)-Si(3)	120.6(4)
C(39)-C(38)-C(37)	121.6(6)
C(38)-C(39)-C(40)	120.7(6)
C(41)-C(40)-C(39)	119.2(7)
C(40)-C(41)-C(42)	120.9(7)
C(41)-C(42)-C(37)	122.0(6)
C(44)-C(43)-C(48)	115.4(5)
C(44)-C(43)-Si(4)	122.9(4)
C(48)-C(43)-Si(4)	121.7(4)
C(45)-C(44)-C(43)	122.3(5)
C(46)-C(45)-C(44)	120.4(6)
C(45)-C(46)-C(47)	120.1(6)
C(46)-C(47)-C(48)	119.6(6)
C(47)-C(48)-C(43)	122.3(6)
C(50)-C(49)-C(54)	115.0(5)
C(50)-C(49)-Si(4)	121.2(4)
C(54)-C(49)-Si(4)	123.8(4)
C(51)-C(50)-C(49)	121.7(6)
C(52)-C(51)-C(50)	121.6(7)
C(53)-C(52)-C(51)	118.3(6)
C(52)-C(53)-C(54)	120.6(6)
C(53)-C(54)-C(49)	122.8(6)
C(56)-C(55)-C(60)	115.8(5)
C(56)-C(55)-Si(5)	122.4(4)
C(60)-C(55)-Si(5)	121.7(4)
C(57)-C(56)-C(55)	121.2(6)
C(56)-C(57)-C(58)	121.0(7)
C(59)-C(58)-C(57)	119.1(7)
C(58)-C(59)-C(60)	120.3(6)
C(59)-C(60)-C(55)	122.5(6)
C(62)-C(61)-C(66)	115.1(5)
C(62)-C(61)-Si(6)	123.0(4)
C(66)-C(61)-Si(6)	121.9(4)
C(63)-C(62)-C(61)	121.0(6)
C(64)-C(63)-C(62)	121.4(6)
C(63)-C(64)-C(65)	119.7(6)
C(64)-C(65)-C(66)	119.2(6)
C(65)-C(66)-C(61)	123.6(6)
C(68)-C(67)-C(72)	115.7(5)
C(68)-C(67)-Si(6)	121.9(4)
C(72)-C(67)-Si(6)	122.3(4)
C(67)-C(68)-C(69)	122.3(5)
C(70)-C(69)-C(68)	120.4(6)
C(71)-C(70)-C(69)	119.5(6)
C(70)-C(71)-C(72)	120.7(6)
C(71)-C(72)-C(67)	121.4(6)
C(74)-C(73)-C(78)	116.0(5)
C(74)-C(73)-Si(7)	121.2(4)
C(78)-C(73)-Si(7)	122.6(5)

C(75)-C(74)-C(73)	121.7(6)
C(76)-C(75)-C(74)	120.4(7)
C(77)-C(76)-C(75)	120.2(6)
C(76)-C(77)-C(78)	118.9(7)
C(73)-C(78)-C(77)	122.8(7)
C(84)-C(79)-C(80)	116.1(5)
C(84)-C(79)-Si(7)	121.0(4)
C(80)-C(79)-Si(7)	122.6(4)
C(81)-C(80)-C(79)	121.6(6)
C(80)-C(81)-C(82)	120.8(7)
C(83)-C(82)-C(81)	118.6(7)
C(82)-C(83)-C(84)	121.1(7)
C(79)-C(84)-C(83)	121.7(6)
C(86)-C(85)-C(90)	115.5(5)
C(86)-C(85)-Si(8)	123.1(4)
C(90)-C(85)-Si(8)	121.4(4)
C(87)-C(86)-C(85)	123.5(6)
C(88)-C(87)-C(86)	119.5(7)
C(87)-C(88)-C(89)	120.4(7)
C(88)-C(89)-C(90)	120.4(7)
C(89)-C(90)-C(85)	120.7(6)
C(92)-C(91)-C(96)	116.0(5)
C(92)-C(91)-Si(8)	124.2(4)
C(96)-C(91)-Si(8)	119.8(4)
C(93)-C(92)-C(91)	122.6(6)
C(94)-C(93)-C(92)	119.9(6)
C(93)-C(94)-C(95)	119.1(6)
C(96)-C(95)-C(94)	121.0(7)
C(95)-C(96)-C(91)	121.3(6)
C(98)-N(1)-C(97)	113.6(7)
C(98)-N(1)-H(1)	105(2)
C(97)-N(1)-H(1)	114(2)
C(100)-N(2)-C(99)	115.0(5)
C(100)-N(2)-H(2)	105(2)
C(99)-N(2)-H(2)	114(2)
C(101)-N(3)-C(102)	112.6(7)
C(101)-N(3)-H(3)	115(3)
C(102)-N(3)-H(3)	105(3)
C(104)-N(4)-C(103)	113.0(6)
C(104)-N(4)-H(4)	114(2)
C(103)-N(4)-H(4)	108.4(19)
C(106)-C(105)-C(107)	116.3(11)
C(107)#1-C(106)-C(105)	125.2(10)
C(106)#1-C(107)-C(105)	118.5(10)
C(114)-C(108)-C(109)	119.8(11)
C(108)-C(109)-C(110)	120.5(11)
C(112)-C(110)-C(109)	116.0(10)
C(113)-C(112)-C(110)	122.8(11)
C(112)-C(113)-C(114)	120.8(12)
C(113)-C(114)-C(108)	120.0(11)
C(120)-C(115)-C(116)	118.2(11)
C(115)-C(116)-C(117)	119.8(12)
C(118)-C(117)-C(116)	119.0(14)
C(117)-C(118)-C(119)	121.6(16)
C(120)-C(119)-C(118)	115.9(14)
C(119)-C(120)-C(115)	124.6(12)
C(126)-C(121)-C(122)	122.3(11)
C(121)-C(122)-C(123)	116.7(11)
C(124)-C(123)-C(122)	118.4(11)
C(123)-C(124)-C(125)	120.2(10)
C(124)-C(125)-C(126)	121.7(10)
C(121)-C(126)-C(125)	119.8(10)
C(132)-C(127)-C(128)	120.5(9)
C(127)-C(128)-C(129)	119.8(9)
C(128)-C(129)-C(130)	121.0(9)
C(129)-C(130)-C(131)	119.2(8)
C(132)-C(131)-C(130)	117.5(9)
C(127)-C(132)-C(131)	122.1(9)
C(138)-C(133)-C(134)	118.6(11)
C(135)-C(134)-C(133)	119.4(12)
C(134)-C(135)-C(136)	120.9(13)
C(135)-C(136)-C(137)	119.0(12)
C(138)-C(137)-C(136)	119.4(12)
C(137)-C(138)-C(133)	122.8(12)
C(142)-O(17)-C(139)	108.7(12)
O(17)-C(139)-C(140)	102.3(13)
C(141)-C(140)-C(139)	113.2(14)

C(140)-C(141)-C(142)	103.2(12)
O(17)-C(142)-C(141)	111.9(12)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2151. 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}
Al(1)	29(1)	33(1)	32(1)	0(1)	2(1)	2(1)
Al(2)	33(1)	33(1)	31(1)	1(1)	5(1)	1(1)
Al(3)	32(1)	32(1)	33(1)	0(1)	6(1)	-1(1)
Al(4)	30(1)	33(1)	33(1)	2(1)	3(1)	0(1)
Si(1)	33(1)	35(1)	39(1)	0(1)	2(1)	5(1)
Si(2)	37(1)	34(1)	37(1)	3(1)	-1(1)	3(1)
Si(3)	38(1)	40(1)	38(1)	0(1)	12(1)	-1(1)
Si(4)	39(1)	38(1)	38(1)	-4(1)	9(1)	2(1)
Si(5)	36(1)	39(1)	38(1)	1(1)	5(1)	-6(1)
Si(6)	38(1)	37(1)	35(1)	4(1)	6(1)	-4(1)
Si(7)	31(1)	44(1)	38(1)	6(1)	-1(1)	1(1)
Si(8)	32(1)	41(1)	34(1)	-1(1)	1(1)	-3(1)
O(1)	31(2)	44(2)	37(2)	1(2)	1(2)	-6(2)
O(2)	28(2)	35(2)	41(2)	2(1)	2(2)	-1(1)
O(3)	30(3)	40(2)	36(2)	2(1)	6(2)	4(2)
O(4)	27(2)	36(2)	43(2)	1(1)	6(2)	-2(2)
O(5)	33(2)	40(2)	49(2)	2(2)	-1(2)	10(2)
O(6)	46(3)	46(2)	38(2)	-3(2)	0(2)	5(2)
O(7)	39(2)	37(2)	39(2)	2(1)	-1(2)	6(2)
O(8)	45(2)	44(2)	41(2)	0(2)	17(2)	-2(2)
O(9)	48(3)	33(2)	52(2)	-1(2)	17(2)	-3(2)
O(10)	42(2)	43(2)	41(2)	-4(2)	13(2)	3(2)
O(11)	39(2)	39(2)	45(2)	0(2)	9(2)	-11(2)
O(12)	43(3)	54(2)	40(2)	1(2)	3(2)	-8(2)
O(13)	40(2)	32(2)	43(2)	5(1)	9(2)	-5(2)
O(14)	37(2)	45(2)	41(2)	4(2)	-2(2)	0(2)
O(15)	36(2)	39(2)	48(2)	9(2)	1(2)	2(2)
O(16)	38(2)	41(2)	33(2)	-3(1)	-1(1)	-5(2)
C(1)	34(3)	36(3)	42(3)	-4(2)	2(2)	5(2)
C(2)	39(4)	72(4)	62(4)	-12(3)	7(3)	-2(3)
C(3)	40(5)	95(5)	90(5)	-17(4)	5(4)	-19(4)
C(4)	56(5)	81(5)	96(6)	-1(4)	28(4)	-9(4)
C(5)	58(5)	78(4)	76(5)	-1(4)	32(4)	3(4)
C(6)	48(4)	57(3)	55(4)	-8(3)	12(3)	3(3)
C(7)	39(4)	46(3)	46(3)	7(2)	3(2)	-1(3)
C(8)	52(5)	48(3)	74(4)	-4(3)	-7(3)	-1(3)
C(9)	69(6)	58(4)	129(7)	-11(4)	-31(4)	-11(4)
C(10)	102(8)	51(4)	155(8)	-25(4)	-34(6)	-13(5)
C(11)	84(7)	40(4)	156(8)	-26(4)	-2(5)	6(4)
C(12)	50(5)	46(3)	107(5)	-12(3)	1(4)	4(3)
C(13)	54(4)	38(3)	47(3)	8(2)	-4(3)	1(3)
C(14)	99(6)	72(4)	60(4)	-7(3)	-25(4)	28(4)
C(15)	170(10)	79(5)	76(5)	-5(4)	-60(6)	17(6)
C(16)	121(9)	107(7)	120(8)	48(6)	-74(7)	-26(6)
C(17)	69(7)	181(10)	128(8)	57(8)	-16(6)	44(6)
C(18)	70(6)	139(7)	67(5)	25(4)	-1(4)	39(5)
C(19)	47(4)	35(3)	43(3)	5(2)	-4(3)	0(2)
C(20)	54(5)	53(4)	77(4)	6(3)	8(3)	-5(3)
C(21)	56(5)	67(5)	123(6)	26(4)	13(4)	-11(4)
C(22)	66(6)	67(5)	117(6)	30(4)	-12(5)	-26(4)
C(23)	95(7)	44(4)	91(5)	5(3)	-6(5)	-18(4)
C(24)	66(5)	50(4)	65(4)	12(3)	11(3)	-4(3)
C(25)	43(4)	45(3)	51(3)	0(2)	13(3)	-8(3)
C(26)	59(5)	83(4)	51(4)	1(3)	0(3)	6(3)
C(27)	92(6)	100(6)	70(5)	21(4)	-23(4)	16(4)
C(28)	107(7)	116(6)	44(4)	10(4)	-11(4)	-22(5)
C(29)	81(6)	87(5)	44(4)	-3(3)	15(3)	-19(4)
C(30)	60(5)	66(4)	43(3)	-1(3)	17(3)	1(3)
C(31)	44(4)	41(3)	47(3)	2(2)	2(3)	-3(3)
C(32)	67(5)	55(4)	80(5)	3(3)	21(4)	-4(3)
C(33)	92(6)	52(4)	119(6)	-4(4)	50(5)	17(4)
C(34)	125(8)	56(5)	95(6)	-6(4)	24(5)	25(5)
C(35)	116(8)	45(4)	103(6)	-19(4)	-2(5)	-11(4)
C(36)	74(5)	52(4)	83(5)	-8(3)	1(4)	-2(3)
C(37)	40(4)	48(3)	36(3)	-2(2)	11(2)	-5(2)
C(38)	55(5)	60(4)	70(4)	4(3)	2(3)	-8(3)
C(39)	66(6)	66(4)	114(6)	9(4)	6(4)	-34(4)
C(40)	51(5)	102(6)	80(5)	-8(4)	-3(4)	-24(4)
C(41)	47(5)	100(6)	66(4)	-1(4)	2(3)	6(4)
C(42)	39(4)	64(4)	58(4)	3(3)	6(3)	2(3)
C(43)	48(4)	38(3)	39(3)	-4(2)	7(2)	2(2)

C(44)	56(4)	58(4)	44(3)	-4(3)	11(3)	4(3)
C(45)	49(5)	82(5)	70(4)	-15(4)	20(3)	6(3)
C(46)	62(5)	70(5)	96(5)	-21(4)	19(4)	20(4)
C(47)	91(7)	44(4)	119(6)	2(4)	26(5)	23(4)
C(48)	66(5)	53(4)	85(5)	-6(3)	34(4)	4(3)
C(49)	51(4)	42(3)	40(3)	-2(2)	12(3)	5(3)
C(50)	56(5)	62(4)	56(4)	-9(3)	1(3)	-13(3)
C(51)	58(5)	90(5)	78(5)	-15(4)	0(4)	-25(4)
C(52)	65(6)	119(6)	62(5)	-23(4)	-17(4)	-7(4)
C(53)	81(6)	96(5)	46(4)	-5(3)	-7(4)	3(4)
C(54)	63(5)	64(4)	46(4)	-4(3)	6(3)	-10(3)
C(55)	36(4)	45(3)	41(3)	1(2)	2(2)	-6(2)
C(56)	48(5)	100(5)	50(4)	-10(3)	7(3)	6(3)
C(57)	48(6)	134(7)	87(6)	-25(5)	10(4)	20(4)
C(58)	51(5)	110(6)	90(6)	1(5)	-9(4)	17(4)
C(59)	54(5)	105(5)	59(4)	3(4)	-13(4)	6(4)
C(60)	50(5)	72(4)	55(4)	-3(3)	0(3)	-3(3)
C(61)	43(4)	39(3)	35(3)	6(2)	2(2)	-1(2)
C(62)	73(5)	54(4)	67(4)	-3(3)	12(3)	-22(3)
C(63)	68(6)	91(5)	98(6)	14(5)	28(4)	-30(4)
C(64)	76(6)	97(5)	71(5)	26(4)	39(4)	-5(4)
C(65)	66(5)	116(6)	46(4)	6(4)	23(3)	-1(4)
C(66)	52(4)	81(4)	47(4)	4(3)	6(3)	-12(3)
C(67)	56(4)	42(3)	35(3)	5(2)	7(3)	-6(3)
C(68)	65(5)	49(3)	51(4)	-5(3)	-7(3)	6(3)
C(69)	60(5)	64(4)	81(5)	9(4)	-12(3)	10(3)
C(70)	87(6)	57(4)	74(5)	8(3)	2(4)	32(4)
C(71)	104(7)	58(4)	91(5)	-18(4)	-14(5)	30(4)
C(72)	67(5)	52(4)	75(4)	-15(3)	-14(3)	8(3)
C(73)	45(4)	39(3)	43(3)	3(2)	2(3)	8(2)
C(74)	65(5)	56(4)	52(4)	-2(3)	17(3)	-17(3)
C(75)	95(6)	82(5)	64(5)	5(4)	34(4)	-24(4)
C(76)	105(7)	80(5)	56(5)	16(4)	32(4)	10(4)
C(77)	89(7)	99(5)	42(4)	9(3)	-7(4)	31(5)
C(78)	54(5)	88(5)	50(4)	16(3)	-4(3)	6(3)
C(79)	36(4)	51(3)	46(3)	3(2)	0(2)	3(3)
C(80)	44(5)	58(4)	107(5)	19(3)	23(4)	6(3)
C(81)	52(6)	98(6)	157(8)	39(5)	45(5)	9(4)
C(82)	53(6)	94(6)	133(7)	20(5)	30(5)	27(4)
C(83)	64(6)	75(5)	139(7)	28(5)	21(5)	28(4)
C(84)	54(5)	60(4)	103(5)	22(4)	24(4)	13(3)
C(85)	41(4)	52(3)	32(3)	-7(2)	2(2)	-8(2)
C(86)	43(4)	73(4)	45(3)	-15(3)	3(3)	-4(3)
C(87)	42(5)	117(6)	53(4)	-20(4)	6(3)	-25(4)
C(88)	65(6)	123(7)	59(4)	-27(4)	16(4)	-49(5)
C(89)	111(7)	66(4)	82(5)	2(4)	7(5)	-45(4)
C(90)	65(5)	60(4)	63(4)	-1(3)	-5(3)	-18(3)
C(91)	37(4)	47(3)	37(3)	-3(2)	1(2)	0(2)
C(92)	60(5)	54(3)	55(4)	-2(3)	12(3)	3(3)
C(93)	72(5)	77(4)	53(4)	6(3)	24(3)	2(4)
C(94)	72(6)	106(6)	63(4)	-10(4)	31(4)	16(4)
C(95)	94(7)	120(6)	103(6)	26(5)	50(5)	61(5)
C(96)	78(6)	94(5)	75(5)	25(4)	30(4)	31(4)
N(1)	70(5)	152(6)	55(3)	-1(4)	17(3)	-14(4)

sh 2283

Table 1. Crystal data and structure refinement for sh2283.

Identification code	sh2283	
Empirical formula	C135.50 H156 Al2 N2 O22 Si8	
Formula weight	2443.30	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.6979(11) Å	α= 90°.
	b = 37.059(3) Å	β= 106.069(3)°.
	c = 25.009(2) Å	γ = 90°.
Volume	13090(2) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	5188	
Crystal size	0.53 x 0.3 x 0.25 mm^3	

Theta range for data collection	1.01 to 26.35°.
Index ranges	-18<=h<=14, -46<=k<=46, -31<=l<=31
Reflections collected	177285
Independent reflections	26675 [R(int) = 0.1291]
Completeness to theta = 26.35°	99.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	26675 / 1 / 1459
Goodness-of-fit on F^2	1.537
Final R indices [I>2sigma(I)]	R1 = 0.1042, wR2 = 0.2245
R indices (all data)	R1 = 0.2158, wR2 = 0.2574
Largest diff. peak and hole	1.407 and -0.570 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2283. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	3370(1)	4593(1)	2182(1)	30(1)
Al(2)	3004(1)	3077(1)	2027(1)	29(1)
Si(1)	2084(1)	4282(1)	989(1)	31(1)
Si(2)	1520(1)	3451(1)	989(1)	32(1)
Si(3)	2933(1)	3360(1)	3261(1)	35(1)
Si(4)	2723(1)	4215(1)	3209(1)	40(1)
Si(5)	4097(1)	5361(1)	2151(1)	33(1)
Si(6)	5465(1)	4748(1)	2250(1)	31(1)
Si(7)	4839(1)	2979(1)	1670(1)	45(1)
Si(8)	3726(1)	2332(1)	1846(1)	50(1)
O(1)	2599(2)	4393(1)	1616(2)	37(1)
O(2)	1945(2)	3848(1)	905(1)	34(1)
O(3)	2045(2)	3280(1)	1577(1)	37(1)
O(4)	3087(2)	3202(1)	2704(2)	45(1)
O(5)	3095(2)	3796(1)	3277(2)	42(1)
O(6)	3166(2)	4415(1)	2776(2)	42(1)
O(7)	3311(2)	5064(1)	2162(1)	32(1)
O(8)	5102(2)	5166(1)	2143(1)	33(1)
O(9)	4572(2)	4489(1)	2222(1)	31(1)
O(10)	4070(2)	3211(1)	1878(2)	39(1)
O(11)	4602(3)	2550(1)	1690(2)	64(1)
O(12)	2956(2)	2610(1)	1951(2)	39(1)
C(1)	878(4)	4485(2)	761(2)	39(1)
C(2)	633(4)	4780(2)	1016(3)	67(2)
C(3)	-277(6)	4938(2)	852(4)	92(3)
C(4)	-926(5)	4810(3)	429(4)	81(3)
C(5)	-726(5)	4508(3)	148(3)	92(3)
C(6)	179(4)	4347(2)	314(3)	66(2)
C(7)	2799(3)	4431(1)	520(2)	33(1)
C(8A)	3114(5)	4786(2)	545(3)	48(1)
C(9A)	3631(5)	4909(2)	181(3)	48(1)
C(8B)	3767(15)	4507(6)	696(10)	48(1)
C(9B)	4334(16)	4636(6)	358(10)	48(1)
C(10)	3852(4)	4682(2)	-187(3)	55(2)
C(11A)	3584(5)	4326(2)	-204(3)	48(1)
C(12A)	3065(5)	4199(2)	155(3)	48(1)
C(11B)	2872(15)	4619(6)	-424(10)	48(1)
C(12B)	2367(16)	4497(6)	-73(10)	48(1)
C(13)	228(4)	3478(1)	939(2)	35(1)
C(14)	-82(4)	3600(2)	1375(3)	64(2)
C(15)	-1031(5)	3605(2)	1366(3)	78(2)
C(16)	-1697(4)	3483(2)	905(3)	61(2)
C(17)	-1418(4)	3356(2)	461(3)	54(2)
C(18)	-477(4)	3352(2)	478(2)	42(2)
C(19)	1673(3)	3169(2)	400(2)	35(1)
C(20)	1876(4)	2810(2)	457(3)	49(2)
C(21)	1984(5)	2601(2)	15(3)	67(2)
C(22)	1867(5)	2751(2)	-500(3)	67(2)
C(23)	1617(6)	3112(2)	-583(3)	81(2)
C(24)	1528(5)	3314(2)	-138(3)	62(2)
C(25)	3810(4)	3174(2)	3888(3)	45(2)
C(26)	3754(5)	2804(2)	4020(3)	74(2)
C(27)	4317(6)	2645(2)	4496(4)	91(3)
C(28)	4970(7)	2852(3)	4851(4)	95(3)
C(29)	5042(6)	3206(3)	4759(3)	79(2)
C(30)	4427(5)	3369(2)	4289(3)	65(2)
C(31)	1742(4)	3257(2)	3351(3)	49(2)
C(32)	1626(5)	3214(2)	3881(3)	75(2)
C(33)	751(6)	3146(3)	3958(4)	111(3)
C(34)	0(6)	3100(3)	3519(5)	117(4)
C(35)	55(5)	3143(3)	2979(5)	106(3)
C(36)	953(4)	3230(2)	2893(3)	74(2)
C(37)	1402(4)	4229(2)	2972(3)	46(2)
C(38)	859(5)	4143(2)	3342(3)	77(2)
C(39)	-120(6)	4161(2)	3149(5)	103(4)
C(40)	-581(5)	4268(2)	2613(5)	85(3)
C(41)	-67(4)	4350(2)	2240(3)	68(2)
C(42)	916(4)	4328(2)	2431(3)	57(2)
C(43)	3158(4)	4419(2)	3910(3)	58(2)
C(44)	3487(6)	4778(2)	3969(4)	107(3)
C(45)	3819(9)	4943(4)	4502(6)	187(7)

C(46)	3805(9)	4751(5)	4959(6)	193(8)
C(47)	3499(8)	4399(4)	4920(4)	139(4)
C(48)	3156(6)	4237(2)	4400(3)	88(3)
C(49)	4338(4)	5644(1)	2792(2)	36(1)
C(50)	5106(5)	5850(3)	2967(3)	113(4)
C(51)	5334(6)	6051(2)	3456(4)	109(4)
C(52)	4790(6)	6053(2)	3772(3)	81(2)
C(53)	4016(8)	5859(4)	3622(4)	188(7)
C(54)	3786(6)	5653(3)	3131(4)	131(4)
C(55)	3759(4)	5645(1)	1514(2)	32(1)
C(56)	2978(4)	5870(2)	1388(3)	48(2)
C(57)	2702(4)	6065(2)	906(3)	56(2)
C(58)	3201(5)	6046(2)	521(3)	56(2)
C(59)	3999(5)	5841(2)	642(3)	76(2)
C(60)	4259(5)	5644(2)	1123(3)	60(2)
C(61)	6074(4)	4606(2)	1725(2)	38(1)
C(62)	6896(4)	4757(2)	1682(3)	54(2)
C(63)	7364(5)	4639(2)	1310(3)	72(2)
C(64)	7000(7)	4361(2)	957(4)	86(3)
C(65)	6151(8)	4211(2)	961(4)	119(4)
C(66)	5698(6)	4333(2)	1342(3)	88(3)
C(67)	6344(4)	4741(2)	2933(3)	46(2)
C(68)	7087(5)	4509(2)	3055(3)	79(2)
C(69)	7775(6)	4480(3)	3562(4)	87(3)
C(70)	7737(6)	4738(2)	3943(3)	70(2)
C(71)	7073(6)	4986(3)	3867(4)	100(3)
C(72)	6370(5)	4996(2)	3333(3)	78(2)
C(73)	6023(4)	3083(2)	2150(3)	78(2)
C(74)	6515(6)	3400(3)	2050(4)	93(3)
C(75)	7336(7)	3537(3)	2420(5)	111(3)
C(76)	7734(7)	3360(4)	2907(7)	132(5)
C(77)	7265(8)	3037(4)	3028(5)	159(6)
C(78)	6391(5)	2892(3)	2633(4)	108(3)
C(79)	4871(5)	3111(2)	968(3)	54(2)
C(80)	5692(6)	3014(2)	782(4)	93(3)
C(81)	5722(9)	3131(3)	242(5)	125(5)
C(82)	5041(9)	3304(4)	-94(5)	149(6)
C(83)	4301(8)	3388(3)	57(4)	138(5)
C(84)	4227(6)	3310(3)	619(4)	109(3)
C(85)	4212(5)	2059(2)	2478(3)	54(2)
C(86)	4823(6)	1780(2)	2497(4)	111(3)
C(87)	5159(7)	1562(3)	2953(5)	130(4)
C(88)	4871(9)	1618(3)	3410(4)	116(4)
C(89)	4250(8)	1885(3)	3417(4)	126(4)
C(90)	3916(6)	2098(2)	2929(3)	93(3)
C(91)	3200(5)	2013(2)	1268(3)	57(2)
C(92)	3613(5)	1932(2)	846(3)	63(2)
C(93)	3210(6)	1683(2)	434(3)	76(2)
C(94)	2383(7)	1510(2)	432(3)	86(3)
C(95)	1955(6)	1585(2)	848(4)	93(3)
C(96)	2368(6)	1831(2)	1256(3)	79(2)
N(1)	4612(3)	3791(1)	2640(2)	39(1)
C(97)	5408(4)	3692(2)	3123(3)	46(2)
C(98)	5536(5)	3963(2)	3597(3)	76(2)
C(99)	6375(6)	3840(2)	4103(4)	94(3)
C(100)	6500(6)	4069(3)	4623(4)	110(3)
C(101)	7343(8)	3908(4)	5180(5)	173(6)
C(102)	8164(7)	3847(3)	5055(5)	134(4)
C(103)	8876(7)	3659(2)	5594(4)	131(4)
C(104)	9016(6)	3813(2)	6152(4)	96(3)
C(105)	9676(6)	3610(2)	6609(3)	90(3)
N(2)	9936(3)	3785(1)	7159(2)	63(2)
O(13)	8525(5)	3393(2)	7641(4)	142(3)
O(14)	7442(4)	3175(2)	6520(3)	106(2)
O(15)	8829(5)	2737(2)	6258(3)	127(3)
O(16)	10731(4)	2864(2)	6938(3)	92(2)
O(17)	10401(4)	3158(1)	7925(2)	94(2)
C(106)	7541(8)	3429(4)	7407(6)	194(7)
C(107)	7086(7)	3132(4)	6954(5)	161(5)
C(108)	7270(7)	2876(3)	6151(5)	138(4)
C(109)	7922(8)	2621(3)	6196(5)	149(5)
C(110)	9525(7)	2475(3)	6373(5)	127(4)
C(111)	10413(7)	2620(2)	6469(4)	117(4)
C(112)	11039(6)	2696(2)	7436(4)	93(3)
C(113)	11198(6)	2943(2)	7891(4)	100(3)
C(114)	9657(12)	2959(3)	8016(6)	179(8)
C(115)	8887(14)	3116(7)	8022(10)	337(17)

O(18)	11747(6)	3969(2)	6944(3)	146(3)
O(19)	11827(4)	3869(2)	8037(3)	120(2)
O(20)	10322(4)	4257(2)	8235(2)	93(2)
O(21)	8800(4)	4412(2)	7276(4)	110(2)
O(22)	10335(7)	4532(2)	6798(3)	142(3)
C(116)	12587(8)	3834(4)	7478(10)	240(11)
C(117)	12655(12)	4018(7)	7847(10)	330(20)
C(118)	11857(9)	4014(3)	8581(4)	136(4)
C(119)	10890(7)	4015(3)	8627(4)	99(3)
C(120)	9365(8)	4273(3)	8249(5)	126(4)
C(121)	8876(7)	4540(3)	7832(5)	119(4)
C(122)	8828(9)	4704(3)	6895(6)	156(6)
C(123)	9804(12)	4809(3)	6975(6)	164(5)
C(124)	11370(8)	4612(4)	6998(5)	153(6)
C(125)	11784(12)	4322(4)	6802(9)	235(9)
C(126)	2765(7)	7108(2)	1031(3)	126(3)
C(127)	1797(6)	7160(2)	812(4)	153(4)
C(128)	1461(5)	7474(3)	518(3)	171(5)
C(129)	2094(8)	7735(2)	445(4)	177(5)
C(130)	3063(7)	7683(2)	664(4)	254(8)
C(131)	3398(4)	7369(3)	957(4)	180(5)
C(132)	700(10)	7718(4)	152(6)	190(5)
C(133)	325(10)	4676(4)	5034(6)	160(5)
C(134)	-207(9)	4780(3)	5338(5)	142(4)
C(135)	666(9)	4872(4)	4630(6)	173(5)
C(136)	719(17)	4398(7)	5013(10)	150(9)

Table 3. Bond lengths [Å] and angles [°] for sh2283.

Al(1)-O(1)	1.717(4)
Al(1)-O(6)	1.726(4)
Al(1)-O(7)	1.747(4)
Al(1)-O(9)	1.785(3)
Al(2)-O(3)	1.714(4)
Al(2)-O(4)	1.727(4)
Al(2)-O(12)	1.740(4)
Al(2)-O(10)	1.778(3)
Si(1)-O(1)	1.596(4)
Si(1)-O(2)	1.626(4)
Si(1)-C(7)	1.861(5)
Si(1)-C(1)	1.864(5)
Si(2)-O(3)	1.591(4)
Si(2)-O(2)	1.635(3)
Si(2)-C(19)	1.870(6)
Si(2)-C(13)	1.871(5)
Si(3)-O(4)	1.584(4)
Si(3)-O(5)	1.630(4)
Si(3)-C(31)	1.866(5)
Si(3)-C(25)	1.867(6)
Si(4)-O(6)	1.593(4)
Si(4)-O(5)	1.641(4)
Si(4)-C(43)	1.854(7)
Si(4)-C(37)	1.867(6)
Si(5)-O(7)	1.600(3)
Si(5)-O(8)	1.650(3)
Si(5)-C(55)	1.859(6)
Si(5)-C(49)	1.866(6)
Si(6)-O(9)	1.613(3)
Si(6)-O(8)	1.635(4)
Si(6)-C(67)	1.835(6)
Si(6)-C(61)	1.858(5)
Si(7)-O(10)	1.617(4)
Si(7)-O(11)	1.633(4)
Si(7)-C(79)	1.836(7)
Si(7)-C(73)	1.861(8)
Si(8)-O(12)	1.605(4)
Si(8)-O(11)	1.654(4)
Si(8)-C(85)	1.846(7)
Si(8)-C(91)	1.862(7)
C(1)-C(2)	1.364(8)
C(1)-C(6)	1.390(8)
C(2)-C(3)	1.412(9)
C(3)-C(4)	1.303(11)
C(4)-C(5)	1.396(11)
C(5)-C(6)	1.412(10)
C(7)-C(12A)	1.387(9)
C(7)-C(8A)	1.390(9)
C(7)-C(8B)	1.40(2)
C(7)-C(12B)	1.46(2)
C(8A)-C(9A)	1.414(10)
C(9A)-C(10)	1.351(10)
C(8B)-C(9B)	1.42(3)
C(9B)-C(10)	1.36(2)
C(10)-C(11A)	1.376(9)
C(10)-C(11B)	1.42(2)
C(11A)-C(12A)	1.409(10)
C(11B)-C(12B)	1.37(3)
C(13)-C(14)	1.370(7)
C(13)-C(18)	1.401(7)
C(14)-C(15)	1.388(8)
C(15)-C(16)	1.367(9)
C(16)-C(17)	1.370(8)
C(17)-C(18)	1.371(7)
C(19)-C(20)	1.364(7)
C(19)-C(24)	1.409(8)
C(20)-C(21)	1.394(8)
C(21)-C(22)	1.368(9)
C(22)-C(23)	1.387(9)
C(23)-C(24)	1.379(8)
C(25)-C(30)	1.357(8)
C(25)-C(26)	1.415(9)
C(26)-C(27)	1.380(10)
C(27)-C(28)	1.351(11)
C(28)-C(29)	1.342(11)

C(29)-C(30)	1.404(9)
C(31)-C(36)	1.389(9)
C(31)-C(32)	1.392(9)
C(32)-C(33)	1.374(9)
C(33)-C(34)	1.335(12)
C(34)-C(35)	1.383(12)
C(35)-C(36)	1.431(10)
C(37)-C(42)	1.392(8)
C(37)-C(38)	1.416(8)
C(38)-C(39)	1.387(10)
C(39)-C(40)	1.381(11)
C(40)-C(41)	1.388(10)
C(41)-C(42)	1.393(8)
C(43)-C(48)	1.400(9)
C(43)-C(44)	1.410(9)
C(44)-C(45)	1.424(12)
C(45)-C(46)	1.353(18)
C(46)-C(47)	1.371(16)
C(47)-C(48)	1.395(12)
C(49)-C(54)	1.326(8)
C(49)-C(50)	1.334(8)
C(50)-C(51)	1.390(9)
C(51)-C(52)	1.272(9)
C(52)-C(53)	1.308(11)
C(53)-C(54)	1.407(11)
C(55)-C(60)	1.375(7)
C(55)-C(56)	1.382(7)
C(56)-C(57)	1.369(8)
C(57)-C(58)	1.365(8)
C(58)-C(59)	1.359(9)
C(59)-C(60)	1.368(8)
C(61)-C(62)	1.364(7)
C(61)-C(66)	1.398(9)
C(62)-C(63)	1.372(9)
C(63)-C(64)	1.368(10)
C(64)-C(65)	1.368(11)
C(65)-C(66)	1.380(9)
C(67)-C(68)	1.356(9)
C(67)-C(72)	1.369(9)
C(68)-C(69)	1.390(10)
C(69)-C(70)	1.363(10)
C(70)-C(71)	1.316(10)
C(71)-C(72)	1.444(10)
C(73)-C(78)	1.375(10)
C(73)-C(74)	1.436(11)
C(74)-C(75)	1.398(11)
C(75)-C(76)	1.364(14)
C(76)-C(77)	1.455(15)
C(77)-C(78)	1.486(14)
C(79)-C(84)	1.321(9)
C(79)-C(80)	1.453(9)
C(80)-C(81)	1.432(12)
C(81)-C(82)	1.287(16)
C(82)-C(83)	1.283(15)
C(83)-C(84)	1.469(12)
C(85)-C(90)	1.324(9)
C(85)-C(86)	1.362(9)
C(86)-C(87)	1.373(11)
C(87)-C(88)	1.340(12)
C(88)-C(89)	1.349(12)
C(89)-C(90)	1.423(11)
C(91)-C(92)	1.388(8)
C(91)-C(96)	1.387(9)
C(92)-C(93)	1.387(10)
C(93)-C(94)	1.373(10)
C(94)-C(95)	1.384(10)
C(95)-C(96)	1.379(10)
N(1)-C(97)	1.478(7)
C(97)-C(98)	1.525(9)
C(98)-C(99)	1.569(10)
C(99)-C(100)	1.522(11)
C(100)-C(101)	1.695(13)
C(101)-C(102)	1.347(12)
C(102)-C(103)	1.619(12)
C(103)-C(104)	1.469(11)
C(104)-C(105)	1.483(10)
C(105)-N(2)	1.471(8)

O(13)-C(115)	1.401(18)
O(13)-C(106)	1.408(12)
O(14)-C(107)	1.339(11)
O(14)-C(108)	1.418(10)
O(15)-C(109)	1.367(11)
O(15)-C(110)	1.381(10)
O(16)-C(112)	1.354(9)
O(16)-C(111)	1.451(9)
O(17)-C(114)	1.389(12)
O(17)-C(113)	1.438(8)
C(106)-C(107)	1.590(14)
C(108)-C(109)	1.329(12)
C(110)-C(111)	1.371(11)
C(112)-C(113)	1.428(11)
C(114)-C(115)	1.28(2)
O(18)-C(125)	1.359(15)
O(18)-C(116)	1.627(16)
O(19)-C(118)	1.454(11)
O(19)-C(117)	1.53(2)
O(20)-C(119)	1.417(9)
O(20)-C(120)	1.418(10)
O(21)-C(121)	1.444(11)
O(21)-C(122)	1.451(14)
O(22)-C(123)	1.431(13)
O(22)-C(124)	1.493(12)
C(116)-C(117)	1.13(2)
C(118)-C(119)	1.456(12)
C(120)-C(121)	1.474(13)
C(122)-C(123)	1.445(14)
C(124)-C(125)	1.391(16)
C(126)-C(127)	1.3900
C(126)-C(131)	1.3900
C(127)-C(128)	1.3900
C(128)-C(129)	1.3900
C(128)-C(132)	1.531(15)
C(129)-C(130)	1.3900
C(129)-C(132)	1.977(17)
C(130)-C(131)	1.3900
C(133)-C(136)	1.19(2)
C(133)-C(134)	1.291(14)
C(133)-C(135)	1.442(15)
C(134)-C(135)#1	1.467(15)
C(135)-C(134)#1	1.467(15)
C(135)-C(136)	1.99(3)

O(1)-Al(1)-O(6)	108.15(18)
O(1)-Al(1)-O(7)	113.03(18)
O(6)-Al(1)-O(7)	112.83(18)
O(1)-Al(1)-O(9)	111.68(17)
O(6)-Al(1)-O(9)	105.90(18)
O(7)-Al(1)-O(9)	105.04(16)
O(3)-Al(2)-O(4)	110.41(18)
O(3)-Al(2)-O(12)	111.33(19)
O(4)-Al(2)-O(12)	111.32(19)
O(3)-Al(2)-O(10)	110.60(18)
O(4)-Al(2)-O(10)	107.56(18)
O(12)-Al(2)-O(10)	105.45(17)
O(1)-Si(1)-O(2)	112.99(19)
O(1)-Si(1)-C(7)	110.2(2)
O(2)-Si(1)-C(7)	106.5(2)
O(1)-Si(1)-C(1)	110.3(2)
O(2)-Si(1)-C(1)	106.6(2)
C(7)-Si(1)-C(1)	110.0(2)
O(3)-Si(2)-O(2)	111.88(19)
O(3)-Si(2)-C(19)	111.8(2)
O(2)-Si(2)-C(19)	105.6(2)
O(3)-Si(2)-C(13)	107.8(2)
O(2)-Si(2)-C(13)	111.1(2)
C(19)-Si(2)-C(13)	108.6(2)
O(4)-Si(3)-O(5)	109.4(2)
O(4)-Si(3)-C(31)	113.4(3)
O(5)-Si(3)-C(31)	109.6(2)
O(4)-Si(3)-C(25)	111.6(2)
O(5)-Si(3)-C(25)	106.5(2)
C(31)-Si(3)-C(25)	106.0(3)
O(6)-Si(4)-O(5)	108.8(2)
O(6)-Si(4)-C(43)	110.8(3)

O(5)-Si(4)-C(43)	105.7(3)
O(6)-Si(4)-C(37)	110.9(3)
O(5)-Si(4)-C(37)	110.3(2)
C(43)-Si(4)-C(37)	110.2(3)
O(7)-Si(5)-O(8)	110.68(18)
O(7)-Si(5)-C(55)	112.4(2)
O(8)-Si(5)-C(55)	105.4(2)
O(7)-Si(5)-C(49)	109.7(2)
O(8)-Si(5)-C(49)	107.3(2)
C(55)-Si(5)-C(49)	111.1(2)
O(9)-Si(6)-O(8)	109.46(17)
O(9)-Si(6)-C(67)	112.7(2)
O(8)-Si(6)-C(67)	106.3(2)
O(9)-Si(6)-C(61)	110.2(2)
O(8)-Si(6)-C(61)	110.7(2)
C(67)-Si(6)-C(61)	107.5(3)
O(10)-Si(7)-O(11)	109.58(19)
O(10)-Si(7)-C(79)	111.9(3)
O(11)-Si(7)-C(79)	110.5(3)
O(10)-Si(7)-C(73)	107.1(3)
O(11)-Si(7)-C(73)	110.6(3)
C(79)-Si(7)-C(73)	107.1(3)
O(12)-Si(8)-O(11)	110.8(2)
O(12)-Si(8)-C(85)	109.5(3)
O(11)-Si(8)-C(85)	109.1(3)
O(12)-Si(8)-C(91)	112.0(3)
O(11)-Si(8)-C(91)	108.1(3)
C(85)-Si(8)-C(91)	107.2(3)
Si(1)-O(1)-Al(1)	161.2(2)
Si(1)-O(2)-Si(2)	155.8(2)
Si(2)-O(3)-Al(2)	151.9(2)
Si(3)-O(4)-Al(2)	166.6(3)
Si(3)-O(5)-Si(4)	153.2(2)
Si(4)-O(6)-Al(1)	164.7(3)
Si(5)-O(7)-Al(1)	131.0(2)
Si(6)-O(8)-Si(5)	131.7(2)
Si(6)-O(9)-Al(1)	130.8(2)
Si(7)-O(10)-Al(2)	130.8(2)
Si(7)-O(11)-Si(8)	132.0(2)
Si(8)-O(12)-Al(2)	130.4(2)
C(2)-C(1)-C(6)	116.0(6)
C(2)-C(1)-Si(1)	122.3(5)
C(6)-C(1)-Si(1)	121.7(5)
C(1)-C(2)-C(3)	123.3(7)
C(4)-C(3)-C(2)	120.3(8)
C(3)-C(4)-C(5)	119.6(7)
C(4)-C(5)-C(6)	120.2(8)
C(1)-C(6)-C(5)	120.5(7)
C(12A)-C(7)-C(8A)	117.7(6)
C(12A)-C(7)-C(8B)	83.4(10)
C(8A)-C(7)-C(8B)	59.7(10)
C(12A)-C(7)-C(12B)	63.8(9)
C(8A)-C(7)-C(12B)	86.1(10)
C(8B)-C(7)-C(12B)	113.8(13)
C(12A)-C(7)-Si(1)	122.8(5)
C(8A)-C(7)-Si(1)	119.4(5)
C(8B)-C(7)-Si(1)	124.4(10)
C(12B)-C(7)-Si(1)	121.7(9)
C(7)-C(8A)-C(9A)	120.5(7)
C(10)-C(9A)-C(8A)	120.8(8)
C(7)-C(8B)-C(9B)	126(2)
C(10)-C(9B)-C(8B)	114.1(19)
C(9A)-C(10)-C(9B)	63.4(10)
C(9A)-C(10)-C(11A)	119.8(7)
C(9B)-C(10)-C(11A)	88.6(11)
C(9A)-C(10)-C(11B)	88.8(10)
C(9B)-C(10)-C(11B)	125.8(14)
C(11A)-C(10)-C(11B)	65.2(10)
C(10)-C(11A)-C(12A)	120.2(7)
C(7)-C(12A)-C(11A)	120.9(7)
C(12B)-C(11B)-C(10)	117(2)
C(11B)-C(12B)-C(7)	122.9(19)
C(14)-C(13)-C(18)	115.6(5)
C(14)-C(13)-Si(2)	121.3(4)
C(18)-C(13)-Si(2)	122.9(4)
C(13)-C(14)-C(15)	123.1(6)
C(16)-C(15)-C(14)	119.3(6)

C(15)-C(16)-C(17)	119.6(6)
C(16)-C(17)-C(18)	120.2(6)
C(17)-C(18)-C(13)	122.2(5)
C(20)-C(19)-C(24)	116.3(5)
C(20)-C(19)-Si(2)	122.3(4)
C(24)-C(19)-Si(2)	121.3(4)
C(19)-C(20)-C(21)	121.9(6)
C(22)-C(21)-C(20)	120.6(6)
C(21)-C(22)-C(23)	119.5(6)
C(24)-C(23)-C(22)	118.9(7)
C(23)-C(24)-C(19)	122.7(6)
C(30)-C(25)-C(26)	114.4(6)
C(30)-C(25)-Si(3)	126.0(5)
C(26)-C(25)-Si(3)	118.8(5)
C(27)-C(26)-C(25)	123.6(8)
C(28)-C(27)-C(26)	118.2(9)
C(29)-C(28)-C(27)	121.2(8)
C(28)-C(29)-C(30)	120.0(8)
C(25)-C(30)-C(29)	122.2(7)
C(36)-C(31)-C(32)	118.8(6)
C(36)-C(31)-Si(3)	120.9(5)
C(32)-C(31)-Si(3)	120.3(5)
C(33)-C(32)-C(31)	121.3(8)
C(34)-C(33)-C(32)	120.1(9)
C(33)-C(34)-C(35)	121.9(8)
C(34)-C(35)-C(36)	118.5(8)
C(31)-C(36)-C(35)	119.1(8)
C(42)-C(37)-C(38)	117.6(6)
C(42)-C(37)-Si(4)	121.7(4)
C(38)-C(37)-Si(4)	120.7(5)
C(39)-C(38)-C(37)	118.7(8)
C(40)-C(39)-C(38)	122.3(7)
C(39)-C(40)-C(41)	120.2(7)
C(40)-C(41)-C(42)	117.5(8)
C(37)-C(42)-C(41)	123.6(6)
C(48)-C(43)-C(44)	116.6(7)
C(48)-C(43)-Si(4)	123.2(6)
C(44)-C(43)-Si(4)	120.2(6)
C(43)-C(44)-C(45)	121.4(9)
C(46)-C(45)-C(44)	118.9(11)
C(45)-C(46)-C(47)	121.5(11)
C(46)-C(47)-C(48)	120.1(11)
C(47)-C(48)-C(43)	121.3(9)
C(54)-C(49)-C(50)	112.8(6)
C(54)-C(49)-Si(5)	124.0(5)
C(50)-C(49)-Si(5)	123.1(4)
C(49)-C(50)-C(51)	124.9(6)
C(52)-C(51)-C(50)	120.6(7)
C(51)-C(52)-C(53)	117.8(8)
C(52)-C(53)-C(54)	121.9(8)
C(49)-C(54)-C(53)	122.0(7)
C(60)-C(55)-C(56)	114.4(5)
C(60)-C(55)-Si(5)	122.6(4)
C(56)-C(55)-Si(5)	123.0(4)
C(57)-C(56)-C(55)	123.0(6)
C(58)-C(57)-C(56)	120.5(6)
C(59)-C(58)-C(57)	118.1(6)
C(58)-C(59)-C(60)	120.5(6)
C(59)-C(60)-C(55)	123.4(6)
C(62)-C(61)-C(66)	115.8(5)
C(62)-C(61)-Si(6)	123.3(5)
C(66)-C(61)-Si(6)	120.9(4)
C(61)-C(62)-C(63)	122.9(7)
C(64)-C(63)-C(62)	119.9(7)
C(63)-C(64)-C(65)	119.7(7)
C(64)-C(65)-C(66)	119.2(8)
C(65)-C(66)-C(61)	122.3(7)
C(68)-C(67)-C(72)	114.5(7)
C(68)-C(67)-Si(6)	122.3(5)
C(72)-C(67)-Si(6)	122.7(5)
C(67)-C(68)-C(69)	126.3(8)
C(70)-C(69)-C(68)	115.0(8)
C(71)-C(70)-C(69)	124.2(8)
C(70)-C(71)-C(72)	117.6(8)
C(67)-C(72)-C(71)	121.7(8)
C(78)-C(73)-C(74)	118.7(8)
C(78)-C(73)-Si(7)	122.0(7)

C(74)-C(73)-Si(7)	118.9(6)
C(75)-C(74)-C(73)	124.4(9)
C(76)-C(75)-C(74)	119.7(11)
C(75)-C(76)-C(77)	118.1(12)
C(76)-C(77)-C(78)	122.1(11)
C(73)-C(78)-C(77)	117.0(10)
C(84)-C(79)-C(80)	115.7(7)
C(84)-C(79)-Si(7)	125.2(6)
C(80)-C(79)-Si(7)	118.9(6)
C(81)-C(80)-C(79)	118.2(9)
C(82)-C(81)-C(80)	123.1(11)
C(83)-C(82)-C(81)	119.9(12)
C(82)-C(83)-C(84)	121.8(10)
C(79)-C(84)-C(83)	120.8(8)
C(90)-C(85)-C(86)	115.0(7)
C(90)-C(85)-Si(8)	121.9(5)
C(86)-C(85)-Si(8)	122.8(6)
C(85)-C(86)-C(87)	123.9(9)
C(88)-C(87)-C(86)	119.4(9)
C(87)-C(88)-C(89)	119.9(9)
C(88)-C(89)-C(90)	118.1(9)
C(85)-C(90)-C(89)	123.6(8)
C(92)-C(91)-C(96)	116.5(7)
C(92)-C(91)-Si(8)	123.5(6)
C(96)-C(91)-Si(8)	119.9(5)
C(93)-C(92)-C(91)	121.5(7)
C(94)-C(93)-C(92)	120.6(7)
C(93)-C(94)-C(95)	119.2(8)
C(96)-C(95)-C(94)	119.4(8)
C(95)-C(96)-C(91)	122.8(7)
N(1)-C(97)-C(98)	111.9(5)
C(97)-C(98)-C(99)	109.6(6)
C(100)-C(99)-C(98)	114.1(7)
C(99)-C(100)-C(101)	113.1(8)
C(102)-C(101)-C(100)	111.5(9)
C(101)-C(102)-C(103)	107.0(10)
C(104)-C(103)-C(102)	120.8(8)
C(103)-C(104)-C(105)	115.1(7)
N(2)-C(105)-C(104)	116.2(6)
C(115)-O(13)-C(106)	120.5(12)
C(107)-O(14)-C(108)	113.1(9)
C(109)-O(15)-C(110)	116.5(8)
C(112)-O(16)-C(111)	114.1(7)
C(114)-O(17)-C(113)	114.0(7)
O(13)-C(106)-C(107)	114.3(8)
O(14)-C(107)-C(106)	108.2(9)
C(109)-C(108)-O(14)	120.4(9)
C(108)-C(109)-O(15)	116.4(10)
C(111)-C(110)-O(15)	111.9(9)
C(110)-C(111)-O(16)	117.8(8)
O(16)-C(112)-C(113)	112.1(8)
C(112)-C(113)-O(17)	116.4(8)
C(115)-C(114)-O(17)	120.1(13)
C(114)-C(115)-O(13)	119.8(15)
C(125)-O(18)-C(116)	115.7(11)
C(118)-O(19)-C(117)	109.6(9)
C(119)-O(20)-C(120)	114.1(8)
C(121)-O(21)-C(122)	112.0(8)
C(123)-O(22)-C(124)	110.3(9)
C(117)-C(116)-O(18)	111.1(17)
C(116)-C(117)-O(19)	97.8(18)
O(19)-C(118)-C(119)	107.3(9)
O(20)-C(119)-C(118)	110.4(8)
O(20)-C(120)-C(121)	107.7(8)
O(21)-C(121)-C(120)	110.7(9)
C(123)-C(122)-O(21)	108.5(10)
O(22)-C(123)-C(122)	111.8(10)
C(125)-C(124)-O(22)	103.5(10)
O(18)-C(125)-C(124)	126.8(16)
C(127)-C(126)-C(131)	120.0
C(126)-C(127)-C(128)	120.0
C(127)-C(128)-C(129)	120.0
C(127)-C(128)-C(132)	154.7(9)
C(129)-C(128)-C(132)	85.1(9)
C(130)-C(129)-C(128)	120.0
C(130)-C(129)-C(132)	170.0(7)
C(128)-C(129)-C(132)	50.5(7)

C(129)-C(130)-C(131)	120.0
C(130)-C(131)-C(126)	120.0
C(128)-C(132)-C(129)	44.5(4)
C(136)-C(133)-C(134)	132(2)
C(136)-C(133)-C(135)	97.9(19)
C(134)-C(133)-C(135)	130.3(15)
C(133)-C(134)-C(135)#1	131.0(13)
C(133)-C(135)-C(134)#1	98.7(11)
C(133)-C(135)-C(136)	36.3(9)
C(134)#1-C(135)-C(136)	135.0(13)
C(133)-C(136)-C(135)	45.8(13)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2283. 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}
Al(1)	28(1)	28(1)	33(1)	3(1)	10(1)	-5(1)
Al(2)	27(1)	30(1)	30(1)	4(1)	8(1)	2(1)
Si(1)	28(1)	27(1)	39(1)	2(1)	8(1)	-2(1)
Si(2)	33(1)	28(1)	33(1)	3(1)	5(1)	-4(1)
Si(3)	37(1)	36(1)	36(1)	2(1)	18(1)	-3(1)
Si(4)	49(1)	35(1)	43(1)	1(1)	26(1)	-7(1)
Si(5)	36(1)	27(1)	37(1)	-3(1)	15(1)	-6(1)
Si(6)	31(1)	33(1)	31(1)	-2(1)	11(1)	-5(1)
Si(7)	40(1)	52(1)	51(1)	7(1)	24(1)	9(1)
Si(8)	67(1)	33(1)	59(1)	14(1)	32(1)	15(1)
O(1)	32(2)	37(2)	40(2)	-6(2)	9(2)	-7(2)
O(2)	37(2)	26(2)	37(2)	4(2)	9(2)	-3(2)
O(3)	34(2)	41(2)	34(2)	11(2)	4(2)	4(2)
O(4)	45(2)	59(3)	30(2)	-3(2)	10(2)	-1(2)
O(5)	45(2)	34(2)	48(3)	7(2)	15(2)	-3(2)
O(6)	37(2)	52(3)	40(2)	10(2)	16(2)	-7(2)
O(7)	35(2)	26(2)	39(2)	1(2)	16(2)	-3(2)
O(8)	29(2)	31(2)	39(2)	0(2)	11(2)	-4(2)
O(9)	31(2)	29(2)	34(2)	5(2)	11(2)	-2(2)
O(10)	29(2)	42(2)	47(3)	-5(2)	14(2)	-3(2)
O(11)	80(3)	42(3)	90(4)	22(2)	60(3)	25(2)
O(12)	51(2)	28(2)	45(2)	10(2)	24(2)	5(2)
C(1)	29(3)	38(4)	48(4)	15(3)	11(3)	3(3)
C(2)	47(4)	56(5)	93(6)	-2(4)	11(4)	12(3)
C(3)	54(5)	84(6)	138(9)	14(6)	26(6)	37(5)
C(4)	40(5)	109(8)	98(7)	52(6)	28(5)	34(5)
C(5)	36(4)	147(9)	76(6)	41(6)	-11(4)	-12(5)
C(6)	47(4)	74(5)	67(5)	12(4)	0(4)	5(4)
C(7)	28(3)	27(3)	41(4)	3(3)	5(3)	3(2)
C(10)	46(4)	55(5)	68(5)	19(4)	23(4)	-10(3)
C(13)	37(3)	35(3)	30(3)	5(3)	5(3)	0(3)
C(14)	38(4)	100(6)	52(5)	-24(4)	7(3)	-20(4)
C(15)	47(4)	120(7)	76(6)	-36(5)	31(4)	-18(4)
C(16)	32(4)	69(5)	82(6)	-1(4)	17(4)	-4(3)
C(17)	37(4)	62(5)	54(5)	0(4)	-1(3)	-2(3)
C(18)	37(3)	45(4)	42(4)	-1(3)	7(3)	0(3)
C(19)	38(3)	29(4)	35(4)	1(3)	7(3)	-6(3)
C(20)	59(4)	39(4)	38(4)	-2(3)	-3(3)	12(3)
C(21)	80(5)	46(5)	58(5)	-9(4)	-9(4)	23(4)
C(22)	94(5)	61(5)	48(5)	-3(4)	26(4)	22(4)
C(23)	152(8)	45(5)	57(5)	2(4)	49(5)	-1(5)
C(24)	108(6)	33(4)	51(5)	-5(3)	34(4)	-8(4)
C(25)	56(4)	35(4)	44(4)	4(3)	16(3)	4(3)
C(26)	86(5)	60(6)	74(6)	2(4)	20(5)	17(4)
C(27)	100(7)	82(7)	88(7)	28(6)	22(6)	19(6)
C(28)	93(7)	123(9)	58(6)	26(6)	5(5)	33(6)
C(29)	92(6)	92(7)	46(5)	10(5)	6(4)	-8(5)
C(30)	81(5)	71(5)	39(4)	6(4)	13(4)	2(4)
C(31)	38(3)	39(4)	73(5)	5(3)	23(4)	-3(3)
C(32)	62(4)	92(6)	89(6)	37(5)	49(4)	6(4)
C(33)	84(6)	153(9)	116(8)	51(7)	62(6)	8(6)
C(34)	57(6)	180(11)	119(9)	11(8)	31(6)	-40(6)
C(35)	51(5)	135(9)	129(9)	-51(7)	21(5)	-2(5)
C(36)	39(4)	84(6)	99(6)	-29(5)	21(4)	-10(4)
C(37)	49(4)	32(4)	68(5)	3(3)	32(4)	-4(3)
C(38)	67(5)	62(5)	124(7)	39(5)	62(5)	12(4)
C(39)	83(6)	61(6)	202(12)	38(7)	101(7)	6(5)
C(40)	50(5)	51(5)	165(10)	1(6)	48(6)	-15(4)
C(41)	41(4)	55(5)	110(7)	-16(4)	23(4)	-8(3)
C(42)	43(4)	59(5)	78(6)	-18(4)	30(4)	-17(3)
C(43)	66(4)	60(5)	58(5)	-18(4)	36(4)	-14(4)
C(44)	106(7)	111(8)	133(9)	-60(6)	80(6)	-51(6)
C(45)	228(13)	223(14)	163(12)	-143(11)	144(11)	-162(11)
C(46)	170(11)	300(20)	146(13)	-147(14)	112(10)	-150(13)
C(47)	145(10)	234(15)	55(7)	-22(8)	57(7)	-22(9)
C(48)	121(7)	105(7)	49(5)	-14(5)	44(5)	-14(5)
C(49)	47(3)	29(3)	35(4)	-2(3)	18(3)	-6(3)
C(50)	82(6)	183(10)	97(7)	-92(7)	63(5)	-78(6)
C(51)	106(7)	147(9)	94(7)	-81(6)	62(6)	-79(6)
C(52)	103(6)	80(6)	59(5)	-34(4)	23(5)	-28(5)
C(53)	171(11)	312(17)	120(9)	-145(11)	105(9)	-129(12)

C(54)	114(7)	209(11)	88(7)	-98(7)	60(6)	-92(7)
C(55)	39(3)	22(3)	36(3)	-9(3)	12(3)	-8(2)
C(56)	65(4)	34(4)	52(4)	8(3)	27(4)	6(3)
C(57)	53(4)	40(4)	70(5)	7(4)	8(4)	4(3)
C(58)	69(5)	47(4)	47(4)	8(3)	12(4)	-10(4)
C(59)	82(5)	99(6)	57(5)	20(5)	36(4)	22(5)
C(60)	70(4)	73(5)	39(4)	21(4)	18(4)	25(4)
C(61)	53(4)	28(3)	40(4)	0(3)	24(3)	-3(3)
C(62)	47(4)	71(5)	48(4)	-4(4)	22(3)	-4(3)
C(63)	45(4)	119(7)	60(5)	18(5)	28(4)	6(4)
C(64)	119(7)	90(7)	75(6)	18(5)	72(6)	40(6)
C(65)	228(11)	63(6)	119(8)	-32(5)	135(9)	-36(7)
C(66)	136(7)	73(6)	87(6)	-23(5)	84(6)	-37(5)
C(67)	52(4)	32(4)	48(4)	-12(3)	5(3)	9(3)
C(68)	46(4)	139(8)	46(5)	32(5)	3(4)	1(5)
C(69)	80(6)	102(7)	86(7)	17(6)	36(5)	3(5)
C(70)	77(6)	76(6)	56(5)	2(5)	16(4)	-10(5)
C(71)	89(6)	136(9)	68(7)	-37(6)	10(5)	-10(6)
C(72)	67(5)	96(7)	65(6)	-5(5)	6(4)	2(4)
C(73)	39(4)	137(8)	65(5)	34(5)	26(4)	13(4)
C(74)	67(5)	141(9)	78(6)	-19(6)	31(5)	-28(5)
C(75)	79(7)	138(10)	130(10)	-29(8)	51(7)	-8(7)
C(76)	64(7)	136(12)	186(15)	-21(10)	16(8)	10(7)
C(77)	88(8)	259(18)	122(10)	6(11)	15(8)	96(10)
C(78)	48(5)	189(10)	80(7)	20(7)	6(5)	56(6)
C(79)	66(4)	44(4)	58(5)	-6(3)	29(4)	-20(3)
C(80)	119(7)	80(6)	108(7)	-33(5)	77(6)	-19(5)
C(81)	160(10)	151(10)	106(9)	-94(8)	109(8)	-116(9)
C(82)	121(10)	251(17)	61(8)	-18(9)	3(7)	-110(11)
C(83)	95(8)	202(12)	106(9)	74(8)	11(7)	-19(8)
C(84)	68(5)	148(9)	117(8)	76(7)	36(5)	14(5)
C(85)	77(5)	34(4)	56(5)	8(3)	27(4)	13(3)
C(86)	118(7)	108(8)	128(8)	64(7)	70(6)	65(6)
C(87)	120(8)	122(9)	135(10)	71(8)	16(8)	64(7)
C(88)	187(11)	60(7)	75(7)	29(6)	-5(7)	13(7)
C(89)	235(12)	74(7)	51(6)	7(5)	8(7)	50(8)
C(90)	149(8)	61(6)	58(6)	2(4)	12(6)	33(5)
C(91)	91(5)	34(4)	54(5)	17(3)	33(4)	23(4)
C(92)	93(5)	49(5)	56(5)	23(4)	36(4)	27(4)
C(93)	121(7)	62(6)	53(5)	10(4)	35(5)	25(5)
C(94)	149(8)	55(5)	61(6)	-12(4)	39(6)	2(5)
C(95)	138(7)	72(6)	82(6)	-29(5)	53(6)	-36(5)
C(96)	114(6)	73(6)	66(6)	-9(5)	52(5)	-2(5)
N(1)	35(3)	30(3)	56(3)	6(2)	20(3)	-2(2)
C(97)	40(3)	41(4)	60(5)	11(3)	20(3)	7(3)
C(98)	72(5)	77(6)	81(6)	25(5)	23(5)	-3(4)
C(99)	92(6)	109(7)	77(7)	11(6)	16(5)	-7(5)
C(100)	111(7)	123(8)	76(7)	9(6)	-5(6)	-15(6)
C(101)	131(10)	296(18)	105(10)	-27(10)	54(8)	3(10)
C(102)	120(8)	154(11)	133(10)	20(8)	43(8)	-1(7)
C(103)	133(8)	90(7)	108(8)	-16(6)	-69(7)	36(6)
C(104)	100(6)	68(6)	101(7)	-7(5)	-5(6)	-8(5)
C(105)	103(6)	81(6)	72(6)	-3(5)	3(5)	41(5)
N(2)	54(3)	56(4)	76(4)	-3(3)	14(3)	-1(3)
O(13)	96(5)	191(8)	161(7)	-85(6)	71(5)	-39(5)
O(14)	78(4)	96(5)	140(6)	-18(4)	24(4)	-8(3)
O(15)	85(4)	100(5)	195(7)	-80(5)	37(5)	-8(4)
O(16)	108(4)	69(4)	112(5)	0(4)	52(4)	16(3)
O(17)	144(5)	70(4)	79(4)	1(3)	50(4)	12(4)
C(106)	92(8)	293(18)	220(14)	-155(13)	79(9)	-22(9)
C(107)	77(7)	259(16)	168(12)	-60(11)	68(8)	-39(8)
C(108)	89(7)	154(11)	154(11)	-82(9)	4(7)	-36(7)
C(109)	111(9)	101(9)	217(14)	-79(9)	18(9)	-1(7)
C(110)	112(8)	83(7)	208(12)	-64(7)	83(8)	3(7)
C(111)	128(8)	79(7)	150(10)	-65(7)	49(7)	2(6)
C(112)	119(7)	84(7)	100(7)	28(6)	71(6)	34(5)
C(113)	142(8)	85(7)	87(7)	7(5)	57(6)	60(6)
C(114)	303(18)	67(7)	277(17)	14(8)	262(17)	10(9)
C(115)	230(20)	420(40)	410(30)	240(30)	190(20)	-30(20)
O(18)	150(7)	136(7)	182(8)	-30(6)	99(6)	-44(6)
O(19)	89(5)	104(5)	142(7)	10(5)	-7(4)	4(4)
O(20)	118(5)	80(4)	92(5)	-11(3)	46(4)	-11(3)
O(21)	72(4)	89(5)	168(7)	-31(5)	31(4)	15(3)
O(22)	249(10)	67(5)	121(6)	-14(4)	72(6)	-38(5)
C(116)	42(7)	177(15)	490(30)	136(19)	57(13)	45(8)
C(117)	89(11)	520(40)	390(30)	-340(30)	53(14)	-59(16)
C(118)	169(12)	124(10)	74(8)	1(7)	-32(8)	-14(8)

C(119)	114(7)	93(7)	74(7)	29(5)	1(6)	-32(6)
C(120)	124(9)	116(9)	174(12)	-30(8)	104(9)	-10(7)
C(121)	91(7)	127(10)	153(11)	-49(9)	58(7)	19(6)
C(122)	149(11)	81(9)	190(14)	-51(9)	-32(10)	50(8)
C(123)	245(17)	68(8)	158(12)	-18(8)	23(12)	-18(10)
C(124)	146(10)	174(14)	168(11)	-70(10)	89(9)	-123(10)
C(125)	225(17)	119(13)	380(30)	-71(16)	118(18)	-116(12)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sh2283.

	x	y	z	U(eq)
H(2)	1097	4885	1319	81
H(3)	-416	5139	1052	111
H(4)	-1531	4921	313	97
H(5)	-1201	4410	-156	110
H(6)	312	4143	118	79
H(8)	2980	4947	809	57
H(9)	3826	5154	195	57
H(8B)	4078	4470	1079	57
H(9B)	4991	4686	500	57
H(10)	4200(40)	4766(16)	-410(20)	66
H(11)	3748	4165	-458	57
H(12)	2896	3951	147	57
H(11B)	2577	4660	-808	57
H(12B)	1708	4453	-222	57
H(14)	373	3684	1699	77
H(15)	-1215	3692	1678	94
H(16)	-2349	3486	892	73
H(17)	-1878	3269	140	64
H(18)	-298	3262	166	50
H(20)	1947	2698	808	59
H(21)	2140	2352	71	81
H(22)	1956	2609	-797	80
H(23)	1509	3217	-941	97
H(24)	1363	3562	-196	74
H(26)	3305	2658	3766	89
H(27)	4246	2397	4572	109
H(28)	5386	2745	5171	114
H(29)	5508	3347	5011	95
H(30)	4443	3623	4250	77
H(32)	2162	3232	4196	90
H(33)	681	3133	4324	133
H(34)	-589	3035	3579	141
H(35)	-492	3116	2673	127
H(36)	1009	3268	2528	89
H(38)	1159	4075	3715	92
H(39)	-487	4097	3393	123
H(40)	-1252	4286	2500	102
H(41)	-374	4418	1867	82
H(42)	1274	4383	2178	69
H(44A)	2966	4931	3746	129
H(44B)	4008	4794	3790	129
H(45)	4047	5184	4536	224
H(46)	4012	4861	5315	231
H(47)	3520	4267	5248	167
H(48)	2917	3998	4378	105
H(50)	5528	5862	2740	136
H(51)	5903	6188	3555	131
H(52)	4940	6189	4107	97
H(53)	3597	5859	3851	226
H(54)	3218	5516	3039	157
H(56)	2617	5889	1648	58
H(57)	2158	6216	839	68
H(58)	2998	6172	178	67
H(59)	4378	5833	390	91
H(60)	4814	5500	1192	72
H(62)	7157	4953	1920	65
H(63)	7940	4751	1298	87
H(64)	7334	4272	709	103
H(65)	5876	4026	705	143
H(66)	5110	4227	1344	106
H(68)	7142	4351	2766	95
H(69)	8237	4293	3637	104
H(70)	8221	4739	4286	84
H(71)	7056	5153	4152	120
H(72)	5914	5184	3257	94
H(74)	6267	3524	1708	111
H(75)	7614	3753	2334	134
H(76)	8301	3445	3160	159
H(77A)	7113	3081	3384	191
H(77B)	7740	2841	3097	191
H(78)	6101	2677	2711	130

H(80)	6195	2877	1013	112
H(81)	6270	3077	125	150
H(82)	5085	3370	-453	178
H(83)	3788	3504	-202	165
H(84)	3708	3404	733	131
H(86)	5029	1733	2175	133
H(87)	5591	1373	2944	156
H(88)	5105	1470	3729	139
H(89)	4042	1929	3738	152
H(90)	3456	2278	2926	111
H(92)	4184	2049	840	76
H(93)	3509	1632	151	91
H(94)	2107	1341	148	104
H(95)	1383	1468	852	112
H(96)	2071	1879	1541	95
H(1A)	4073	3813	2749	58
H(1B)	4531	3616	2375	58
H(1C)	4741	4004	2496	58
H(97A)	5998	3680	3007	55
H(97B)	5290	3450	3258	55
H(98A)	4946	3979	3713	92
H(98B)	5673	4205	3470	92
H(99A)	6267	3587	4194	113
H(99B)	6969	3847	3990	113
H(10A)	5889	4081	4717	132
H(10B)	6672	4318	4543	132
H(10C)	7451	4084	5488	207
H(10D)	7118	3680	5306	207
H(10E)	8435	4077	4968	161
H(10F)	8058	3686	4727	161
H(10G)	8657	3407	5608	157
H(10H)	9506	3646	5525	157
H(10I)	8393	3827	6232	115
H(10J)	9256	4062	6151	115
H(10K)	9387	3373	6645	108
H(10L)	10264	3563	6501	108
H(2A)	10471	3918	7198	94
H(2B)	10043	3613	7429	94
H(2C)	9456	3931	7189	94
H(10M)	7411	3670	7233	233
H(10N)	7227	3417	7709	233
H(10O)	7237	2887	7113	194
H(10P)	6388	3159	6832	194
H(10Q)	6687	2756	6186	166
H(10R)	7126	2973	5768	166
H(10S)	7734	2468	5859	178
H(10T)	7919	2467	6518	178
H(11A)	9486	2336	6704	152
H(11B)	9413	2306	6055	152
H(11C)	10441	2752	6130	140
H(11D)	10871	2419	6522	140
H(11E)	11636	2567	7453	112
H(11F)	10564	2515	7471	112
H(11G)	11716	3108	7870	120
H(11H)	11421	2804	8241	120
H(11I)	9494	2770	7726	215
H(11J)	9899	2834	8377	215
H(11K)	8978	3217	8400	404
H(11L)	8393	2928	7970	404
H(11M)	12448	3585	7579	288
H(11N)	13194	3829	7379	288
H(11O)	12563	4275	7736	402
H(11P)	13268	3988	8134	402
H(11Q)	12114	4263	8619	163
H(11R)	12266	3863	8878	163
H(11S)	10623	3769	8560	119
H(11T)	10891	4089	9008	119
H(12A)	9332	4346	8624	151
H(12B)	9062	4034	8162	151
H(12C)	8235	4586	7873	142
H(12D)	9231	4770	7894	142
H(12E)	8548	4625	6507	187
H(12F)	8457	4912	6969	187
H(12G)	9826	5032	6762	196
H(12H)	10096	4861	7374	196
H(12I)	11522	4842	6842	184
H(12J)	11584	4625	7409	184

H(12K)	11535	4330	6392	282
H(12L)	12466	4381	6887	282

sh 2125

Table 1. Crystal data and structure refinement for sh2125.

Identification code	sh2125	
Empirical formula	C164 H158 Al6 O28 Si12	
Formula weight	3075.86	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.613(3) Å	α= 61.86(3)°.
	b = 18.079(4) Å	β= 78.94(3)°.
	c = 18.574(4) Å	γ = 73.01(3)°.
Volume	4129.7(15) $Å^3$	
Z	1	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.193 mm^{-1}	
F(000)	1612	
Crystal size	0.3 x 0.22 x 0.2 mm^3	
Theta range for data collection	1.72 to 24.03°.	
Index ranges	-15<=h<=15, -20<=k<=20, -20<=l<=20	
Reflections collected	32320	
Independent reflections	12013 [R(int) = 0.1128]	
Completeness to theta = 24.03°	92.2 %	
Absorption correction	N/A	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12013 / 0 / 912	
Goodness-of-fit on F^2	1.479	
Final R indices [I>2sigma(I)]	R1 = 0.0749, wR2 = 0.1899	
R indices (all data)	R1 = 0.0966, wR2 = 0.2008	
Largest diff. peak and hole	0.759 and -0.473 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sh2125. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	5190(1)	4660(1)	856(1)	26(1)
Al(2)	4157(1)	6670(1)	-33(1)	28(1)
Al(3)	3371(1)	4112(1)	2291(1)	30(1)
Si(1)	5943(1)	7647(1)	-662(1)	32(1)
Si(2)	7702(1)	6460(1)	-1293(1)	35(1)
Si(3)	2240(1)	7594(1)	742(1)	36(1)
Si(4)	2309(1)	5873(1)	2413(1)	45(1)
Si(5)	3860(1)	2696(1)	4138(1)	43(1)
Si(6)	6088(1)	2697(1)	3670(1)	50(1)
O(1)	4376(2)	4628(1)	191(1)	28(1)
O(2)	4410(2)	5683(1)	886(1)	30(1)
O(3)	6007(2)	3641(2)	790(2)	29(1)
O(4)	4591(2)	3972(2)	1846(2)	31(1)
O(5)	5056(2)	7213(2)	-379(2)	41(1)
O(6)	3048(2)	5187(2)	2120(2)	39(1)
O(7)	6882(2)	7084(2)	-956(2)	44(1)
O(8)	2061(2)	6800(2)	1629(2)	54(1)
O(9)	3076(2)	7254(2)	190(2)	40(1)
O(10)	5040(2)	2517(2)	4041(2)	64(1)
O(11)	3407(2)	3404(2)	3304(2)	53(1)
O(12)	2736(2)	3914(2)	1737(2)	61(1)
O(13)	6134(2)	4633(2)	1478(2)	38(1)
O(14)	6084(3)	3725(2)	3111(2)	62(1)
C(1)	6507(4)	5336(3)	1370(3)	52(1)
C(2)	6252(10)	5586(6)	2036(4)	167(5)
C(3)	6388(10)	5072(5)	2874(5)	164(5)
C(4)	5914(9)	4369(5)	3399(5)	149(5)
C(5)	5642(3)	8735(2)	-1549(3)	40(1)
C(6)	5942(4)	8868(3)	-2356(3)	59(1)
C(7)	5647(5)	9655(4)	-3015(4)	91(2)
C(8)	5032(5)	10337(4)	-2872(5)	92(2)
C(9)	4744(5)	10223(3)	-2084(5)	80(2)
C(10)	5038(4)	9426(3)	-1420(3)	59(1)
C(11)	6241(4)	7741(3)	228(3)	43(1)
C(12)	7165(5)	7704(3)	343(4)	67(2)
C(13)	7374(6)	7764(4)	1021(5)	91(2)
C(14)	6627(7)	7889(4)	1576(5)	103(3)
C(15)	5726(7)	7961(5)	1459(4)	104(3)
C(16)	5515(5)	7873(4)	805(4)	79(2)
C(17)	8565(3)	7102(3)	-2008(3)	49(1)
C(18)	8681(4)	7832(4)	-1988(4)	74(2)
C(19)	9345(6)	8287(5)	-2517(5)	105(3)
C(20)	9886(6)	8035(7)	-3095(6)	128(4)
C(21)	9786(5)	7339(7)	-3122(4)	106(3)
C(22)	9130(4)	6864(4)	-2599(3)	75(2)
C(23)	8281(3)	5536(3)	-364(3)	42(1)
C(24)	8773(4)	5651(3)	135(3)	56(1)
C(25)	9154(4)	4982(4)	845(4)	77(2)
C(26)	9054(4)	4178(4)	1080(4)	87(2)
C(27)	8574(5)	4018(3)	606(5)	96(3)
C(28)	8197(4)	4699(3)	-128(4)	61(1)
C(29)	1093(3)	8054(3)	229(3)	41(1)
C(30)	707(4)	8928(3)	-193(3)	60(1)
C(31)	-143(5)	9244(4)	-598(4)	77(2)
C(32)	-565(5)	8715(5)	-603(5)	99(3)
C(33)	-224(5)	7835(5)	-220(7)	136(4)
C(34)	605(5)	7519(4)	199(5)	90(2)
C(35)	2541(3)	8441(3)	905(3)	46(1)
C(36)	2986(4)	9062(3)	265(4)	73(2)
C(37)	3198(5)	9708(4)	361(5)	91(2)
C(38)	3000(5)	9752(5)	1093(6)	96(2)
C(39)	2546(7)	9185(6)	1716(5)	112(3)
C(40)	2305(6)	8523(4)	1632(4)	91(2)
C(41)	1184(4)	5500(3)	2885(4)	73(2)
C(42A)	1120(8)	4753(6)	3575(6)	85(3)
C(43A)	273(10)	4451(8)	3919(8)	113(4)
C(44)	-473(9)	4815(8)	3558(8)	158(4)
C(45A)	-443(10)	5362(8)	2789(9)	173(5)
C(46A)	292(8)	5861(7)	2390(7)	74(3)
C(42B)	862(16)	5579(13)	3706(13)	76(5)
C(43B)	-70(16)	5245(14)	4066(14)	80(6)

C(46B)	723(16)	5302(13)	2594(12)	90(5)
C(47)	2890(6)	6014(3)	3151(3)	81(2)
C(48)	3551(8)	6428(9)	2951(6)	155(4)
C(49)	4016(8)	6527(8)	3485(7)	147(4)
C(50)	3773(15)	6295(9)	4186(6)	244(10)
C(51A)	3646(12)	5434(11)	4486(11)	103(2)
C(52A)	3098(12)	5377(10)	3956(10)	103(2)
C(51B)	2537(13)	6430(10)	4297(10)	103(2)
C(52B)	2080(12)	6205(10)	3770(10)	103(2)
C(53)	3489(4)	1677(3)	4446(3)	49(1)
C(54)	2716(5)	1671(3)	4141(4)	74(2)
C(55)	2351(6)	948(5)	4431(6)	114(3)
C(56)	2770(8)	204(5)	5026(7)	119(3)
C(57)	3556(9)	173(4)	5337(5)	121(3)
C(58)	3926(6)	908(3)	5038(4)	90(2)
C(59)	3448(4)	3039(3)	4987(3)	51(1)
C(60)	2635(8)	3005(10)	5379(8)	214(8)
C(61)	2311(11)	3246(9)	6035(7)	209(8)
C(62)	2755(7)	3545(7)	6258(5)	131(4)
C(63A)	3629(10)	3133(8)	6233(8)	80(2)
C(64A)	3997(10)	2917(8)	5586(8)	80(2)
C(63B)	3445(10)	4070(8)	5512(9)	80(2)
C(64B)	3733(10)	3767(8)	4882(8)	80(2)
C(65)	6581(4)	2223(3)	2932(3)	50(1)
C(66)	6064(4)	1808(3)	2736(3)	55(1)
C(67)	6485(5)	1421(3)	2203(3)	68(2)
C(68)	7403(5)	1443(3)	1859(3)	70(2)
C(69)	7911(5)	1878(4)	2016(4)	81(2)
C(70)	7517(4)	2272(4)	2536(4)	81(2)
C(71)	6838(4)	2263(4)	4539(3)	72(2)
C(72)	6578(6)	1711(4)	5316(3)	88(2)
C(73)	7212(9)	1346(6)	5956(4)	150(4)
C(74A)	8079(16)	1620(16)	5825(13)	95(6)
C(75A)	8404(17)	2057(16)	5038(13)	71(6)
C(76A)	7726(12)	2594(13)	4404(10)	68(5)
C(74B)	7840(20)	2070(20)	5893(19)	109(9)
C(75B)	8142(13)	2550(12)	5091(11)	84(5)
C(76B)	7494(19)	2889(16)	4480(15)	44(6)
C(74C)	8146(14)	1196(13)	5815(11)	56(5)
C(75C)	8433(15)	1612(15)	5068(13)	68(5)
C(76C)	7833(11)	2127(11)	4423(9)	69(4)
C(77A)	8798(16)	8778(13)	1770(12)	112(6)
C(77B)	9306(16)	8424(13)	2006(13)	111(5)
C(78A)	9738(12)	8057(10)	2479(11)	95(4)
C(78B)	9745(14)	8079(12)	3117(12)	122(6)
C(79A)	9122(17)	8533(14)	3414(13)	131(6)
C(79B)	8461(17)	8906(13)	3156(13)	118(6)
C(80A)	8061(13)	9081(11)	2695(13)	106(5)
C(80B)	8188(12)	9096(10)	2083(11)	96(4)

Table 3. Bond lengths [Å] and angles [°] for sh2125.

Al(1)-O(1)#1	1.867(3)
Al(1)-O(4)	1.884(3)
Al(1)-O(2)	1.887(2)
Al(1)-O(1)	1.902(3)
Al(1)-O(3)	1.925(2)
Al(1)-O(13)	1.938(3)
Al(1)-Al(1)#1	2.921(2)
Al(2)-O(5)	1.714(3)
Al(2)-O(9)	1.723(3)
Al(2)-O(2)	1.794(3)
Al(2)-O(3)#1	1.818(3)
Al(3)-O(11)	1.707(3)
Al(3)-O(12)	1.717(3)
Al(3)-O(6)	1.743(3)
Al(3)-O(4)	1.816(3)
Si(1)-O(5)	1.586(3)
Si(1)-O(7)	1.625(3)
Si(1)-C(5)	1.869(4)
Si(1)-C(11)	1.879(4)
Si(2)-O(12)#1	1.592(3)
Si(2)-O(7)	1.638(3)
Si(2)-C(17)	1.859(5)
Si(2)-C(23)	1.870(5)
Si(3)-O(9)	1.612(3)
Si(3)-O(8)	1.634(3)
Si(3)-C(29)	1.861(5)
Si(3)-C(35)	1.875(5)
Si(4)-O(8)	1.614(3)
Si(4)-O(6)	1.621(2)
Si(4)-C(41)	1.861(6)
Si(4)-C(47)	1.888(7)
Si(5)-O(11)	1.583(3)
Si(5)-O(10)	1.648(4)
Si(5)-C(53)	1.866(5)
Si(5)-C(59)	1.891(5)
Si(6)-O(10)	1.613(4)
Si(6)-O(14)	1.645(4)
Si(6)-C(71)	1.845(6)
Si(6)-C(65)	1.872(5)
O(1)-Al(1)#1	1.867(3)
O(3)-Al(2)#1	1.818(3)
O(12)-Si(2)#1	1.592(3)
O(13)-C(1)	1.441(5)
O(14)-C(4)	1.440(7)
C(1)-C(2)	1.457(8)
C(2)-C(3)	1.406(10)
C(3)-C(4)	1.460(11)
C(5)-C(10)	1.398(6)
C(5)-C(6)	1.403(7)
C(6)-C(7)	1.381(7)
C(7)-C(8)	1.403(9)
C(8)-C(9)	1.376(9)
C(9)-C(10)	1.394(8)
C(11)-C(12)	1.385(7)
C(11)-C(16)	1.410(7)
C(12)-C(13)	1.409(8)
C(13)-C(14)	1.395(11)
C(14)-C(15)	1.334(11)
C(15)-C(16)	1.396(9)
C(17)-C(18)	1.399(8)
C(17)-C(22)	1.399(7)
C(18)-C(19)	1.386(9)
C(19)-C(20)	1.382(12)
C(20)-C(21)	1.333(12)
C(21)-C(22)	1.390(11)
C(23)-C(24)	1.393(7)
C(23)-C(28)	1.399(7)
C(24)-C(25)	1.377(7)
C(25)-C(26)	1.350(10)
C(26)-C(27)	1.397(10)
C(27)-C(28)	1.410(9)
C(29)-C(30)	1.383(6)
C(29)-C(34)	1.383(8)
C(30)-C(31)	1.404(8)
C(31)-C(32)	1.285(9)

C(32)-C(33)	1.376(10)
C(33)-C(34)	1.392(9)
C(35)-C(40)	1.393(7)
C(35)-C(36)	1.402(7)
C(36)-C(37)	1.385(8)
C(37)-C(38)	1.370(10)
C(38)-C(39)	1.346(11)
C(39)-C(40)	1.424(9)
C(41)-C(46B)	1.16(2)
C(41)-C(42A)	1.369(11)
C(41)-C(46A)	1.538(13)
C(41)-C(42B)	1.57(2)
C(42A)-C(43A)	1.414(15)
C(43A)-C(44)	1.232(15)
C(44)-C(45A)	1.299(15)
C(45A)-C(46A)	1.466(16)
C(42B)-C(43B)	1.55(3)
C(47)-C(48)	1.287(12)
C(47)-C(52A)	1.414(17)
C(47)-C(52B)	1.568(17)
C(48)-C(49)	1.405(12)
C(49)-C(50)	1.180(13)
C(50)-C(51A)	1.441(18)
C(50)-C(51B)	1.74(2)
C(51A)-C(52A)	1.44(2)
C(51B)-C(52B)	1.53(2)
C(53)-C(58)	1.363(7)
C(53)-C(54)	1.363(8)
C(54)-C(55)	1.384(10)
C(55)-C(56)	1.335(12)
C(56)-C(57)	1.357(12)
C(57)-C(58)	1.405(11)
C(59)-C(60)	1.270(9)
C(59)-C(64A)	1.392(14)
C(59)-C(64B)	1.411(14)
C(60)-C(61)	1.434(11)
C(61)-C(62)	1.185(13)
C(61)-C(63A)	1.96(2)
C(62)-C(63A)	1.281(14)
C(62)-C(63B)	1.619(17)
C(63A)-C(64A)	1.399(17)
C(63B)-C(64B)	1.459(18)
C(65)-C(66)	1.400(7)
C(65)-C(70)	1.430(7)
C(66)-C(67)	1.420(7)
C(67)-C(68)	1.374(8)
C(68)-C(69)	1.376(9)
C(69)-C(70)	1.402(8)
C(71)-C(72)	1.368(8)
C(71)-C(76C)	1.394(17)
C(71)-C(76A)	1.514(18)
C(71)-C(76B)	1.64(3)
C(72)-C(73)	1.427(11)
C(73)-C(74C)	1.31(2)
C(73)-C(74A)	1.43(2)
C(73)-C(74B)	1.75(3)
C(74A)-C(75A)	1.36(3)
C(75A)-C(76A)	1.46(3)
C(74B)-C(75B)	1.39(3)
C(75B)-C(76B)	1.41(3)
C(74C)-C(75C)	1.28(3)
C(75C)-C(76C)	1.39(3)
C(77A)-C(77B)	0.86(2)
C(77A)-C(80B)	1.13(2)
C(77A)-C(78A)	1.83(2)
C(77B)-C(78A)	1.02(2)
C(77B)-C(80B)	1.76(2)
C(77B)-C(78B)	2.03(3)
C(78A)-C(78B)	1.21(2)
C(78B)-C(79A)	1.27(2)
C(79A)-C(79B)	1.05(2)
C(79A)-C(80A)	1.95(3)
C(79B)-C(80A)	1.00(2)
C(79B)-C(80B)	1.96(3)
C(80A)-C(80B)	1.10(2)

O(1)#1-Al(1)-O(4)	171.88(14)

O(1)#1-Al(1)-O(2)	86.22(11)
O(4)-Al(1)-O(2)	91.62(11)
O(1)#1-Al(1)-O(1)	78.43(13)
O(4)-Al(1)-O(1)	93.95(13)
O(2)-Al(1)-O(1)	94.24(11)
O(1)#1-Al(1)-O(3)	91.77(11)
O(4)-Al(1)-O(3)	90.40(11)
O(2)-Al(1)-O(3)	177.98(13)
O(1)-Al(1)-O(3)	85.58(11)
O(1)#1-Al(1)-O(13)	98.78(13)
O(4)-Al(1)-O(13)	89.07(13)
O(2)-Al(1)-O(13)	91.09(12)
O(1)-Al(1)-O(13)	173.79(12)
O(3)-Al(1)-O(13)	88.98(12)
O(1)#1-Al(1)-Al(1)#1	39.65(9)
O(4)-Al(1)-Al(1)#1	132.67(12)
O(2)-Al(1)-Al(1)#1	90.35(9)
O(1)-Al(1)-Al(1)#1	38.78(8)
O(3)-Al(1)-Al(1)#1	88.26(9)
O(13)-Al(1)-Al(1)#1	138.17(11)
O(5)-Al(2)-O(9)	113.57(14)
O(5)-Al(2)-O(2)	113.54(14)
O(9)-Al(2)-O(2)	105.20(13)
O(5)-Al(2)-O(3)#1	109.74(14)
O(9)-Al(2)-O(3)#1	108.89(14)
O(2)-Al(2)-O(3)#1	105.47(12)
O(11)-Al(3)-O(12)	114.77(19)
O(11)-Al(3)-O(6)	112.90(15)
O(12)-Al(3)-O(6)	112.56(16)
O(11)-Al(3)-O(4)	106.86(15)
O(12)-Al(3)-O(4)	104.40(15)
O(6)-Al(3)-O(4)	104.20(14)
O(5)-Si(1)-O(7)	112.10(16)
O(5)-Si(1)-C(5)	110.11(18)
O(7)-Si(1)-C(5)	107.03(18)
O(5)-Si(1)-C(11)	108.21(19)
O(7)-Si(1)-C(11)	108.91(19)
C(5)-Si(1)-C(11)	110.49(18)
O(12)#1-Si(2)-O(7)	112.82(18)
O(12)#1-Si(2)-C(17)	110.2(2)
O(7)-Si(2)-C(17)	107.84(19)
O(12)#1-Si(2)-C(23)	108.3(2)
O(7)-Si(2)-C(23)	105.65(17)
C(17)-Si(2)-C(23)	112.0(2)
O(9)-Si(3)-O(8)	110.87(14)
O(9)-Si(3)-C(29)	109.55(17)
O(8)-Si(3)-C(29)	106.7(2)
O(9)-Si(3)-C(35)	111.2(2)
O(8)-Si(3)-C(35)	109.2(2)
C(29)-Si(3)-C(35)	109.17(19)
O(8)-Si(4)-O(6)	109.18(15)
O(8)-Si(4)-C(41)	109.2(2)
O(6)-Si(4)-C(41)	109.7(2)
O(8)-Si(4)-C(47)	107.4(2)
O(6)-Si(4)-C(47)	109.9(2)
C(41)-Si(4)-C(47)	111.3(3)
O(11)-Si(5)-O(10)	110.91(19)
O(11)-Si(5)-C(53)	108.8(2)
O(10)-Si(5)-C(53)	109.8(2)
O(11)-Si(5)-C(59)	111.89(19)
O(10)-Si(5)-C(59)	106.8(2)
C(53)-Si(5)-C(59)	108.5(2)
O(10)-Si(6)-O(14)	113.8(2)
O(10)-Si(6)-C(71)	107.5(2)
O(14)-Si(6)-C(71)	108.6(3)
O(10)-Si(6)-C(65)	109.9(2)
O(14)-Si(6)-C(65)	103.24(19)
C(71)-Si(6)-C(65)	114.0(2)
Al(1)#1-O(1)-Al(1)	101.57(13)
Al(2)-O(2)-Al(1)	121.29(13)
Al(2)#1-O(3)-Al(1)	120.86(14)
Al(3)-O(4)-Al(1)	132.58(14)
Si(1)-O(5)-Al(2)	175.55(19)
Si(4)-O(6)-Al(3)	144.24(19)
Si(1)-O(7)-Si(2)	170.6(2)
Si(4)-O(8)-Si(3)	157.7(2)
Si(3)-O(9)-Al(2)	157.50(19)

Si(6)-O(10)-Si(5)	158.6(3)
Si(5)-O(11)-Al(3)	158.1(2)
Si(2)#1-O(12)-Al(3)	168.1(2)
C(1)-O(13)-Al(1)	128.2(3)
C(4)-O(14)-Si(6)	126.9(4)
O(13)-C(1)-C(2)	115.4(5)
C(3)-C(2)-C(1)	128.9(9)
C(2)-C(3)-C(4)	123.9(8)
O(14)-C(4)-C(3)	113.4(7)
C(10)-C(5)-C(6)	118.3(4)
C(10)-C(5)-Si(1)	119.7(4)
C(6)-C(5)-Si(1)	121.8(3)
C(7)-C(6)-C(5)	121.6(5)
C(6)-C(7)-C(8)	119.2(6)
C(9)-C(8)-C(7)	120.0(5)
C(8)-C(9)-C(10)	120.7(5)
C(9)-C(10)-C(5)	120.2(5)
C(12)-C(11)-C(16)	116.8(5)
C(12)-C(11)-Si(1)	122.5(4)
C(16)-C(11)-Si(1)	120.7(4)
C(11)-C(12)-C(13)	121.5(6)
C(14)-C(13)-C(12)	119.2(7)
C(15)-C(14)-C(13)	120.3(6)
C(14)-C(15)-C(16)	121.0(7)
C(15)-C(16)-C(11)	121.2(7)
C(18)-C(17)-C(22)	117.1(6)
C(18)-C(17)-Si(2)	122.5(4)
C(22)-C(17)-Si(2)	120.4(5)
C(19)-C(18)-C(17)	121.2(7)
C(20)-C(19)-C(18)	119.9(8)
C(21)-C(20)-C(19)	119.6(8)
C(20)-C(21)-C(22)	122.1(8)
C(21)-C(22)-C(17)	120.0(7)
C(24)-C(23)-C(28)	117.5(5)
C(24)-C(23)-Si(2)	122.1(3)
C(28)-C(23)-Si(2)	120.3(4)
C(25)-C(24)-C(23)	122.6(5)
C(26)-C(25)-C(24)	119.8(7)
C(25)-C(26)-C(27)	120.6(6)
C(26)-C(27)-C(28)	119.7(6)
C(23)-C(28)-C(27)	119.8(6)
C(30)-C(29)-C(34)	115.5(5)
C(30)-C(29)-Si(3)	123.8(4)
C(34)-C(29)-Si(3)	120.5(3)
C(29)-C(30)-C(31)	121.7(5)
C(32)-C(31)-C(30)	119.9(5)
C(31)-C(32)-C(33)	122.8(6)
C(32)-C(33)-C(34)	117.5(7)
C(29)-C(34)-C(33)	122.6(5)
C(40)-C(35)-C(36)	116.4(5)
C(40)-C(35)-Si(3)	123.4(4)
C(36)-C(35)-Si(3)	120.1(4)
C(37)-C(36)-C(35)	121.5(6)
C(38)-C(37)-C(36)	121.1(7)
C(39)-C(38)-C(37)	119.3(6)
C(38)-C(39)-C(40)	120.8(7)
C(35)-C(40)-C(39)	120.8(7)
C(46B)-C(41)-C(42A)	86.3(12)
C(46B)-C(41)-C(46A)	38.6(10)
C(42A)-C(41)-C(46A)	111.3(8)
C(46B)-C(41)-C(42B)	122.7(14)
C(42A)-C(41)-C(42B)	63.4(9)
C(46A)-C(41)-C(42B)	107.6(9)
C(46B)-C(41)-Si(4)	125.9(11)
C(42A)-C(41)-Si(4)	125.2(6)
C(46A)-C(41)-Si(4)	121.0(5)
C(42B)-C(41)-Si(4)	111.2(9)
C(41)-C(42A)-C(43A)	125.5(10)
C(44)-C(43A)-C(42A)	120.9(14)
C(43A)-C(44)-C(45A)	119.7(15)
C(44)-C(45A)-C(46A)	124.0(14)
C(45A)-C(46A)-C(41)	113.3(10)
C(43B)-C(42B)-C(41)	108.0(15)
C(48)-C(47)-C(52A)	102.6(10)
C(48)-C(47)-C(52B)	114.3(8)
C(52A)-C(47)-C(52B)	70.6(9)
C(48)-C(47)-Si(4)	125.0(5)

C(52A)-C(47)-Si(4)	124.4(8)
C(52B)-C(47)-Si(4)	107.6(8)
C(47)-C(48)-C(49)	126.6(10)
C(50)-C(49)-C(48)	122.4(13)
C(49)-C(50)-C(51A)	106.4(12)
C(49)-C(50)-C(51B)	108.5(14)
C(51A)-C(50)-C(51B)	76.4(10)
C(52A)-C(51A)-C(50)	111.9(14)
C(47)-C(52A)-C(51A)	124.9(15)
C(52B)-C(51B)-C(50)	117.6(12)
C(51B)-C(52B)-C(47)	107.1(13)
C(58)-C(53)-C(54)	116.0(5)
C(58)-C(53)-Si(5)	121.9(5)
C(54)-C(53)-Si(5)	121.9(4)
C(53)-C(54)-C(55)	123.2(6)
C(56)-C(55)-C(54)	120.3(8)
C(55)-C(56)-C(57)	118.7(8)
C(56)-C(57)-C(58)	120.8(7)
C(53)-C(58)-C(57)	121.0(8)
C(60)-C(59)-C(64A)	100.4(8)
C(60)-C(59)-C(64B)	110.3(8)
C(64A)-C(59)-C(64B)	63.5(8)
C(60)-C(59)-Si(5)	124.0(5)
C(64A)-C(59)-Si(5)	127.3(6)
C(64B)-C(59)-Si(5)	116.0(6)
C(59)-C(60)-C(61)	125.2(9)
C(62)-C(61)-C(60)	123.9(10)
C(62)-C(61)-C(63A)	38.9(7)
C(60)-C(61)-C(63A)	91.9(8)
C(61)-C(62)-C(63A)	105.5(11)
C(61)-C(62)-C(63B)	110.6(9)
C(63A)-C(62)-C(63B)	64.3(9)
C(62)-C(63A)-C(64A)	120.3(12)
C(62)-C(63A)-C(61)	35.5(6)
C(64A)-C(63A)-C(61)	91.4(9)
C(59)-C(64A)-C(63A)	124.2(12)
C(64B)-C(63B)-C(62)	114.4(11)
C(59)-C(64B)-C(63B)	119.3(11)
C(66)-C(65)-C(70)	116.6(5)
C(66)-C(65)-Si(6)	122.6(4)
C(70)-C(65)-Si(6)	120.8(4)
C(65)-C(66)-C(67)	120.5(5)
C(68)-C(67)-C(66)	121.7(6)
C(67)-C(68)-C(69)	118.8(5)
C(68)-C(69)-C(70)	121.1(6)
C(69)-C(70)-C(65)	121.1(6)
C(72)-C(71)-C(76C)	110.3(8)
C(72)-C(71)-C(76A)	118.7(8)
C(76C)-C(71)-C(76A)	31.5(7)
C(72)-C(71)-C(76B)	115.3(10)
C(76C)-C(71)-C(76B)	52.9(11)
C(76A)-C(71)-C(76B)	21.7(9)
C(72)-C(71)-Si(6)	122.5(5)
C(76C)-C(71)-Si(6)	121.0(7)
C(76A)-C(71)-Si(6)	118.6(7)
C(76B)-C(71)-Si(6)	115.5(9)
C(71)-C(72)-C(73)	120.3(8)
C(74C)-C(73)-C(72)	122.0(11)
C(74C)-C(73)-C(74A)	31.5(10)
C(72)-C(73)-C(74A)	120.9(11)
C(74C)-C(73)-C(74B)	60.0(13)
C(72)-C(73)-C(74B)	113.0(12)
C(74A)-C(73)-C(74B)	28.6(11)
C(75A)-C(74A)-C(73)	117.6(19)
C(74A)-C(75A)-C(76A)	120(2)
C(75A)-C(76A)-C(71)	114.2(16)
C(75B)-C(74B)-C(73)	111(2)
C(74B)-C(75B)-C(76B)	118(2)
C(75B)-C(76B)-C(71)	117.3(18)
C(75C)-C(74C)-C(73)	114.5(17)
C(74C)-C(75C)-C(76C)	125(2)
C(71)-C(76C)-C(75C)	122.3(15)
C(77B)-C(77A)-C(80B)	123(3)
C(77B)-C(77A)-C(78A)	13.2(17)
C(80B)-C(77A)-C(78A)	110.0(16)
C(77A)-C(77B)-C(78A)	156(3)
C(77A)-C(77B)-C(80B)	32.7(17)

C(78A)-C(77B)-C(80B)	122.9(19)
C(77A)-C(77B)-C(78B)	130(2)
C(78A)-C(77B)-C(78B)	26.2(12)
C(80B)-C(77B)-C(78B)	97.6(11)
C(77B)-C(78A)-C(78B)	132(2)
C(77B)-C(78A)-C(77A)	11.2(14)
C(78B)-C(78A)-C(77A)	121.3(15)
C(78A)-C(78B)-C(79A)	128(2)
C(78A)-C(78B)-C(77B)	21.8(10)
C(79A)-C(78B)-C(77B)	106.0(16)
C(79B)-C(79A)-C(78B)	123(2)
C(79B)-C(79A)-C(80A)	17.6(14)
C(78B)-C(79A)-C(80A)	105.5(17)
C(80A)-C(79B)-C(79A)	144(3)
C(80A)-C(79B)-C(80B)	22.9(13)
C(79A)-C(79B)-C(80B)	122(2)
C(79B)-C(80A)-C(80B)	136(2)
C(79B)-C(80A)-C(79A)	18.5(14)
C(80B)-C(80A)-C(79A)	118.8(16)
C(80A)-C(80B)-C(77A)	134(2)
C(80A)-C(80B)-C(77B)	110.2(16)
C(77A)-C(80B)-C(77B)	24.1(13)
C(80A)-C(80B)-C(79B)	20.7(12)
C(77A)-C(80B)-C(79B)	114.3(17)
C(77B)-C(80B)-C(79B)	90.5(11)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for sh2125. 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}
Al(1)	27(1)	24(1)	20(1)	-9(1)	-3(1)	1(1)
Al(2)	29(1)	23(1)	25(1)	-10(1)	-1(1)	1(1)
Al(3)	33(1)	28(1)	24(1)	-11(1)	1(1)	-3(1)
Si(1)	34(1)	27(1)	32(1)	-14(1)	-2(1)	-3(1)
Si(2)	27(1)	40(1)	39(1)	-21(1)	-2(1)	-3(1)
Si(3)	35(1)	30(1)	36(1)	-17(1)	2(1)	4(1)
Si(4)	55(1)	33(1)	33(1)	-16(1)	11(1)	2(1)
Si(5)	43(1)	43(1)	29(1)	-11(1)	2(1)	-3(1)
Si(6)	50(1)	50(1)	37(1)	-11(1)	-7(1)	-5(1)
O(1)	29(2)	26(1)	24(1)	-8(1)	-1(1)	-6(1)
O(2)	36(2)	28(1)	20(1)	-11(1)	0(1)	0(1)
O(3)	28(2)	27(1)	24(1)	-10(1)	-7(1)	6(1)
O(4)	32(2)	25(1)	23(1)	-6(1)	0(1)	2(1)
O(5)	46(2)	31(1)	40(2)	-12(1)	0(1)	-10(1)
O(6)	42(2)	30(1)	36(2)	-17(1)	8(1)	-1(1)
O(7)	38(2)	41(2)	46(2)	-22(1)	3(1)	1(1)
O(8)	62(2)	36(2)	40(2)	-14(1)	8(2)	9(1)
O(9)	37(2)	37(2)	35(2)	-18(1)	1(1)	10(1)
O(10)	40(2)	82(2)	61(2)	-33(2)	3(2)	-5(2)
O(11)	55(2)	45(2)	31(2)	-3(1)	8(1)	-3(1)
O(12)	47(2)	79(2)	81(3)	-57(2)	-9(2)	-6(2)
O(13)	43(2)	30(1)	38(2)	-12(1)	-17(1)	-1(1)
O(14)	98(3)	51(2)	36(2)	-17(2)	-12(2)	-13(2)
C(1)	55(3)	48(3)	54(3)	-18(2)	-15(2)	-14(2)
C(2)	378(17)	135(7)	54(4)	-36(5)	4(7)	-173(9)
C(3)	369(17)	92(5)	70(5)	-17(4)	-48(7)	-120(8)
C(4)	307(14)	96(6)	60(5)	-44(4)	26(6)	-80(7)
C(5)	42(3)	29(2)	47(3)	-14(2)	-10(2)	-8(2)
C(6)	68(4)	45(3)	40(3)	-7(2)	-1(2)	-3(2)
C(7)	103(5)	68(4)	52(4)	5(3)	-2(3)	-7(4)
C(8)	107(6)	44(3)	83(5)	10(3)	-26(4)	-11(3)
C(9)	99(5)	35(3)	100(5)	-28(3)	-32(4)	5(3)
C(10)	71(4)	39(2)	68(3)	-27(3)	-12(3)	-2(2)
C(11)	58(3)	32(2)	43(3)	-19(2)	-13(2)	-4(2)
C(12)	80(5)	67(3)	71(4)	-44(3)	-21(3)	-8(3)
C(13)	97(6)	95(5)	112(6)	-63(5)	-51(5)	-7(4)
C(14)	156(8)	91(5)	84(5)	-61(4)	-54(5)	7(5)
C(15)	131(7)	123(6)	82(5)	-78(5)	-12(5)	-3(5)
C(16)	88(5)	93(4)	67(4)	-54(4)	-4(3)	-6(3)
C(17)	30(3)	57(3)	37(3)	-7(2)	-8(2)	0(2)
C(18)	62(4)	64(3)	73(4)	-10(3)	1(3)	-23(3)
C(19)	76(5)	92(5)	117(7)	-11(5)	-4(5)	-43(4)
C(20)	72(6)	125(7)	99(7)	15(6)	11(5)	-25(5)
C(21)	53(4)	147(7)	55(4)	-11(5)	13(3)	-4(5)
C(22)	50(4)	103(4)	43(3)	-20(3)	6(3)	-3(3)
C(23)	29(3)	42(2)	46(3)	-17(2)	1(2)	-2(2)
C(24)	44(3)	58(3)	55(3)	-19(3)	-8(2)	-7(2)
C(25)	54(4)	88(4)	55(4)	-11(3)	-15(3)	1(3)
C(26)	37(4)	80(5)	79(5)	9(4)	-12(3)	5(3)
C(27)	61(5)	36(3)	123(6)	0(3)	10(4)	11(3)
C(28)	42(3)	42(3)	87(4)	-24(3)	1(3)	-2(2)
C(29)	34(3)	36(2)	51(3)	-27(2)	0(2)	5(2)
C(30)	60(4)	40(2)	73(4)	-25(3)	-18(3)	4(2)
C(31)	69(4)	54(3)	100(5)	-38(3)	-36(3)	25(3)
C(32)	65(5)	92(5)	157(7)	-76(5)	-50(4)	22(4)
C(33)	68(6)	93(5)	276(13)	-97(7)	-78(7)	11(4)
C(34)	67(4)	44(3)	154(7)	-37(4)	-40(4)	2(3)
C(35)	38(3)	43(2)	55(3)	-27(2)	-6(2)	4(2)
C(36)	78(4)	61(3)	85(4)	-43(3)	16(3)	-17(3)
C(37)	88(5)	66(4)	130(6)	-56(4)	20(4)	-27(3)
C(38)	73(5)	89(5)	164(8)	-85(6)	-28(5)	-9(4)
C(39)	158(9)	126(6)	105(6)	-83(6)	-9(6)	-51(6)
C(40)	137(7)	97(5)	67(4)	-54(4)	9(4)	-48(4)
C(41)	53(4)	57(3)	66(4)	-14(3)	25(3)	6(3)
C(47)	161(7)	42(3)	32(3)	-18(2)	-2(4)	-14(3)
C(48)	135(9)	283(15)	76(6)	-81(8)	-4(6)	-88(9)
C(49)	141(9)	216(11)	126(9)	-98(9)	-26(7)	-53(8)
C(50)	520(30)	254(14)	63(6)	-72(8)	32(10)	-267(18)
C(53)	62(3)	42(2)	32(2)	-12(2)	-2(2)	-4(2)
C(54)	83(5)	48(3)	86(4)	-21(3)	-25(4)	-9(3)
C(55)	103(6)	76(5)	181(9)	-63(6)	-30(6)	-22(4)

C(56)	153(9)	69(5)	135(8)	-47(5)	22(7)	-42(5)
C(57)	206(11)	35(3)	79(5)	5(3)	-25(6)	-14(5)
C(58)	133(6)	47(3)	64(4)	3(3)	-40(4)	-10(3)
C(59)	52(3)	55(3)	41(3)	-21(2)	-1(2)	-6(2)
C(60)	190(11)	406(19)	257(13)	-298(15)	167(10)	-215(12)
C(61)	277(16)	305(16)	180(11)	-202(12)	183(11)	-217(14)
C(62)	134(8)	170(8)	115(7)	-116(7)	-29(6)	33(6)
C(65)	54(3)	40(2)	41(3)	-6(2)	1(2)	-12(2)
C(66)	59(3)	49(3)	38(3)	-6(2)	-2(2)	-9(2)
C(67)	82(5)	58(3)	60(4)	-28(3)	-7(3)	-8(3)
C(68)	82(5)	55(3)	51(3)	-21(3)	7(3)	3(3)
C(69)	64(4)	65(3)	85(4)	-24(3)	27(3)	-10(3)
C(70)	53(4)	74(4)	122(6)	-56(4)	26(4)	-22(3)
C(71)	59(4)	93(4)	39(3)	-14(3)	1(3)	-14(3)
C(72)	109(6)	102(5)	39(3)	-11(3)	-10(3)	-39(4)
C(73)	221(13)	156(8)	34(4)	12(4)	-43(6)	-63(8)