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

Identification code	shelxs1577	
Empirical formula	C32 H40 Ga2 O5 Si2	
Formula weight	700.26	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.891(2) Å	α= 90°.
	b = 17.099(3) Å	β= 98.94(3)°.
	c = 21.162(4) Å	γ = 90°.
Volume	3535.6(12) $Å^3$	
Z	4	
Density (calculated)	1.316 Mg/m^3	
Absorption coefficient	1.626 mm^{-1}	
F(000)	1448	
Crystal size	0.5 x 0.4 x 0.4 mm^3	
Theta range for data collection	2.28 to 24.02°.	
Index ranges	-11<=h<=11, -19<=k<=19, -24<=l<=24	
Reflections collected	17347	
Independent reflections	5220 [R(int) = 0.0369]	
Completeness to theta = 24.02°	93.7 %	
Absorption correction	Emperical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5220 / 0 / 384	
Goodness-of-fit on F^2	1.148	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1360	
R indices (all data)	R1 = 0.0619, wR2 = 0.1447	
Largest diff. peak and hole	0.405 and -0.390 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for shelxs1577. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	3229(1)	1671(1)	225(1)	61(1)
Ga(2)	3119(1)	3338(1)	-90(1)	59(1)
Si(1)	6428(1)	1580(1)	127(1)	48(1)
Si(2)	6381(1)	3450(1)	19(1)	49(1)
O(1)	4971(3)	1350(2)	324(2)	62(1)
O(2)	6663(3)	2516(2)	100(2)	61(1)
O(3)	4788(3)	3661(2)	-195(2)	60(1)
O(4)	2890(3)	2338(2)	-507(2)	66(1)
O(5)	3281(4)	2674(2)	646(2)	70(1)
C(1)	6575(4)	1183(2)	-682(2)	52(1)
C(2)	5990(5)	462(3)	-898(3)	72(1)
C(3)	6059(6)	183(3)	-1499(3)	89(2)
C(4)	6699(7)	615(4)	-1917(3)	96(2)
C(5)	7293(7)	1304(4)	-1715(3)	94(2)
C(6)	7219(6)	1588(3)	-1115(2)	73(1)
C(7)	7808(4)	1163(2)	748(2)	54(1)
C(8)	8884(5)	718(3)	593(2)	67(1)
C(9)	9886(5)	407(3)	1055(3)	80(2)
C(10)	9822(6)	542(3)	1683(3)	89(2)
C(11)	8790(7)	978(4)	1852(3)	101(2)
C(12)	7795(6)	1287(4)	1393(2)	86(2)
C(13)	7028(4)	3906(2)	809(2)	55(1)
C(14)	6541(6)	4637(3)	973(2)	74(1)
C(15)	6960(7)	4968(3)	1558(3)	94(2)
C(16)	7902(7)	4591(4)	2002(3)	96(2)
C(17)	8433(6)	3888(4)	1854(3)	89(2)
C(18)	7984(5)	3550(3)	1264(3)	71(1)
C(19)	7331(4)	3825(2)	-620(2)	53(1)
C(20)	8592(5)	4198(3)	-490(2)	69(1)
C(21)	9303(5)	4445(3)	-968(3)	84(2)
C(22)	8778(6)	4317(4)	-1584(3)	90(2)

C(23)	7558(7)	3946(4)	-1747(3)	100(2)
C(24)	6832(6)	3717(4)	-1256(3)	86(2)
C(25)	2215(5)	2158(3)	-1155(3)	76(1)
C(26A)	2668(11)	1316(6)	-1339(5)	94(3)
C(27A)	620(10)	2123(6)	-1090(5)	102(3)
C(28A)	2461(12)	2785(7)	-1600(5)	107(3)
C(26B)	2110(30)	1239(15)	-1205(12)	112(8)
C(27B)	980(30)	2618(15)	-1349(13)	123(7)
C(28B)	3340(20)	2460(10)	-1579(9)	83(5)
C(29)	3058(6)	2849(3)	1298(3)	79(2)
C(30A)	3520(20)	3741(10)	1455(9)	72(4)
C(31A)	1310(20)	2733(15)	1202(12)	112(7)
C(32A)	3970(20)	2288(11)	1781(8)	82(4)
C(30B)	2800(30)	3754(14)	1292(12)	95(7)
C(31B)	1830(20)	2437(11)	1457(9)	72(4)
C(32B)	4430(20)	2609(13)	1689(10)	87(6)
C(30C)	3970(30)	3570(16)	1555(13)	93(8)
C(31C)	1650(20)	2947(12)	1358(10)	65(5)
C(32C)	3410(30)	2088(14)	1697(11)	89(7)

Table 3. Bond lengths [Å] and angles [°] for shelxs1577.

Ga(1)-O(1)	1.790(3)
Ga(1)-O(4)	1.912(3)
Ga(1)-O(5)	1.929(3)
Ga(1)-Ga(2)	2.9250(8)
Ga(2)-O(3)	1.787(3)
Ga(2)-O(5)	1.915(3)
Ga(2)-O(4)	1.921(3)
Si(1)-O(1)	1.609(3)
Si(1)-O(2)	1.620(3)
Si(1)-C(1)	1.868(4)
Si(1)-C(7)	1.881(4)
Si(2)-O(3)	1.611(3)
Si(2)-O(2)	1.626(3)
Si(2)-C(13)	1.865(5)
Si(2)-C(19)	1.876(4)
O(4)-C(25)	1.461(6)
O(5)-C(29)	1.462(6)
C(1)-C(6)	1.381(6)
C(1)-C(2)	1.408(6)
C(2)-C(3)	1.368(8)
C(3)-C(4)	1.380(9)
C(4)-C(5)	1.356(9)
C(5)-C(6)	1.373(8)
C(7)-C(12)	1.383(7)
C(7)-C(8)	1.388(6)
C(8)-C(9)	1.386(7)
C(9)-C(10)	1.361(8)
C(10)-C(11)	1.356(8)
C(11)-C(12)	1.376(8)
C(13)-C(18)	1.382(6)
C(13)-C(14)	1.403(6)
C(14)-C(15)	1.365(8)
C(15)-C(16)	1.375(9)
C(16)-C(17)	1.368(9)
C(17)-C(18)	1.384(8)
C(19)-C(24)	1.371(7)
C(19)-C(20)	1.389(6)
C(20)-C(21)	1.385(7)
C(21)-C(22)	1.344(8)
C(22)-C(23)	1.359(9)
C(23)-C(24)	1.407(8)
C(25)-C(27B)	1.46(3)
C(25)-C(28A)	1.471(12)
C(25)-C(26A)	1.575(12)
C(25)-C(26B)	1.58(3)
C(25)-C(27A)	1.606(11)
C(25)-C(28B)	1.619(19)
C(29)-C(31C)	1.427(19)
C(29)-C(31B)	1.484(19)
C(29)-C(32B)	1.53(2)
C(29)-C(32C)	1.56(2)
C(29)-C(30B)	1.57(2)
C(29)-C(30C)	1.57(3)
C(29)-C(32A)	1.580(18)
C(29)-C(30A)	1.611(18)
C(29)-C(31A)	1.72(2)

O(1)-Ga(1)-O(4)	108.77(14)
O(1)-Ga(1)-O(5)	105.20(15)
O(4)-Ga(1)-O(5)	80.40(13)
O(1)-Ga(1)-Ga(2)	109.05(10)
O(4)-Ga(1)-Ga(2)	40.37(9)
O(5)-Ga(1)-Ga(2)	40.27(9)
O(3)-Ga(2)-O(5)	108.75(15)
O(3)-Ga(2)-O(4)	105.26(14)

O(5)-Ga(2)-O(4)	80.54(14)	C(9)-C(8)-C(7)	122.3(5)
O(3)-Ga(2)-Ga(1)	109.09(9)	C(10)-C(9)-C(8)	119.2(5)
O(5)-Ga(2)-Ga(1)	40.63(9)	C(11)-C(10)-C(9)	120.1(5)
O(4)-Ga(2)-Ga(1)	40.15(9)	C(10)-C(11)-C(12)	120.6(5)
O(1)-Si(1)-O(2)	112.91(16)	C(11)-C(12)-C(7)	121.6(5)
O(1)-Si(1)-C(1)	110.46(19)	C(18)-C(13)-C(14)	116.3(4)
O(2)-Si(1)-C(1)	107.13(17)	C(18)-C(13)-Si(2)	122.9(4)
O(1)-Si(1)-C(7)	108.00(17)	C(14)-C(13)-Si(2)	120.8(4)
O(2)-Si(1)-C(7)	107.82(19)	C(15)-C(14)-C(13)	121.7(5)
C(1)-Si(1)-C(7)	110.51(18)	C(14)-C(15)-C(16)	120.2(6)
O(3)-Si(2)-O(2)	113.18(17)	C(17)-C(16)-C(15)	119.9(5)
O(3)-Si(2)-C(13)	110.02(18)	C(16)-C(17)-C(18)	119.5(5)
O(2)-Si(2)-C(13)	106.64(18)	C(13)-C(18)-C(17)	122.3(5)
O(3)-Si(2)-C(19)	107.38(18)	C(24)-C(19)-C(20)	115.6(4)
O(2)-Si(2)-C(19)	108.39(18)	C(24)-C(19)-Si(2)	121.1(4)
C(13)-Si(2)-C(19)	111.27(19)	C(20)-C(19)-Si(2)	123.3(4)
Si(1)-O(1)-Ga(1)	141.22(19)	C(21)-C(20)-C(19)	122.5(5)
Si(1)-O(2)-Si(2)	162.0(2)	C(22)-C(21)-C(20)	119.7(5)
Si(2)-O(3)-Ga(2)	141.10(18)	C(21)-C(22)-C(23)	121.1(5)
C(25)-O(4)-Ga(1)	129.2(3)	C(22)-C(23)-C(24)	118.5(6)
C(25)-O(4)-Ga(2)	128.5(3)	C(19)-C(24)-C(23)	122.7(5)
Ga(1)-O(4)-Ga(2)	99.49(15)	C(27B)-C(25)-O(4)	113.0(11)
C(29)-O(5)-Ga(2)	129.9(3)	C(27B)-C(25)-C(28A)	69.0(12)
C(29)-O(5)-Ga(1)	128.3(3)	O(4)-C(25)-C(28A)	110.5(6)
Ga(2)-O(5)-Ga(1)	99.09(15)	C(27B)-C(25)-C(26A)	133.0(12)
C(6)-C(1)-C(2)	115.6(4)	O(4)-C(25)-C(26A)	108.6(5)
C(6)-C(1)-Si(1)	122.4(3)	C(28A)-C(25)-C(26A)	115.2(7)
C(2)-C(1)-Si(1)	122.0(3)	C(27B)-C(25)-C(26B)	118.2(14)
C(3)-C(2)-C(1)	122.0(5)	O(4)-C(25)-C(26B)	106.8(10)
C(2)-C(3)-C(4)	120.2(5)	C(28A)-C(25)-C(26B)	134.3(11)
C(5)-C(4)-C(3)	118.8(6)	C(26A)-C(25)-C(26B)	24.7(9)
C(4)-C(5)-C(6)	121.1(6)	C(27B)-C(25)-C(27A)	41.6(10)
C(5)-C(6)-C(1)	122.2(5)	O(4)-C(25)-C(27A)	103.8(5)
C(12)-C(7)-C(8)	116.2(4)	C(28A)-C(25)-C(27A)	110.2(7)
C(12)-C(7)-Si(1)	120.9(3)	C(26A)-C(25)-C(27A)	107.9(6)
C(8)-C(7)-Si(1)	122.9(3)	C(26B)-C(25)-C(27A)	84.8(10)

C(27B)-C(25)-C(28B)	106.9(13)
O(4)-C(25)-C(28B)	101.5(7)
C(28A)-C(25)-C(28B)	38.5(7)
C(26A)-C(25)-C(28B)	84.7(8)
C(26B)-C(25)-C(28B)	109.0(12)
C(27A)-C(25)-C(28B)	146.0(9)
C(31C)-C(29)-O(5)	113.6(9)
C(31C)-C(29)-C(31B)	36.3(10)
O(5)-C(29)-C(31B)	111.4(8)
C(31C)-C(29)-C(32B)	141.2(13)
O(5)-C(29)-C(32B)	101.7(9)
C(31B)-C(29)-C(32B)	116.0(12)
C(31C)-C(29)-C(32C)	101.0(12)
O(5)-C(29)-C(32C)	106.6(9)
C(31B)-C(29)-C(32C)	66.7(12)
C(32B)-C(29)-C(32C)	51.7(12)
C(31C)-C(29)-C(30B)	73.9(12)
O(5)-C(29)-C(30B)	104.0(9)
C(31B)-C(29)-C(30B)	109.3(12)
C(32B)-C(29)-C(30B)	113.6(13)
C(32C)-C(29)-C(30B)	148.2(13)
C(31C)-C(29)-C(30C)	113.0(13)
O(5)-C(29)-C(30C)	108.8(10)
C(31B)-C(29)-C(30C)	137.6(12)
C(32B)-C(29)-C(30C)	67.1(14)
C(32C)-C(29)-C(30C)	113.5(15)
C(30B)-C(29)-C(30C)	46.8(12)
C(31C)-C(29)-C(32A)	118.9(12)
O(5)-C(29)-C(32A)	109.3(7)
C(31B)-C(29)-C(32A)	88.5(12)
C(32B)-C(29)-C(32A)	28.1(8)
C(32C)-C(29)-C(32A)	24.0(9)
C(30B)-C(29)-C(32A)	133.0(13)
C(30C)-C(29)-C(32A)	90.7(14)
C(31C)-C(29)-C(30A)	96.7(11)
O(5)-C(29)-C(30A)	108.0(7)
C(31B)-C(29)-C(30A)	128.0(10)
C(32B)-C(29)-C(30A)	86.8(12)
C(32C)-C(29)-C(30A)	130.2(13)
C(30B)-C(29)-C(30A)	27.0(9)
C(30C)-C(29)-C(30A)	19.8(10)
C(32A)-C(29)-C(30A)	109.1(11)
C(31C)-C(29)-C(31A)	17.8(11)
O(5)-C(29)-C(31A)	99.3(9)
C(31B)-C(29)-C(31A)	29.7(10)
C(32B)-C(29)-C(31A)	145.4(13)
C(32C)-C(29)-C(31A)	96.0(13)
C(30B)-C(29)-C(31A)	87.1(13)
C(30C)-C(29)-C(31A)	129.9(14)
C(32A)-C(29)-C(31A)	118.1(12)
C(30A)-C(29)-C(31A)	112.2(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for shelxs1577. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ga(1)	54(1)	54(1)	78(1)	8(1)	24(1)	-3(1)
Ga(2)	51(1)	52(1)	75(1)	6(1)	11(1)	9(1)
Si(1)	54(1)	38(1)	55(1)	7(1)	16(1)	6(1)
Si(2)	54(1)	38(1)	55(1)	6(1)	7(1)	-2(1)
O(1)	61(2)	51(2)	79(2)	13(1)	23(2)	4(1)
O(2)	76(2)	38(2)	70(2)	5(1)	16(2)	2(1)
O(3)	57(2)	49(2)	71(2)	11(1)	5(2)	0(1)
O(4)	66(2)	56(2)	70(2)	3(2)	-3(2)	-7(1)
O(5)	87(2)	58(2)	71(2)	4(2)	37(2)	12(2)
C(1)	53(2)	46(2)	56(3)	4(2)	6(2)	9(2)
C(2)	83(3)	48(3)	84(4)	-1(2)	16(3)	8(2)
C(3)	104(4)	62(3)	95(4)	-27(3)	-4(4)	6(3)
C(4)	112(5)	108(5)	65(4)	-20(3)	5(4)	16(4)
C(5)	115(5)	111(5)	62(4)	-1(3)	28(3)	-7(4)
C(6)	86(3)	77(3)	60(3)	-5(2)	22(3)	-13(3)
C(7)	61(2)	44(2)	56(3)	8(2)	12(2)	1(2)
C(8)	65(3)	71(3)	64(3)	1(2)	8(2)	12(2)
C(9)	67(3)	83(4)	85(4)	10(3)	-1(3)	16(3)
C(10)	85(4)	85(4)	89(5)	23(3)	-9(3)	2(3)
C(11)	116(5)	132(6)	54(3)	17(3)	9(3)	23(4)
C(12)	99(4)	104(4)	58(3)	12(3)	21(3)	32(3)
C(13)	62(3)	45(2)	61(3)	5(2)	14(2)	-11(2)
C(14)	102(4)	48(3)	70(3)	0(2)	9(3)	-1(2)
C(15)	135(5)	64(3)	85(4)	-20(3)	23(4)	-4(3)
C(16)	124(5)	103(5)	58(4)	-15(3)	9(4)	-31(4)
C(17)	87(4)	109(5)	64(4)	7(3)	-9(3)	-3(3)
C(18)	68(3)	77(3)	65(3)	2(2)	0(3)	6(2)
C(19)	58(2)	41(2)	57(3)	10(2)	5(2)	1(2)
C(20)	65(3)	73(3)	70(3)	10(2)	10(2)	-4(2)
C(21)	63(3)	91(4)	100(5)	28(3)	22(3)	-5(3)
C(22)	79(4)	105(4)	91(5)	48(3)	28(3)	12(3)

C(23)	107(5)	135(6)	56(4)	27(3)	10(3)	-1(4)
C(24)	83(4)	108(4)	64(4)	19(3)	-1(3)	-19(3)
C(25)	66(3)	73(3)	81(4)	-8(3)	-10(3)	-9(3)
C(29)	85(4)	83(4)	77(3)	-2(3)	44(3)	11(3)

Table 1. Crystal data and structure refinement for **2**.

Identification code	shelxs1396	
Empirical formula	C79 H70 Ga2 O8 Si6	
Formula weight	1455.33	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.040(2) Å	α= 76.28(3)°.
	b = 12.070(2) Å	β= 76.04(3)°.
	c = 16.070(3) Å	γ = 89.01(3)°.
Volume	1834.3(6) $Å^3$	
Z	1	
Density (calculated)	1.317 Mg/m^3	
Absorption coefficient	0.887 mm^{-1}	
F(000)	754	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	1.93 to 23.95°.	
Index ranges	-10<=h<=10, -13<=k<=13, -18<=l<=18	
Reflections collected	11625	
Independent reflections	5377 [R(int) = 0.0314]	
Completeness to theta = 23.95°	94.0 %	
Absorption correction	Emprirical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5377 / 0 / 434	
Goodness-of-fit on F^2	0.932	
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0690	
R indices (all data)	R1 = 0.0452, wR2 = 0.0730	
Largest diff. peak and hole	0.330 and -0.205 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for shelxs1396. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	1182(1)	4965(1)	380(1)	34(1)
Si(1)	1051(1)	4503(1)	2391(1)	34(1)
Si(2)	-104(1)	6964(1)	2274(1)	34(1)
Si(3)	-568(1)	7257(1)	320(1)	30(1)
O(1)	674(2)	4249(1)	1532(1)	41(1)
O(2)	820(2)	5848(1)	2403(1)	43(1)
O(3)	-377(2)	7278(1)	1289(1)	39(1)
O(4)	320(2)	4059(1)	-192(1)	33(1)
C(1)	2880(3)	4228(2)	2367(2)	37(1)
C(2)	3558(3)	3465(3)	1897(2)	54(1)
C(3)	4908(4)	3208(3)	1874(2)	72(1)
C(4)	5613(4)	3696(3)	2335(2)	68(1)
C(5)	4980(3)	4456(3)	2809(2)	57(1)
C(6)	3638(3)	4718(2)	2823(2)	45(1)
C(7)	-91(3)	3572(2)	3399(2)	43(1)
C(8)	-1405(4)	3271(3)	3427(2)	67(1)
C(9)	-2275(4)	2594(4)	4162(3)	84(1)
C(10)	-1843(5)	2205(4)	4896(3)	108(2)
C(11)	-569(6)	2504(6)	4911(3)	178(3)
C(12)	325(5)	3180(5)	4166(3)	127(2)
C(13)	889(3)	8161(2)	2422(2)	39(1)
C(14)	2288(4)	8160(3)	2308(2)	62(1)
C(15)	3003(4)	9060(3)	2446(3)	86(1)
C(16)	2315(6)	9956(3)	2700(3)	86(1)
C(17)	943(5)	9977(3)	2816(2)	76(1)
C(18)	231(4)	9087(2)	2682(2)	59(1)
C(19)	-1796(3)	6723(2)	3092(2)	41(1)
C(20)	-1904(4)	6105(3)	3954(2)	65(1)
C(21)	-3142(5)	5965(3)	4588(2)	84(1)
C(22)	-4290(4)	6449(3)	4362(3)	81(1)
C(23)	-4228(4)	7049(3)	3524(3)	72(1)

C(24)	-2984(3)	7183(3)	2886(2)	55(1)
C(25)	765(3)	8227(2)	-535(2)	33(1)
C(26)	1109(3)	8094(2)	-1403(2)	45(1)
C(27)	2132(3)	8770(2)	-2045(2)	51(1)
C(28)	2838(3)	9594(2)	-1845(2)	49(1)
C(29)	2513(3)	9755(2)	-999(2)	51(1)
C(30)	1485(3)	9077(2)	-352(2)	42(1)
C(31)	-2350(3)	7531(2)	233(2)	35(1)
C(32)	-2710(3)	8447(2)	-379(2)	42(1)
C(33)	-4064(3)	8610(3)	-410(2)	56(1)
C(34)	-5095(4)	7854(3)	151(2)	65(1)
C(35)	-4770(4)	6934(3)	748(2)	66(1)
C(36)	-3424(3)	6782(2)	790(2)	49(1)
C(37)	4008(6)	727(5)	4775(4)	104(2)
C(38)	4088(6)	352(5)	5640(3)	109(2)
C(39)	4938(6)	362(5)	4130(3)	115(2)
C(40)	3044(10)	1372(7)	4575(6)	98(3)

Table 3. Bond lengths [Å] and angles [°] for shelxs1396.

Ga(1)-O(1)	1.7987(17)
Ga(1)-O(4)	1.9191(16)
Ga(1)-O(4)#1	1.9338(17)
Ga(1)-Ga(1)#1	2.9109(9)
Ga(1)-H(41)	1.3800
Si(1)-O(1)	1.6117(17)
Si(1)-O(2)	1.6396(18)
Si(1)-C(1)	1.853(3)
Si(1)-C(7)	1.867(3)
Si(2)-O(2)	1.6227(19)
Si(2)-O(3)	1.6270(17)
Si(2)-C(19)	1.859(3)
Si(2)-C(13)	1.862(3)
Si(3)-O(3)	1.6205(16)
Si(3)-O(4)#1	1.6571(16)
Si(3)-C(31)	1.846(3)
Si(3)-C(25)	1.858(3)
O(4)-Si(3)#1	1.6570(16)
O(4)-Ga(1)#1	1.9338(17)
C(1)-C(2)	1.394(4)
C(1)-C(6)	1.400(4)
C(2)-C(3)	1.379(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.368(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.380(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.375(4)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.362(4)
C(7)-C(12)	1.371(4)
C(8)-C(9)	1.376(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.334(6)
C(9)-H(9)	0.9300
C(10)-C(11)	1.342(7)
C(10)-H(10)	0.9300
C(11)-C(12)	1.396(6)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.371(4)
C(13)-C(18)	1.386(4)
C(14)-C(15)	1.401(5)
C(14)-H(14)	0.9300
C(15)-C(16)	1.365(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.345(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.386(5)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(24)	1.385(4)
C(19)-C(20)	1.388(4)
C(20)-C(21)	1.388(5)
C(20)-H(20)	0.9300
C(21)-C(22)	1.371(6)
C(21)-H(21)	0.9300
C(22)-C(23)	1.356(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.395(4)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-C(30)	1.390(4)
C(25)-C(26)	1.401(3)
C(26)-C(27)	1.381(4)
C(26)-H(26)	0.9300

C(27)-C(28)	1.371(4)	C(34)-H(34)	0.9300
C(27)-H(27)	0.9300	C(35)-C(36)	1.377(4)
C(28)-C(29)	1.378(4)	C(35)-H(35)	0.9300
C(28)-H(28)	0.9300	C(36)-H(36)	0.9300
C(29)-C(30)	1.387(4)	C(37)-C(40)	1.286(9)
C(29)-H(29)	0.9300	C(37)-C(39)	1.369(6)
C(30)-H(30)	0.9300	C(37)-C(38)	1.378(7)
C(31)-C(32)	1.401(3)	C(38)-C(39)#2	1.352(7)
C(31)-C(36)	1.402(4)	C(38)-H(38)	0.9300
C(32)-C(33)	1.381(4)	C(39)-C(38)#2	1.352(7)
C(32)-H(32)	0.9300	C(39)-H(39)	0.9300
C(33)-C(34)	1.382(5)	C(40)-H(40A)	0.9600
C(33)-H(33)	0.9300	C(40)-H(40B)	0.9600
C(34)-C(35)	1.375(5)	C(40)-H(40C)	0.9600

O(1)-Ga(1)-O(4)	104.37(8)	C(19)-Si(2)-C(13)	110.22(12)
O(1)-Ga(1)-O(4)#1	104.20(8)	O(3)-Si(3)-O(4)#1	107.81(9)
O(4)-Ga(1)-O(4)#1	81.86(7)	O(3)-Si(3)-C(31)	111.78(11)
O(1)-Ga(1)-Ga(1)#1	109.06(7)	O(4)#1-Si(3)-C(31)	104.70(11)
O(4)-Ga(1)-Ga(1)#1	41.12(5)	O(3)-Si(3)-C(25)	109.09(11)
O(4)#1-Ga(1)-Ga(1)#1	40.74(5)	O(4)#1-Si(3)-C(25)	108.24(10)
O(1)-Ga(1)-H(41)	122.9	C(31)-Si(3)-C(25)	114.88(11)
O(4)-Ga(1)-H(41)	119.1	Si(1)-O(1)-Ga(1)	131.96(11)
O(4)#1-Ga(1)-H(41)	116.3	Si(2)-O(2)-Si(1)	149.79(13)
Ga(1)#1-Ga(1)-H(41)	128.0	Si(3)-O(3)-Si(2)	165.60(12)
O(1)-Si(1)-O(2)	110.01(9)	Si(3)#1-O(4)-Ga(1)	131.72(10)
O(1)-Si(1)-C(1)	110.46(11)	Si(3)#1-O(4)-Ga(1)#1	129.21(10)
O(2)-Si(1)-C(1)	107.56(11)	Ga(1)-O(4)-Ga(1)#1	98.14(7)
O(1)-Si(1)-C(7)	108.62(11)	C(2)-C(1)-C(6)	116.5(3)
O(2)-Si(1)-C(7)	109.68(12)	C(2)-C(1)-Si(1)	119.7(2)
C(1)-Si(1)-C(7)	110.50(12)	C(6)-C(1)-Si(1)	123.8(2)
O(2)-Si(2)-O(3)	110.46(9)	C(3)-C(2)-C(1)	122.1(3)
O(2)-Si(2)-C(19)	111.44(11)	C(3)-C(2)-H(2)	118.9
O(3)-Si(2)-C(19)	108.20(12)	C(1)-C(2)-H(2)	118.9
O(2)-Si(2)-C(13)	106.85(12)	C(4)-C(3)-C(2)	119.8(3)
O(3)-Si(2)-C(13)	109.68(10)	C(4)-C(3)-H(3)	120.1

C(2)-C(3)-H(3)	120.1	C(14)-C(15)-H(15)	119.8
C(3)-C(4)-C(5)	120.0(3)	C(17)-C(16)-C(15)	119.7(3)
C(3)-C(4)-H(4)	120.0	C(17)-C(16)-H(16)	120.1
C(5)-C(4)-H(4)	120.0	C(15)-C(16)-H(16)	120.1
C(6)-C(5)-C(4)	120.1(3)	C(16)-C(17)-C(18)	120.1(4)
C(6)-C(5)-H(5)	120.0	C(16)-C(17)-H(17)	120.0
C(4)-C(5)-H(5)	120.0	C(18)-C(17)-H(17)	120.0
C(5)-C(6)-C(1)	121.5(3)	C(13)-C(18)-C(17)	122.1(4)
C(5)-C(6)-H(6)	119.2	C(13)-C(18)-H(18)	119.0
C(1)-C(6)-H(6)	119.2	C(17)-C(18)-H(18)	119.0
C(8)-C(7)-C(12)	115.8(3)	C(24)-C(19)-C(20)	117.1(3)
C(8)-C(7)-Si(1)	122.0(2)	C(24)-C(19)-Si(2)	122.2(2)
C(12)-C(7)-Si(1)	122.2(3)	C(20)-C(19)-Si(2)	120.6(2)
C(7)-C(8)-C(9)	123.4(3)	C(21)-C(20)-C(19)	121.7(4)
C(7)-C(8)-H(8)	118.3	C(21)-C(20)-H(20)	119.2
C(9)-C(8)-H(8)	118.3	C(19)-C(20)-H(20)	119.2
C(10)-C(9)-C(8)	119.8(4)	C(22)-C(21)-C(20)	119.5(3)
C(10)-C(9)-H(9)	120.1	C(22)-C(21)-H(21)	120.3
C(8)-C(9)-H(9)	120.1	C(20)-C(21)-H(21)	120.3
C(9)-C(10)-C(11)	119.1(4)	C(23)-C(22)-C(21)	120.6(3)
C(9)-C(10)-H(10)	120.5	C(23)-C(22)-H(22)	119.7
C(11)-C(10)-H(10)	120.5	C(21)-C(22)-H(22)	119.7
C(10)-C(11)-C(12)	121.4(4)	C(22)-C(23)-C(24)	119.9(4)
C(10)-C(11)-H(11)	119.3	C(22)-C(23)-H(23)	120.1
C(12)-C(11)-H(11)	119.3	C(24)-C(23)-H(23)	120.1
C(7)-C(12)-C(11)	120.4(4)	C(19)-C(24)-C(23)	121.3(3)
C(7)-C(12)-H(12)	119.8	C(19)-C(24)-H(24)	119.3
C(11)-C(12)-H(12)	119.8	C(23)-C(24)-H(24)	119.3
C(14)-C(13)-C(18)	116.8(3)	C(30)-C(25)-C(26)	117.1(2)
C(14)-C(13)-Si(2)	122.3(2)	C(30)-C(25)-Si(3)	123.02(18)
C(18)-C(13)-Si(2)	120.9(2)	C(26)-C(25)-Si(3)	119.81(19)
C(13)-C(14)-C(15)	121.0(3)	C(27)-C(26)-C(25)	121.2(3)
C(13)-C(14)-H(14)	119.5	C(27)-C(26)-H(26)	119.4
C(15)-C(14)-H(14)	119.5	C(25)-C(26)-H(26)	119.4
C(16)-C(15)-C(14)	120.4(4)	C(28)-C(27)-C(26)	120.4(3)
C(16)-C(15)-H(15)	119.8	C(28)-C(27)-H(27)	119.8

C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(29)	119.8(3)
C(27)-C(28)-H(28)	120.1
C(29)-C(28)-H(28)	120.1
C(28)-C(29)-C(30)	120.0(3)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(25)	121.5(2)
C(29)-C(30)-H(30)	119.3
C(25)-C(30)-H(30)	119.3
C(32)-C(31)-C(36)	116.7(3)
C(32)-C(31)-Si(3)	123.7(2)
C(36)-C(31)-Si(3)	119.56(19)
C(33)-C(32)-C(31)	121.0(3)
C(33)-C(32)-H(32)	119.5
C(31)-C(32)-H(32)	119.5
C(32)-C(33)-C(34)	120.6(3)
C(32)-C(33)-H(33)	119.7
C(34)-C(33)-H(33)	119.7
C(35)-C(34)-C(33)	119.7(3)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	119.8(3)
C(34)-C(35)-H(35)	120.1
C(36)-C(35)-H(35)	120.1
C(35)-C(36)-C(31)	122.2(3)
C(35)-C(36)-H(36)	118.9
C(31)-C(36)-H(36)	118.9
C(40)-C(37)-C(39)	120.1(7)
C(40)-C(37)-C(38)	120.8(6)
C(39)-C(37)-C(38)	119.0(6)
C(39)#2-C(38)-C(37)	121.9(5)
C(39)#2-C(38)-H(38)	119.1
C(37)-C(38)-H(38)	119.1
C(38)#2-C(39)-C(37)	119.1(6)
C(38)#2-C(39)-H(39)	120.5
C(37)-C(39)-H(39)	120.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z #2 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for shelxs1396. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ga(1)	37(1)	34(1)	31(1)	-8(1)	-13(1)	6(1)
Si(1)	42(1)	35(1)	27(1)	-3(1)	-15(1)	3(1)
Si(2)	43(1)	36(1)	24(1)	-8(1)	-8(1)	3(1)
Si(3)	39(1)	30(1)	23(1)	-5(1)	-8(1)	7(1)
O(1)	54(1)	39(1)	33(1)	-4(1)	-22(1)	5(1)
O(2)	53(1)	39(1)	40(1)	-10(1)	-16(1)	7(1)
O(3)	51(1)	40(1)	26(1)	-10(1)	-11(1)	6(1)
O(4)	42(1)	32(1)	28(1)	-9(1)	-14(1)	9(1)
C(1)	45(2)	36(1)	28(1)	2(1)	-13(1)	-2(1)
C(2)	56(2)	62(2)	59(2)	-25(2)	-31(2)	18(2)
C(3)	60(3)	92(3)	80(2)	-41(2)	-32(2)	34(2)
C(4)	45(2)	91(3)	73(2)	-16(2)	-26(2)	14(2)
C(5)	55(2)	65(2)	56(2)	-10(2)	-29(2)	-3(2)
C(6)	48(2)	48(2)	41(2)	-8(1)	-17(1)	1(1)
C(7)	47(2)	45(2)	35(2)	-2(1)	-14(1)	-3(1)
C(8)	51(2)	100(3)	49(2)	-17(2)	-11(2)	-17(2)
C(9)	59(3)	113(3)	74(3)	-31(2)	6(2)	-34(2)
C(10)	95(4)	131(4)	64(3)	21(2)	0(2)	-51(3)
C(11)	123(5)	278(8)	77(3)	101(4)	-50(3)	-89(5)
C(12)	87(4)	193(5)	66(3)	67(3)	-43(2)	-60(3)
C(13)	47(2)	41(2)	26(1)	-2(1)	-10(1)	-1(1)
C(14)	56(3)	57(2)	67(2)	-6(2)	-14(2)	-5(2)
C(15)	69(3)	73(3)	111(3)	11(2)	-43(2)	-27(2)
C(16)	133(4)	52(2)	86(3)	6(2)	-69(3)	-30(2)
C(17)	117(4)	45(2)	81(3)	-22(2)	-44(2)	-3(2)
C(18)	70(2)	48(2)	65(2)	-21(2)	-22(2)	3(2)
C(19)	52(2)	37(1)	32(1)	-11(1)	-3(1)	-4(1)
C(20)	68(2)	80(2)	36(2)	-7(2)	-1(2)	4(2)
C(21)	95(3)	94(3)	39(2)	-2(2)	13(2)	-3(2)
C(22)	72(3)	81(3)	71(3)	-26(2)	27(2)	-16(2)
C(23)	51(2)	80(2)	81(3)	-28(2)	2(2)	3(2)

C(24)	52(2)	58(2)	50(2)	-15(2)	-3(2)	5(2)
C(25)	36(2)	32(1)	30(1)	-5(1)	-9(1)	9(1)
C(26)	56(2)	42(2)	34(2)	-10(1)	-4(1)	-5(1)
C(27)	66(2)	47(2)	32(2)	-9(1)	2(1)	-3(2)
C(28)	49(2)	45(2)	45(2)	-6(1)	1(1)	-3(1)
C(29)	51(2)	47(2)	54(2)	-14(1)	-11(1)	-5(1)
C(30)	48(2)	45(2)	33(1)	-11(1)	-8(1)	4(1)
C(31)	40(2)	36(1)	29(1)	-10(1)	-9(1)	10(1)
C(32)	50(2)	41(2)	37(2)	-8(1)	-14(1)	11(1)
C(33)	57(2)	63(2)	48(2)	-7(2)	-22(2)	25(2)
C(34)	37(2)	95(3)	61(2)	-16(2)	-12(2)	21(2)
C(35)	43(2)	80(2)	60(2)	-2(2)	0(2)	5(2)
C(36)	45(2)	51(2)	41(2)	1(1)	-5(1)	12(1)
C(37)	95(4)	116(4)	100(4)	-50(3)	6(3)	-36(3)
C(38)	103(4)	153(5)	65(3)	-53(3)	20(3)	-38(3)
C(39)	101(4)	159(5)	83(3)	-54(3)	11(3)	-29(4)
C(40)	111(9)	92(6)	102(7)	-34(5)	-38(6)	23(6)

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Table 1. Crystal data and structure refinement for **3**.

Identification code	shelxs1572	
Empirical formula	C86 H78 Ga2 O10 Si6	
Formula weight	1579.46	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.184(2) Å	α= 67.46(3)°.
	b = 13.513(3) Å	β= 74.13(3)°.
	c = 17.014(3) Å	γ = 80.54(3)°.
Volume	2075.4(7) Å^3	
Z	1	
Density (calculated)	1.264 Mg/m^3	
Absorption coefficient	0.791 mm^{-1}	
F(000)	820	
Crystal size	0.6 x 0.4 x 0.3 mm^3	
Theta range for data collection	2.45 to 24.05°.	
Index ranges	-10<=h<=10, -15<=k<=15, -19<=l<=19	
Reflections collected	13059	
Independent reflections	6060 [R(int) = 0.0368]	
Completeness to theta = 24.05°	92.2 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6060 / 0 / 454	
Goodness-of-fit on F^2	0.898	
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.1347	
R indices (all data)	R1 = 0.0511, wR2 = 0.1420	
Largest diff. peak and hole	0.965 and -0.607 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for shelxs1572. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	9237(1)	9372(1)	5855(1)	26(1)
Si(1)	7487(1)	10480(1)	7250(1)	30(1)
Si(2)	8270(1)	8344(1)	8669(1)	32(1)
Si(3)	8847(1)	7123(1)	7291(1)	32(1)
O(1)	7910(3)	9992(2)	6477(2)	33(1)
O(2)	7886(3)	9615(2)	8150(2)	38(1)
O(3)	8699(3)	7682(2)	8011(2)	40(1)
O(4)	9522(3)	7941(2)	6323(2)	36(1)
O(5)	10895(2)	10084(2)	5328(1)	29(1)
C(1)	5600(4)	10801(3)	7470(2)	34(1)
C(2)	5050(5)	11777(4)	6957(3)	52(1)
C(3)	3643(5)	12026(4)	7079(3)	65(1)
C(4)	2758(5)	11317(4)	7714(4)	63(1)
C(5)	3249(5)	10347(4)	8243(3)	62(1)
C(6)	4660(4)	10089(3)	8121(3)	47(1)
C(7)	8430(4)	11724(3)	6902(3)	37(1)
C(8)	8570(5)	12139(4)	7505(3)	49(1)
C(9)	9277(6)	13057(4)	7246(4)	67(1)
C(10)	9865(6)	13567(4)	6369(4)	74(2)
C(11)	9744(6)	13180(4)	5763(4)	72(2)
C(12)	9022(5)	12264(3)	6021(3)	51(1)
C(13)	6768(4)	7768(3)	9570(2)	38(1)
C(14)	6062(5)	8335(4)	10117(3)	52(1)
C(15)	5035(5)	7887(5)	10847(3)	60(1)
C(16)	4700(5)	6860(5)	11050(3)	63(1)
C(17)	5342(6)	6280(4)	10523(3)	67(1)
C(18)	6393(5)	6734(4)	9784(3)	54(1)
C(19)	7088(4)	6836(3)	7355(2)	38(1)
C(20)	5982(5)	7580(4)	7475(3)	51(1)
C(21)	4649(5)	7418(4)	7521(3)	62(1)
C(22)	4380(6)	6502(5)	7438(4)	72(2)

C(23)	5427(7)	5751(4)	7317(4)	76(2)
C(24)	6767(6)	5910(4)	7277(3)	60(1)
C(25)	10032(4)	5891(3)	7576(2)	37(1)
C(26)	11160(4)	5683(3)	6967(3)	43(1)
C(27)	12079(5)	4783(3)	7216(3)	53(1)
C(28)	11892(5)	4095(3)	8068(3)	53(1)
C(29)	10781(6)	4285(4)	8683(3)	65(1)
C(30)	9867(5)	5163(3)	8439(3)	59(1)
C(31)	9739(4)	8207(3)	9167(2)	38(1)
C(32)	9627(5)	8684(4)	9782(3)	52(1)
C(33)	10634(6)	8501(4)	10237(3)	66(1)
C(34)	11778(7)	7855(5)	10078(4)	77(2)
C(35)	11926(6)	7372(5)	9474(4)	76(2)
C(36)	10915(5)	7554(4)	9018(3)	57(1)
C(37)	12122(4)	9905(3)	5680(2)	39(1)
C(38)	11618(5)	9715(4)	6651(3)	54(1)
C(39)	12882(6)	10935(5)	5199(4)	70(2)
C(40)	12965(5)	8926(4)	5523(3)	60(1)
C(41)	5885(12)	14255(9)	5037(7)	138(3)
C(42)	6418(15)	15039(11)	5201(9)	176(5)
C(43)	4869(16)	14004(11)	4865(9)	172(4)

Table 3. Bond lengths [Å] and angles [°] for shelxs1572.

Ga(1)-O(1)	1.782(2)	C(11)-C(12)	1.404(7)
Ga(1)-O(4)	1.795(2)	C(13)-C(18)	1.394(6)
Ga(1)-O(5)#1	1.894(2)	C(13)-C(14)	1.403(6)
Ga(1)-O(5)	1.904(3)	C(14)-C(15)	1.387(7)
Ga(1)-Ga(1)#1	2.8920(14)	C(15)-C(16)	1.373(8)
Si(1)-O(1)	1.615(2)	C(16)-C(17)	1.377(8)
Si(1)-O(2)	1.640(3)	C(17)-C(18)	1.411(7)
Si(1)-C(1)	1.866(4)	C(19)-C(24)	1.406(6)
Si(1)-C(7)	1.885(4)	C(19)-C(20)	1.407(6)
Si(2)-O(3)	1.617(3)	C(20)-C(21)	1.387(7)
Si(2)-O(2)	1.640(3)	C(21)-C(22)	1.375(8)
Si(2)-C(31)	1.863(4)	C(22)-C(23)	1.377(8)
Si(2)-C(13)	1.868(4)	C(23)-C(24)	1.396(8)
Si(3)-O(4)	1.625(3)	C(25)-C(26)	1.392(6)
Si(3)-O(3)	1.633(3)	C(25)-C(30)	1.402(6)
Si(3)-C(19)	1.860(4)	C(26)-C(27)	1.408(6)
Si(3)-C(25)	1.872(4)	C(27)-C(28)	1.369(7)
O(5)-C(37)	1.476(4)	C(28)-C(29)	1.380(7)
O(5)-Ga(1)#1	1.894(2)	C(29)-C(30)	1.386(6)
C(1)-C(2)	1.399(6)	C(31)-C(36)	1.392(6)
C(1)-C(6)	1.405(6)	C(31)-C(32)	1.396(6)
C(2)-C(3)	1.394(7)	C(32)-C(33)	1.384(7)
C(3)-C(4)	1.362(8)	C(33)-C(34)	1.367(8)
C(4)-C(5)	1.380(7)	C(34)-C(35)	1.379(8)
C(5)-C(6)	1.399(7)	C(35)-C(36)	1.389(7)
C(7)-C(8)	1.390(6)	C(37)-C(38)	1.520(5)
C(7)-C(12)	1.397(6)	C(37)-C(40)	1.526(6)
C(8)-C(9)	1.397(7)	C(37)-C(39)	1.530(6)
C(9)-C(10)	1.385(8)	C(41)-C(43)	1.277(15)
C(10)-C(11)	1.363(8)	C(41)-C(42)	1.411(15)
		C(42)-C(43)#2	1.678(17)
		C(43)-C(42)#2	1.678(17)
O(1)-Ga(1)-O(4)	116.73(11)	O(1)-Ga(1)-O(5)#1	110.10(11)

O(4)-Ga(1)-O(5)#1	115.42(11)	C(3)-C(2)-C(1)	121.7(4)
O(1)-Ga(1)-O(5)	115.94(11)	C(4)-C(3)-C(2)	120.3(5)
O(4)-Ga(1)-O(5)	112.72(12)	C(3)-C(4)-C(5)	120.2(5)
O(5)#1-Ga(1)-O(5)	80.82(11)	C(4)-C(5)-C(6)	119.9(5)
O(1)-Ga(1)-Ga(1)#1	120.86(8)	C(5)-C(6)-C(1)	121.4(4)
O(4)-Ga(1)-Ga(1)#1	122.37(8)	C(8)-C(7)-C(12)	117.4(4)
O(5)#1-Ga(1)-Ga(1)#1	40.54(7)	C(8)-C(7)-Si(1)	121.7(3)
O(5)-Ga(1)-Ga(1)#1	40.28(7)	C(12)-C(7)-Si(1)	120.9(3)
O(1)-Si(1)-O(2)	111.19(13)	C(7)-C(8)-C(9)	121.6(4)
O(1)-Si(1)-C(1)	108.26(15)	C(10)-C(9)-C(8)	119.6(5)
O(2)-Si(1)-C(1)	108.91(16)	C(11)-C(10)-C(9)	120.1(5)
O(1)-Si(1)-C(7)	109.45(16)	C(10)-C(11)-C(12)	120.3(5)
O(2)-Si(1)-C(7)	108.22(16)	C(7)-C(12)-C(11)	120.9(4)
C(1)-Si(1)-C(7)	110.83(17)	C(18)-C(13)-C(14)	117.5(4)
O(3)-Si(2)-O(2)	111.12(13)	C(18)-C(13)-Si(2)	122.2(3)
O(3)-Si(2)-C(31)	108.02(17)	C(14)-C(13)-Si(2)	120.1(3)
O(2)-Si(2)-C(31)	110.06(16)	C(15)-C(14)-C(13)	121.7(5)
O(3)-Si(2)-C(13)	110.58(17)	C(16)-C(15)-C(14)	119.7(5)
O(2)-Si(2)-C(13)	108.94(16)	C(15)-C(16)-C(17)	120.8(4)
C(31)-Si(2)-C(13)	108.08(17)	C(16)-C(17)-C(18)	119.5(5)
O(4)-Si(3)-O(3)	109.48(14)	C(13)-C(18)-C(17)	120.9(4)
O(4)-Si(3)-C(19)	111.15(16)	C(24)-C(19)-C(20)	116.0(4)
O(3)-Si(3)-C(19)	106.41(17)	C(24)-C(19)-Si(3)	124.2(3)
O(4)-Si(3)-C(25)	108.68(16)	C(20)-C(19)-Si(3)	119.9(3)
O(3)-Si(3)-C(25)	107.34(16)	C(21)-C(20)-C(19)	122.7(4)
C(19)-Si(3)-C(25)	113.64(18)	C(22)-C(21)-C(20)	119.5(5)
Si(1)-O(1)-Ga(1)	146.49(17)	C(21)-C(22)-C(23)	120.1(5)
Si(2)-O(2)-Si(1)	144.49(17)	C(22)-C(23)-C(24)	120.4(5)
Si(2)-O(3)-Si(3)	168.6(2)	C(23)-C(24)-C(19)	121.4(5)
Si(3)-O(4)-Ga(1)	129.12(15)	C(26)-C(25)-C(30)	116.7(4)
C(37)-O(5)-Ga(1)#1	128.7(2)	C(26)-C(25)-Si(3)	122.5(3)
C(37)-O(5)-Ga(1)	128.4(2)	C(30)-C(25)-Si(3)	120.7(3)
Ga(1)#1-O(5)-Ga(1)	99.19(11)	C(25)-C(26)-C(27)	121.1(4)
C(2)-C(1)-C(6)	116.6(4)	C(28)-C(27)-C(26)	120.6(4)
C(2)-C(1)-Si(1)	120.1(3)	C(27)-C(28)-C(29)	119.3(4)
C(6)-C(1)-Si(1)	123.3(3)	C(28)-C(29)-C(30)	120.2(4)

C(29)-C(30)-C(25)	122.1(4)
C(36)-C(31)-C(32)	117.4(4)
C(36)-C(31)-Si(2)	122.4(3)
C(32)-C(31)-Si(2)	119.8(3)
C(33)-C(32)-C(31)	121.4(5)
C(34)-C(33)-C(32)	119.9(5)
C(33)-C(34)-C(35)	120.3(5)
C(34)-C(35)-C(36)	119.8(5)
C(35)-C(36)-C(31)	121.1(5)
O(5)-C(37)-C(38)	106.7(3)
O(5)-C(37)-C(40)	108.0(3)
C(38)-C(37)-C(40)	111.5(4)
O(5)-C(37)-C(39)	106.4(3)
C(38)-C(37)-C(39)	110.9(4)
C(40)-C(37)-C(39)	112.8(4)
C(43)-C(41)-C(42)	145.9(12)
C(41)-C(42)-C(43)#2	102.0(11)
C(41)-C(43)-C(42)#2	112.1(11)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1 #2 -x+1,-y+3,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for shelxs1572. 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}
Ga(1)	28(1)	26(1)	20(1)	-5(1)	-3(1)	-1(1)
Si(1)	34(1)	29(1)	25(1)	-9(1)	-5(1)	3(1)
Si(2)	36(1)	34(1)	22(1)	-7(1)	-6(1)	1(1)
Si(3)	38(1)	26(1)	25(1)	-5(1)	-4(1)	0(1)
O(1)	32(2)	36(1)	27(1)	-12(1)	-2(1)	1(1)
O(2)	47(2)	35(1)	30(1)	-11(1)	-13(1)	6(1)
O(3)	49(2)	39(1)	32(1)	-13(1)	-7(1)	1(1)
O(4)	43(2)	28(1)	28(1)	-7(1)	0(1)	1(1)
O(5)	27(1)	36(1)	22(1)	-7(1)	-7(1)	-4(1)
C(1)	37(2)	36(2)	30(2)	-18(2)	-5(2)	5(2)
C(2)	44(3)	50(2)	49(2)	-11(2)	-6(2)	9(2)
C(3)	49(3)	62(3)	70(3)	-15(3)	-17(2)	21(2)
C(4)	36(3)	80(4)	78(3)	-41(3)	-11(2)	11(2)
C(5)	43(3)	68(3)	68(3)	-25(3)	3(2)	-6(2)
C(6)	39(3)	46(2)	46(2)	-12(2)	-6(2)	-1(2)
C(7)	36(2)	32(2)	44(2)	-15(2)	-13(2)	4(2)
C(8)	50(3)	53(3)	52(2)	-24(2)	-16(2)	-3(2)
C(9)	73(4)	63(3)	88(4)	-40(3)	-33(3)	-5(3)
C(10)	80(4)	50(3)	95(4)	-21(3)	-24(3)	-22(3)
C(11)	83(4)	50(3)	71(3)	-4(2)	-9(3)	-25(3)
C(12)	67(3)	41(2)	41(2)	-10(2)	-8(2)	-12(2)
C(13)	36(2)	46(2)	25(2)	-7(2)	-7(2)	-1(2)
C(14)	49(3)	67(3)	41(2)	-25(2)	-4(2)	-5(2)
C(15)	46(3)	95(4)	40(2)	-31(3)	-2(2)	-2(3)
C(16)	38(3)	92(4)	39(2)	-8(2)	3(2)	-9(2)
C(17)	54(3)	63(3)	63(3)	-4(2)	0(2)	-18(2)
C(18)	49(3)	54(3)	44(2)	-11(2)	4(2)	-8(2)
C(19)	42(2)	35(2)	30(2)	-5(2)	-7(2)	-7(2)
C(20)	48(3)	52(3)	52(3)	-18(2)	-10(2)	-2(2)
C(21)	39(3)	76(3)	65(3)	-19(3)	-14(2)	-2(2)
C(22)	60(4)	75(4)	73(4)	-3(3)	-30(3)	-15(3)

C(23)	81(5)	60(3)	99(4)	-19(3)	-42(3)	-25(3)
C(24)	65(4)	45(2)	73(3)	-19(2)	-26(3)	-1(2)
C(25)	42(2)	29(2)	35(2)	-8(2)	-9(2)	-1(2)
C(26)	50(3)	31(2)	42(2)	-11(2)	-10(2)	1(2)
C(27)	42(3)	44(2)	71(3)	-24(2)	-10(2)	5(2)
C(28)	54(3)	33(2)	69(3)	-11(2)	-29(2)	8(2)
C(29)	82(4)	46(3)	48(3)	2(2)	-19(3)	6(2)
C(30)	71(3)	41(2)	40(2)	-2(2)	-3(2)	12(2)
C(31)	37(2)	40(2)	30(2)	-1(2)	-9(2)	-5(2)
C(32)	56(3)	53(3)	53(3)	-17(2)	-23(2)	-7(2)
C(33)	68(4)	76(3)	63(3)	-20(3)	-31(3)	-14(3)
C(34)	66(4)	101(4)	61(3)	-8(3)	-35(3)	-17(3)
C(35)	44(3)	102(4)	64(3)	-12(3)	-19(2)	12(3)
C(36)	51(3)	74(3)	38(2)	-14(2)	-13(2)	8(2)
C(37)	32(2)	53(2)	31(2)	-11(2)	-13(2)	-3(2)
C(38)	47(3)	84(3)	35(2)	-21(2)	-18(2)	-1(2)
C(39)	51(3)	88(4)	69(3)	-7(3)	-24(3)	-33(3)
C(40)	44(3)	83(3)	51(3)	-24(2)	-20(2)	19(2)

Table 1. Crystal data and structure refinement for **4**.

Identification code	shelxs1531	
Empirical formula	C42 H46 Ga N O4 Si3	
Formula weight	782.79	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.332(2) Å	α= 85.14(3)°.
	b = 11.009(2) Å	β= 78.91(3)°.
	c = 21.428(4) Å	γ = 68.84(3)°.
Volume	2014.4(7) Å^3	
Z	2	
Density (calculated)	1.291 Mg/m^3	
Absorption coefficient	0.813 mm^{-1}	
F(000)	820	
Crystal size	0.6 x 0.5 x 0.3	
Theta range for data collection	1.94 to 22.50°.	
Index ranges	-9<=h<=10, -11<=k<=11, 0<=l<=23	
Reflections collected	5250	
Independent reflections	5250 [R(int) = 0.0000]	
Completeness to theta = 22.50°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5250 / 0 / 460	
Goodness-of-fit on F^2	1.399	
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1664	
R indices (all data)	R1 = 0.0878, wR2 = 0.1858	
Largest diff. peak and hole	1.772 and -0.496 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for shelxs1531. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	860(1)	7684(1)	3266(1)	56(1)
Si(1)	908(2)	7735(1)	1801(1)	40(1)
Si(2)	2122(2)	4788(1)	1825(1)	37(1)
Si(3)	1392(2)	4614(2)	3305(1)	44(1)
O(1)	1530(4)	7864(3)	2430(2)	48(1)
O(2)	933(4)	6257(3)	1747(2)	47(1)
O(3)	1835(4)	4286(4)	2553(2)	47(1)
O(4)	1499(5)	5953(4)	3467(2)	58(1)
C(1)	-1136(6)	8866(5)	1814(2)	44(1)
C(2)	-1468(7)	10186(6)	1883(3)	66(2)
C(3)	-2926(9)	11079(7)	1873(4)	84(2)
C(4)	-4070(9)	10707(10)	1804(4)	91(3)
C(5)	-3816(9)	9459(11)	1736(4)	101(3)
C(6)	-2332(8)	8497(7)	1750(4)	81(2)
C(7)	2163(6)	8103(5)	1079(3)	43(1)
C(8)	3687(7)	7974(6)	1079(3)	61(2)
C(9)	4601(8)	8220(7)	535(4)	79(2)
C(10)	4066(10)	8568(8)	-11(4)	83(2)
C(11)	2538(11)	8711(8)	-26(3)	84(2)
C(12)	1622(8)	8470(6)	515(3)	63(2)
C(13)	1749(5)	3736(5)	1293(3)	37(1)
C(14)	1492(7)	4158(6)	687(3)	52(2)
C(15)	1312(8)	3365(8)	267(3)	74(2)
C(16)	1378(8)	2147(8)	447(5)	82(2)
C(17)	1591(8)	1708(6)	1042(5)	75(2)
C(18)	1786(6)	2493(6)	1469(3)	55(2)
C(19)	4182(6)	4713(5)	1619(3)	40(1)
C(20)	5059(7)	4374(6)	1018(3)	58(2)
C(21)	6569(8)	4349(7)	875(4)	77(2)
C(22)	7218(8)	4669(8)	1315(4)	83(2)
C(23)	6389(8)	5005(7)	1909(4)	74(2)

C(24)	4885(7)	5006(6)	2064(3)	57(2)
C(25)	2810(7)	3256(5)	3689(3)	47(1)
C(26)	2560(10)	2990(8)	4329(4)	86(2)
C(27)	3594(12)	2016(9)	4638(4)	109(3)
C(28)	4951(11)	1251(8)	4288(5)	92(3)
C(29)	5239(8)	1472(7)	3655(5)	82(2)
C(30)	4195(7)	2448(6)	3353(3)	66(2)
C(31)	-611(7)	4557(6)	3581(3)	51(2)
C(32)	-1204(8)	3894(7)	3251(4)	72(2)
C(33)	-2638(9)	3772(9)	3479(4)	93(3)
C(34)	-3467(9)	4330(10)	4020(5)	101(3)
C(35)	-2957(10)	5015(9)	4354(4)	102(3)
C(36)	-1528(8)	5160(7)	4141(4)	81(2)
N(1)	2380(7)	8224(5)	3657(3)	71(2)
C(37)	3958(8)	7597(7)	3279(4)	78(2)
C(38)	5289(10)	7972(9)	3449(5)	117(3)
C(39)	2413(14)	7645(10)	4337(5)	116(3)
C(40)	917(17)	7958(11)	4772(5)	164(5)
C(41)	1897(11)	9640(8)	3688(5)	106(3)
C(42)	1880(13)	10321(9)	3063(5)	124(4)

Table 3. Bond lengths [Å] and angles [°] for shelxs1531.

Ga(1)-O(1)	1.798(4)
Ga(1)-O(4)	1.820(4)
Ga(1)-N(1)	2.054(6)
Si(1)-O(1)	1.603(4)
Si(1)-O(2)	1.633(4)
Si(1)-C(1)	1.861(6)
Si(1)-C(7)	1.863(5)
Si(2)-O(2)	1.613(4)
Si(2)-O(3)	1.617(4)
Si(2)-C(13)	1.851(5)
Si(2)-C(19)	1.860(5)
Si(3)-O(4)	1.585(4)
Si(3)-O(3)	1.621(4)
Si(3)-C(25)	1.857(6)
Si(3)-C(31)	1.870(6)
C(1)-C(6)	1.351(8)
C(1)-C(2)	1.386(8)
C(2)-C(3)	1.364(9)
C(3)-C(4)	1.310(11)
C(4)-C(5)	1.324(11)
C(5)-C(6)	1.412(11)
C(7)-C(12)	1.371(8)
C(7)-C(8)	1.377(8)
C(8)-C(9)	1.375(9)
C(9)-C(10)	1.331(10)
C(10)-C(11)	1.384(11)
C(11)-C(12)	1.370(9)
C(13)-C(14)	1.377(8)
C(13)-C(18)	1.378(7)
C(14)-C(15)	1.378(9)
C(15)-C(16)	1.347(10)
C(16)-C(17)	1.350(10)
C(17)-C(18)	1.389(9)
C(19)-C(24)	1.373(8)
C(19)-C(20)	1.387(8)
C(20)-C(21)	1.373(9)
C(21)-C(22)	1.346(10)
C(22)-C(23)	1.359(10)
C(23)-C(24)	1.379(9)
C(25)-C(26)	1.370(9)
C(25)-C(30)	1.378(8)
C(26)-C(27)	1.377(11)
C(27)-C(28)	1.359(12)
C(28)-C(29)	1.350(11)
C(29)-C(30)	1.376(10)
C(31)-C(32)	1.367(9)
C(31)-C(36)	1.395(9)
C(32)-C(33)	1.383(9)
C(33)-C(34)	1.324(12)
C(34)-C(35)	1.337(12)
C(35)-C(36)	1.386(11)
N(1)-C(41)	1.461(9)
N(1)-C(37)	1.484(9)
N(1)-C(39)	1.540(10)
C(37)-C(38)	1.554(9)
C(39)-C(40)	1.465(14)
C(41)-C(42)	1.478(11)

O(1)-Ga(1)-O(4)	108.17(17)
O(1)-Ga(1)-N(1)	101.3(2)
O(4)-Ga(1)-N(1)	100.4(2)
O(1)-Si(1)-O(2)	110.3(2)
O(1)-Si(1)-C(1)	111.2(2)
O(2)-Si(1)-C(1)	107.6(2)
O(1)-Si(1)-C(7)	110.5(2)
O(2)-Si(1)-C(7)	108.4(2)

C(1)-Si(1)-C(7)	108.7(2)	C(13)-C(14)-C(15)	121.7(6)
O(2)-Si(2)-O(3)	110.0(2)	C(16)-C(15)-C(14)	119.9(7)
O(2)-Si(2)-C(13)	107.9(2)	C(15)-C(16)-C(17)	120.2(7)
O(3)-Si(2)-C(13)	109.7(2)	C(16)-C(17)-C(18)	120.5(7)
O(2)-Si(2)-C(19)	110.8(2)	C(13)-C(18)-C(17)	120.4(6)
O(3)-Si(2)-C(19)	107.8(2)	C(24)-C(19)-C(20)	117.5(5)
C(13)-Si(2)-C(19)	110.5(2)	C(24)-C(19)-Si(2)	120.5(4)
O(4)-Si(3)-O(3)	114.3(2)	C(20)-C(19)-Si(2)	121.9(4)
O(4)-Si(3)-C(25)	109.3(2)	C(21)-C(20)-C(19)	120.8(6)
O(3)-Si(3)-C(25)	105.4(2)	C(22)-C(21)-C(20)	120.4(7)
O(4)-Si(3)-C(31)	112.0(3)	C(21)-C(22)-C(23)	120.1(6)
O(3)-Si(3)-C(31)	106.3(2)	C(22)-C(23)-C(24)	120.1(7)
C(25)-Si(3)-C(31)	109.1(3)	C(19)-C(24)-C(23)	120.9(6)
Si(1)-O(1)-Ga(1)	133.6(2)	C(26)-C(25)-C(30)	115.1(6)
Si(2)-O(2)-Si(1)	137.4(2)	C(26)-C(25)-Si(3)	122.4(5)
Si(2)-O(3)-Si(3)	148.6(3)	C(30)-C(25)-Si(3)	122.5(5)
Si(3)-O(4)-Ga(1)	143.1(3)	C(25)-C(26)-C(27)	124.5(8)
C(6)-C(1)-C(2)	117.0(6)	C(28)-C(27)-C(26)	118.3(8)
C(6)-C(1)-Si(1)	124.5(5)	C(29)-C(28)-C(27)	119.2(8)
C(2)-C(1)-Si(1)	118.4(4)	C(28)-C(29)-C(30)	121.8(8)
C(3)-C(2)-C(1)	121.7(7)	C(29)-C(30)-C(25)	121.1(7)
C(4)-C(3)-C(2)	120.5(8)	C(32)-C(31)-C(36)	117.9(6)
C(3)-C(4)-C(5)	120.2(8)	C(32)-C(31)-Si(3)	121.3(5)
C(4)-C(5)-C(6)	121.4(8)	C(36)-C(31)-Si(3)	120.8(5)
C(1)-C(6)-C(5)	119.1(7)	C(31)-C(32)-C(33)	121.3(7)
C(12)-C(7)-C(8)	117.0(6)	C(34)-C(33)-C(32)	119.4(8)
C(12)-C(7)-Si(1)	121.2(4)	C(33)-C(34)-C(35)	121.7(8)
C(8)-C(7)-Si(1)	121.8(5)	C(34)-C(35)-C(36)	120.6(8)
C(9)-C(8)-C(7)	120.6(7)	C(35)-C(36)-C(31)	119.0(8)
C(10)-C(9)-C(8)	121.8(7)	C(41)-N(1)-C(37)	113.8(6)
C(9)-C(10)-C(11)	119.0(7)	C(41)-N(1)-C(39)	108.9(6)
C(12)-C(11)-C(10)	119.4(7)	C(37)-N(1)-C(39)	107.2(7)
C(11)-C(12)-C(7)	122.2(7)	C(41)-N(1)-Ga(1)	111.5(5)
C(14)-C(13)-C(18)	117.3(5)	C(37)-N(1)-Ga(1)	106.9(4)
C(14)-C(13)-Si(2)	120.3(4)	C(39)-N(1)-Ga(1)	108.4(5)
C(18)-C(13)-Si(2)	122.3(4)	N(1)-C(37)-C(38)	116.2(7)

C(40)-C(39)-N(1)	117.1(9)	Symmetry transformations used to generate
N(1)-C(41)-C(42)	114.7(7)	equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for shelxs1531. 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}
Ga(1)	54(1)	51(1)	58(1)	-11(1)	1(1)	-17(1)
Si(1)	33(1)	36(1)	50(1)	-3(1)	-2(1)	-13(1)
Si(2)	31(1)	38(1)	42(1)	-6(1)	2(1)	-17(1)
Si(3)	44(1)	47(1)	42(1)	-2(1)	3(1)	-22(1)
O(1)	44(2)	46(2)	57(2)	-1(2)	-9(2)	-20(2)
O(2)	37(2)	39(2)	65(3)	-9(2)	-2(2)	-15(2)
O(3)	46(2)	55(2)	45(2)	-5(2)	1(2)	-25(2)
O(4)	72(3)	54(2)	52(2)	0(2)	-6(2)	-30(2)
C(1)	38(3)	51(4)	42(3)	-6(3)	-1(3)	-15(3)
C(2)	47(4)	52(4)	83(5)	-2(3)	4(3)	-8(3)
C(3)	59(5)	61(5)	95(6)	2(4)	10(4)	10(4)
C(4)	46(5)	103(7)	96(6)	-19(5)	-8(4)	7(5)
C(5)	38(5)	146(9)	121(7)	-34(6)	-10(4)	-29(5)
C(6)	51(4)	82(5)	116(7)	-28(4)	-5(4)	-28(4)
C(7)	37(3)	36(3)	54(4)	-9(3)	3(3)	-14(2)
C(8)	49(4)	65(4)	68(4)	7(3)	-1(3)	-26(3)
C(9)	48(4)	85(5)	98(6)	0(5)	7(4)	-28(4)
C(10)	80(6)	87(6)	71(6)	-6(4)	25(5)	-35(5)
C(11)	114(7)	96(6)	37(4)	-4(4)	0(4)	-39(5)
C(12)	57(4)	73(5)	60(4)	-11(3)	-2(3)	-29(3)
C(13)	23(3)	34(3)	51(4)	-8(2)	5(2)	-9(2)
C(14)	47(4)	55(4)	54(4)	-7(3)	-6(3)	-17(3)
C(15)	58(4)	97(6)	61(5)	-28(4)	-13(3)	-15(4)
C(16)	51(4)	86(6)	111(7)	-55(5)	-13(4)	-18(4)
C(17)	58(4)	46(4)	126(7)	-21(4)	-11(4)	-24(3)
C(18)	41(3)	50(4)	73(4)	-9(3)	0(3)	-18(3)
C(19)	32(3)	38(3)	51(4)	-1(2)	0(3)	-17(2)
C(20)	42(4)	75(4)	60(4)	-9(3)	7(3)	-30(3)
C(21)	50(4)	86(5)	81(5)	-9(4)	22(4)	-21(4)
C(22)	38(4)	96(6)	116(7)	0(5)	-3(4)	-30(4)
C(23)	52(4)	82(5)	100(6)	1(4)	-25(4)	-33(4)

C(24)	48(4)	66(4)	64(4)	-6(3)	-7(3)	-27(3)
C(25)	58(4)	47(3)	42(4)	-1(3)	-4(3)	-27(3)
C(26)	89(6)	88(6)	61(5)	-3(4)	-5(4)	-9(5)
C(27)	129(8)	99(7)	73(6)	21(5)	-24(6)	-13(6)
C(28)	100(7)	78(6)	106(7)	26(5)	-52(6)	-30(5)
C(29)	53(4)	67(5)	118(7)	9(5)	-11(5)	-16(4)
C(30)	52(4)	63(4)	79(5)	3(4)	-2(4)	-23(4)
C(31)	39(3)	53(4)	56(4)	6(3)	5(3)	-18(3)
C(32)	54(4)	84(5)	82(5)	-8(4)	5(4)	-36(4)
C(33)	59(5)	127(7)	106(7)	8(6)	-5(5)	-56(5)
C(34)	49(5)	123(8)	127(8)	24(6)	9(5)	-44(5)
C(35)	71(6)	113(7)	95(7)	-8(5)	35(5)	-23(5)
C(36)	66(5)	85(5)	80(5)	-12(4)	28(4)	-29(4)
N(1)	97(5)	56(3)	64(4)	-8(3)	-22(3)	-28(3)
C(37)	71(5)	66(5)	102(6)	-15(4)	-22(4)	-26(4)
C(38)	97(7)	122(8)	166(10)	9(6)	-66(7)	-61(6)
C(39)	162(10)	115(8)	94(7)	-5(6)	-37(7)	-69(7)
C(40)	245(16)	122(9)	86(7)	-6(6)	25(9)	-43(9)
C(41)	126(8)	65(5)	138(9)	-25(5)	-38(6)	-32(5)
C(42)	202(12)	82(6)	127(8)	20(6)	-63(8)	-84(7)

Table 2. Crystal data and structure refinement for 5.

Identification code	sh1543	
Empirical formula	C78 H76 Ga N O8 Si6 x 0.5 C4 H8 O	
Formula weight	1429.71	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/c	
Unit cell dimensions	a = 27.764(6) Å	α= 90°.
	b = 13.641(3) Å	β= 92.38(3)°.
	c = 21.844(4) Å	γ = 90°.
Volume	8266(3) $Å^3$	
Z	4	
Density (calculated)	1.149 Mg/m^3	
Absorption coefficient	0.471 mm^{-1}	
F(000)	3000	
Crystal size	0.6 x 0.5 x 0.3 mm^3	
Theta range for data collection	1.89 to 24.06°.	
Index ranges	-31<=h<=31, -15<=k<=15, -24<=l<=22	
Reflections collected	49309	
Independent reflections	12759 [R(int) = 0.0591]	
Completeness to theta = 24.06°	97.4 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12759 / 0 / 938	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0559, wR2 = 0.1806	
R indices (all data)	R1 = 0.0876, wR2 = 0.1965	
Largest diff. peak and hole	1.047 and -0.485 $e.Å^{-3}$	

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	7306(1)	3417(1)	665(1)	29(1)
Si(1)	8242(1)	4635(1)	1107(1)	33(1)
Si(2)	8844(1)	3391(1)	233(1)	33(1)
Si(3)	8127(1)	1724(1)	546(1)	32(1)
Si(4)	6414(1)	3180(1)	1581(1)	34(1)
Si(5)	5976(1)	1974(1)	551(1)	33(1)
Si(6)	6514(1)	3312(1)	-405(1)	33(1)
O(1)	7691(1)	4445(2)	897(2)	38(1)
O(2)	8616(1)	4325(2)	579(2)	43(1)
O(3)	8621(1)	2373(2)	472(2)	38(1)
O(4)	7649(1)	2366(2)	439(2)	41(1)
O(5)	6928(1)	3081(3)	1291(2)	41(1)
O(6)	5976(1)	2710(2)	1138(2)	41(1)
O(7)	6239(1)	2491(2)	-12(2)	40(1)
O(8)	6932(1)	3861(2)	-5(2)	35(1)
C(1)	8409(2)	3936(3)	1820(2)	38(1)
C(2)	8067(2)	3448(4)	2156(3)	47(1)
C(3)	8198(2)	2894(4)	2668(3)	58(2)
C(4)	8678(3)	2822(5)	2858(3)	68(2)
C(5)	9017(3)	3300(5)	2549(4)	76(2)
C(6)	8887(2)	3850(5)	2029(3)	62(2)
C(7)	8323(2)	5989(3)	1211(2)	38(1)
C(8)	7994(2)	6541(4)	1531(3)	51(1)
C(9)	8035(3)	7544(4)	1588(3)	66(2)
C(10)	8412(3)	8026(5)	1338(4)	86(2)
C(11)	8742(3)	7519(5)	1025(5)	102(3)
C(12)	8699(3)	6499(5)	966(4)	75(2)
C(13)	9505(2)	3359(4)	406(3)	44(1)
C(14A)	9787(5)	2649(14)	104(11)	97(7)
C(15A)	10295(6)	2587(17)	194(12)	112(7)
C(17A)	10280(7)	3820(20)	908(9)	90(5)

C(18A)	9768(5)	3950(14)	788(10)	80(5)
C(14B)	9717(7)	2665(17)	699(17)	149(12)
C(15B)	10237(7)	2659(17)	831(17)	151(12)
C(17B)	10270(6)	4229(15)	531(15)	134(11)
C(18B)	9771(7)	4243(17)	378(15)	139(12)
C(16)	10516(3)	3296(10)	637(6)	108(4)
C(19)	8717(2)	3525(4)	-606(2)	43(1)
C(20)	8647(2)	4422(5)	-886(3)	59(2)
C(21)	8583(3)	4522(7)	-1518(4)	84(2)
C(22)	8592(3)	3712(7)	-1882(4)	85(2)
C(23)	8647(3)	2807(7)	-1628(3)	87(2)
C(24)	8710(3)	2706(5)	-999(3)	65(2)
C(25)	8192(2)	1153(3)	1318(2)	38(1)
C(26)	7791(2)	801(4)	1616(3)	54(2)
C(27)	7845(3)	304(5)	2168(3)	73(2)
C(28)	8287(4)	136(5)	2431(3)	82(2)
C(29)	8695(3)	477(5)	2153(3)	74(2)
C(30)	8644(2)	986(4)	1604(3)	54(2)
C(31)	8130(2)	739(3)	-45(2)	35(1)
C(32)	8455(2)	-35(4)	-10(3)	61(2)
C(33)	8466(3)	-740(5)	-468(4)	84(2)
C(34)	8150(3)	-691(5)	-962(3)	74(2)
C(35)	7821(3)	53(5)	-1006(3)	66(2)
C(36)	7810(2)	752(4)	-550(3)	51(1)
C(37)	6247(2)	4481(4)	1732(2)	40(1)
C(38)	6594(2)	5129(4)	1974(3)	58(2)
C(39)	6481(3)	6086(5)	2123(3)	77(2)
C(40)	6016(4)	6419(5)	2025(4)	88(3)
C(41)	5668(3)	5800(5)	1769(4)	90(2)
C(42)	5783(2)	4848(5)	1623(3)	68(2)
C(43)	6420(2)	2489(4)	2319(2)	40(1)
C(44)	6828(2)	1994(4)	2543(3)	53(1)
C(45)	6827(3)	1462(5)	3089(3)	71(2)
C(46)	6423(3)	1426(5)	3417(3)	74(2)
C(47)	6023(3)	1927(6)	3223(4)	83(2)
C(48)	6018(2)	2444(5)	2673(3)	64(2)

C(49)	5337(2)	1723(4)	297(2)	39(1)
C(50)	5124(2)	2173(4)	-218(3)	61(2)
C(51)	4644(2)	1979(6)	-404(4)	78(2)
C(52)	4374(2)	1328(5)	-92(4)	66(2)
C(53)	4579(2)	858(5)	418(3)	67(2)
C(54)	5053(2)	1052(5)	613(3)	58(2)
C(55)	6317(2)	830(3)	743(2)	38(1)
C(56)	6663(2)	469(4)	363(3)	52(2)
C(57)	6919(2)	-383(4)	496(4)	68(2)
C(58)	6832(3)	-893(5)	1010(4)	75(2)
C(59)	6493(3)	-577(5)	1405(4)	78(2)
C(60)	6227(2)	302(4)	1281(3)	59(2)
C(61)	6055(2)	4261(4)	-660(2)	41(1)
C(62)	5813(2)	4780(4)	-227(3)	59(2)
C(63)	5498(2)	5528(5)	-378(5)	83(2)
C(64)	5420(3)	5778(6)	-975(6)	102(3)
C(65)	5635(3)	5259(6)	-1427(5)	90(3)
C(66)	5956(2)	4501(5)	-1270(3)	61(2)
C(67)	6749(2)	2659(4)	-1076(2)	41(1)
C(68)	7197(2)	2843(5)	-1316(3)	55(2)
C(69)	7345(3)	2360(6)	-1831(3)	73(2)
C(70)	7056(3)	1676(5)	-2113(3)	72(2)
C(71)	6617(3)	1454(5)	-1889(3)	75(2)
C(72)	6467(2)	1944(5)	-1376(3)	61(2)
N(1)	7100(2)	5916(4)	-368(3)	67(2)
C(73)	7630(3)	5907(6)	-322(4)	101(3)
C(74)	7867(3)	6890(8)	-446(6)	140(5)
C(75)	6898(3)	6218(7)	-963(6)	129(5)
C(76)	7063(6)	5665(10)	-1474(5)	168(7)
C(77A)	7090(5)	6494(9)	292(7)	65(3)
C(77B)	6719(5)	6621(10)	-95(7)	68(4)
C(78)	6665(4)	6420(6)	530(4)	106(3)
O(9)	5000	9930(20)	2500	199(13)
C(79)	4827(12)	9340(20)	2062(14)	164(14)
C(80)	4926(11)	8470(20)	2184(12)	170(12)
C(81)	54(10)	6210(30)	3060(18)	182(13)

O(10)	0	6950(30)	2500	245(19)
C(82)	-16(12)	5365(19)	2775(13)	152(15)

Table 4. Bond lengths [Å] and angles [°] for 5.

Ga(1)-O(4)	1.801(3)
Ga(1)-O(5)	1.817(3)
Ga(1)-O(1)	1.822(3)
Ga(1)-O(8)	1.860(3)
Si(1)-O(1)	1.601(3)
Si(1)-O(2)	1.638(4)
Si(1)-C(1)	1.868(5)
Si(1)-C(7)	1.873(5)
Si(2)-O(3)	1.615(3)
Si(2)-O(2)	1.624(3)
Si(2)-C(13)	1.859(5)
Si(2)-C(19)	1.861(6)
Si(3)-O(4)	1.600(3)
Si(3)-O(3)	1.647(3)
Si(3)-C(25)	1.860(5)
Si(3)-C(31)	1.863(5)
Si(4)-O(5)	1.590(3)
Si(4)-O(6)	1.652(3)
Si(4)-C(43)	1.866(5)
Si(4)-C(37)	1.867(5)
Si(5)-O(7)	1.617(3)
Si(5)-O(6)	1.629(3)
Si(5)-C(55)	1.865(5)
Si(5)-C(49)	1.867(5)
Si(6)-O(8)	1.608(3)
Si(6)-O(7)	1.621(3)
Si(6)-C(67)	1.858(5)
Si(6)-C(61)	1.885(5)
C(1)-C(2)	1.392(7)
C(1)-C(6)	1.392(8)
C(2)-C(3)	1.386(8)
C(3)-C(4)	1.382(9)
C(4)-C(5)	1.351(10)
C(5)-C(6)	1.395(9)
C(7)-C(12)	1.379(8)
C(7)-C(8)	1.395(7)
C(8)-C(9)	1.378(8)
C(9)-C(10)	1.368(10)
C(10)-C(11)	1.356(11)
C(11)-C(12)	1.402(9)
C(13)-C(14B)	1.27(2)
C(13)-C(18A)	1.353(17)
C(13)-C(18B)	1.42(2)
C(13)-C(14A)	1.424(16)
C(14A)-C(15A)	1.42(2)
C(15A)-C(16)	1.48(2)
C(17A)-C(16)	1.15(2)
C(17A)-C(18A)	1.44(3)
C(14B)-C(15B)	1.46(3)
C(15B)-C(16)	1.25(2)
C(17B)-C(18B)	1.41(2)
C(17B)-C(16)	1.46(2)
C(19)-C(20)	1.378(8)
C(19)-C(24)	1.408(8)
C(20)-C(21)	1.393(10)
C(21)-C(22)	1.362(12)
C(22)-C(23)	1.360(12)
C(23)-C(24)	1.386(9)
C(25)-C(26)	1.396(7)
C(25)-C(30)	1.397(8)

C(26)-C(27)	1.387(9)	C(62)-C(63)	1.374(9)
C(27)-C(28)	1.352(11)	C(63)-C(64)	1.356(13)
C(28)-C(29)	1.387(11)	C(64)-C(65)	1.371(13)
C(29)-C(30)	1.388(9)	C(65)-C(66)	1.398(10)
C(31)-C(36)	1.387(7)	C(67)-C(68)	1.392(8)
C(31)-C(32)	1.389(7)	C(67)-C(72)	1.397(8)
C(32)-C(33)	1.388(9)	C(68)-C(69)	1.380(9)
C(33)-C(34)	1.365(10)	C(69)-C(70)	1.361(11)
C(34)-C(35)	1.367(10)	C(70)-C(71)	1.368(11)
C(35)-C(36)	1.381(8)	C(71)-C(72)	1.384(9)
C(37)-C(42)	1.392(8)	N(1)-C(75)	1.455(11)
C(37)-C(38)	1.395(7)	N(1)-C(73)	1.470(10)
C(38)-C(39)	1.386(9)	N(1)-C(77B)	1.567(15)
C(39)-C(40)	1.377(11)	N(1)-C(77A)	1.644(15)
C(40)-C(41)	1.384(11)	C(73)-C(74)	1.523(10)
C(41)-C(42)	1.378(9)	C(75)-C(76)	1.439(17)
C(43)-C(48)	1.384(8)	C(77A)-C(78)	1.313(16)
C(43)-C(44)	1.391(8)	C(77B)-C(78)	1.406(16)
C(44)-C(45)	1.398(9)	O(9)-C(79)#1	1.33(3)
C(45)-C(46)	1.358(10)	O(9)-C(79)	1.33(3)
C(46)-C(47)	1.356(11)	C(79)-C(80)	1.24(3)
C(47)-C(48)	1.392(9)	C(80)-C(80)#1	1.43(5)
C(49)-C(50)	1.394(8)	C(81)-C(82)	1.32(4)
C(49)-C(54)	1.407(8)	C(81)-O(10)	1.59(4)
C(50)-C(51)	1.401(8)	O(10)-C(81)#2	1.59(4)
C(51)-C(52)	1.363(10)	C(82)-C(82)#2	1.21(5)
C(52)-C(53)	1.387(10)		
C(53)-C(54)	1.394(8)	O(4)-Ga(1)-O(5)	109.55(16)
C(55)-C(56)	1.385(8)	O(4)-Ga(1)-O(1)	112.20(15)
C(55)-C(60)	1.410(8)	O(5)-Ga(1)-O(1)	109.60(16)
C(56)-C(57)	1.387(8)	O(4)-Ga(1)-O(8)	109.10(15)
C(57)-C(58)	1.351(10)	O(5)-Ga(1)-O(8)	110.72(15)
C(58)-C(59)	1.372(11)	O(1)-Ga(1)-O(8)	105.62(14)
C(59)-C(60)	1.428(9)	O(1)-Si(1)-O(2)	112.41(19)
C(61)-C(62)	1.379(8)	O(1)-Si(1)-C(1)	111.0(2)
C(61)-C(66)	1.389(8)	O(2)-Si(1)-C(1)	108.2(2)

O(1)-Si(1)-C(7)	107.7(2)	Si(3)-O(4)-Ga(1)	147.2(2)
O(2)-Si(1)-C(7)	105.3(2)	Si(4)-O(5)-Ga(1)	146.6(2)
C(1)-Si(1)-C(7)	112.2(2)	Si(5)-O(6)-Si(4)	132.7(2)
O(3)-Si(2)-O(2)	111.22(18)	Si(5)-O(7)-Si(6)	160.2(2)
O(3)-Si(2)-C(13)	107.6(2)	Si(6)-O(8)-Ga(1)	129.88(19)
O(2)-Si(2)-C(13)	108.9(2)	C(2)-C(1)-C(6)	116.7(5)
O(3)-Si(2)-C(19)	110.0(2)	C(2)-C(1)-Si(1)	122.2(4)
O(2)-Si(2)-C(19)	108.7(2)	C(6)-C(1)-Si(1)	121.1(4)
C(13)-Si(2)-C(19)	110.4(2)	C(3)-C(2)-C(1)	121.7(5)
O(4)-Si(3)-O(3)	112.33(18)	C(4)-C(3)-C(2)	119.9(6)
O(4)-Si(3)-C(25)	114.3(2)	C(5)-C(4)-C(3)	119.9(6)
O(3)-Si(3)-C(25)	105.4(2)	C(4)-C(5)-C(6)	120.4(6)
O(4)-Si(3)-C(31)	108.7(2)	C(1)-C(6)-C(5)	121.5(6)
O(3)-Si(3)-C(31)	107.0(2)	C(12)-C(7)-C(8)	116.4(5)
C(25)-Si(3)-C(31)	108.9(2)	C(12)-C(7)-Si(1)	122.6(4)
O(5)-Si(4)-O(6)	112.52(19)	C(8)-C(7)-Si(1)	121.0(4)
O(5)-Si(4)-C(43)	109.0(2)	C(9)-C(8)-C(7)	121.8(6)
O(6)-Si(4)-C(43)	106.8(2)	C(10)-C(9)-C(8)	120.2(6)
O(5)-Si(4)-C(37)	112.6(2)	C(11)-C(10)-C(9)	120.1(6)
O(6)-Si(4)-C(37)	106.9(2)	C(10)-C(11)-C(12)	119.6(7)
C(43)-Si(4)-C(37)	108.8(2)	C(7)-C(12)-C(11)	121.9(7)
O(7)-Si(5)-O(6)	110.11(18)	C(14B)-C(13)-C(18A)	84.7(17)
O(7)-Si(5)-C(55)	107.1(2)	C(14B)-C(13)-C(18B)	115.1(13)
O(6)-Si(5)-C(55)	110.7(2)	C(18A)-C(13)-C(18B)	41.4(12)
O(7)-Si(5)-C(49)	108.0(2)	C(14B)-C(13)-C(14A)	58.3(15)
O(6)-Si(5)-C(49)	108.5(2)	C(18A)-C(13)-C(14A)	113.4(10)
C(55)-Si(5)-C(49)	112.4(2)	C(18B)-C(13)-C(14A)	105.2(15)
O(8)-Si(6)-O(7)	112.32(18)	C(14B)-C(13)-Si(2)	123.4(9)
O(8)-Si(6)-C(67)	112.5(2)	C(18A)-C(13)-Si(2)	128.0(8)
O(7)-Si(6)-C(67)	106.0(2)	C(18B)-C(13)-Si(2)	118.9(9)
O(8)-Si(6)-C(61)	107.8(2)	C(14A)-C(13)-Si(2)	118.6(8)
O(7)-Si(6)-C(61)	107.7(2)	C(15A)-C(14A)-C(13)	122.6(15)
C(67)-Si(6)-C(61)	110.5(2)	C(14A)-C(15A)-C(16)	115.7(15)
Si(1)-O(1)-Ga(1)	138.4(2)	C(16)-C(17A)-C(18A)	123.8(17)
Si(2)-O(2)-Si(1)	143.2(2)	C(13)-C(18A)-C(17A)	122.9(15)
Si(2)-O(3)-Si(3)	145.7(2)	C(13)-C(14B)-C(15B)	122.4(16)