Table 1. Crystal data and structure refinement for 1.

Empirical formula	C40 H56 Al2 B2 O2
Formula weight	644.43
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 11.2190(2) A alpha = 90 deg b = 16.5510(5) A beta = 114.0490(13)deg c = 11.6130(4) A gamma = 90 deg
Volume	1969.19(10) A^3
Z, Calculated density	2, 1.087 Mg/m^3
Absorption coefficient	0.105 mm^-1
F(000)	696
Crystal size	0.92 x 0.30 x 0.40 mm
Theta range for data collection	2.13 to 27.52 deg.
Limiting indices	-14<=h<=14, -20<=k<=21, -15<=l<=15
Reflections collected / unique	8324 / 4506 [R(int) = 0.025]
Completeness to theta = 27.52	99.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4506 / 0 / 217
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0599, wR2 = 0.1435
R indices (all data)	R1 = 0.1171, wR2 = 0.1679
Extinction coefficient	0.047(5)
Largest diff. peak and hole	0.357 and -0.257 e.A^-3

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

	x	y	z	U(eq)
Al(1)	911(1)	-5(1)	4427(1)	66(1)
O(1)	-687(1)	476(1)	4208(1)	59(1)
B(1)	-1442(2)	1014(1)	3277(2)	55(1)
C(1)	2425(2)	677(2)	4812(2)	96(1)
C(2)	596(2)	-798(2)	3106(2)	86(1)
C(11)	-2987(2)	998(1)	2824(2)	53(1)
C(12)	-3648(2)	1682(1)	2976(2)	58(1)
C(121)	-2939(2)	2440(1)	3605(2)	80(1)
C(13)	-5006(2)	1668(1)	2561(2)	64(1)
C(14)	-5743(2)	1001(1)	1972(2)	64(1)
C(141)	-7214(2)	1013(2)	1516(2)	90(1)
C(15)	-5085(2)	336(1)	1816(2)	63(1)
C(16)	-3736(2)	319(1)	2226(2)	58(1)
C(161)	-3155(2)	-452(1)	1970(2)	74(1)
C(21)	-730(2)	1626(1)	2728(2)	55(1)
C(22)	-964(2)	1610(1)	1437(2)	59(1)
C(221)	-1751(2)	941(1)	592(2)	78(1)
C(23)	-434(2)	2200(1)	936(2)	65(1)
C(24)	325(2)	2821(1)	1659(2)	67(1)
C(241)	867(2)	3470(2)	1095(3)	98(1)
C(25)	586(2)	2821(1)	2924(2)	69(1)
C(26)	90(2)	2240(1)	3475(2)	62(1)
C(261)	434(2)	2330(2)	4877(2)	87(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

Al(1)-O(1)#1	1.8741(14)
Al(1)-O(1)	1.8821(13)
Al(1)-C(1)	1.933(2)
Al(1)-C(2)	1.939(3)
Al(1)-Al(1)#1	2.8585(12)
O(1)-B(1)	1.389(2)
O(1)-Al(1)#1	1.8741(14)
B(1)-C(21)	1.577(3)
B(1)-C(11)	1.593(3)
C(11)-C(12)	1.404(3)
C(11)-C(16)	1.405(3)
C(12)-C(13)	1.399(3)
C(12)-C(121)	1.505(3)
C(13)-C(14)	1.382(3)
C(14)-C(15)	1.379(3)
C(14)-C(141)	1.513(3)
C(15)-C(16)	1.389(2)
C(16)-C(161)	1.517(3)
C(21)-C(26)	1.407(3)
C(21)-C(22)	1.413(3)
C(22)-C(23)	1.389(3)
C(22)-C(221)	1.504(3)
C(23)-C(24)	1.379(3)
C(24)-C(25)	1.376(3)
C(24)-C(241)	1.509(3)
C(25)-C(26)	1.391(3)
C(26)-C(261)	1.520(3)
O(1)#1-Al(1)-O(1)	80.89(6)
O(1)#1-Al(1)-C(1)	117.09(9)
O(1)-Al(1)-C(1)	118.84(10)
O(1)#1-Al(1)-C(2)	110.09(9)
O(1)-Al(1)-C(2)	108.84(8)
C(1)-Al(1)-C(2)	116.00(11)
O(1)#1-Al(1)-Al(1)#1	40.55(4)
O(1)-Al(1)-Al(1)#1	40.34(4)
C(1)-Al(1)-Al(1)#1	128.04(9)
C(2)-Al(1)-Al(1)#1	115.96(8)
B(1)-O(1)-Al(1)#1	132.48(13)
B(1)-O(1)-Al(1)	128.41(13)
Al(1)#1-O(1)-Al(1)	99.11(6)
O(1)-B(1)-C(21)	118.51(16)
O(1)-B(1)-C(11)	118.87(17)
C(21)-B(1)-C(11)	122.61(16)
C(12)-C(11)-C(16)	117.81(17)
C(12)-C(11)-B(1)	120.32(17)
C(16)-C(11)-B(1)	121.83(17)
C(13)-C(12)-C(11)	120.05(18)
C(13)-C(12)-C(121)	117.83(18)
C(11)-C(12)-C(121)	122.11(17)
C(14)-C(13)-C(12)	122.13(19)
C(15)-C(14)-C(13)	117.31(18)
C(15)-C(14)-C(141)	122.0(2)
C(13)-C(14)-C(141)	120.7(2)
C(14)-C(15)-C(16)	122.52(19)
C(15)-C(16)-C(11)	120.18(18)
C(15)-C(16)-C(161)	116.35(18)

C(11)-C(16)-C(161)	123.46(17)
C(26)-C(21)-C(22)	117.41(17)
C(26)-C(21)-B(1)	121.76(17)
C(22)-C(21)-B(1)	120.70(17)
C(23)-C(22)-C(21)	120.32(18)
C(23)-C(22)-C(221)	118.83(18)
C(21)-C(22)-C(221)	120.82(18)
C(24)-C(23)-C(22)	122.2(2)
C(25)-C(24)-C(23)	117.37(19)
C(25)-C(24)-C(241)	121.0(2)
C(23)-C(24)-C(241)	121.6(2)
C(24)-C(25)-C(26)	122.7(2)
C(25)-C(26)-C(21)	119.92(19)
C(25)-C(26)-C(261)	116.80(18)
C(21)-C(26)-C(261)	123.23(18)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Al(1)	49(1)	76(1)	61(1)	16(1)	11(1)	0(1)
O(1)	50(1)	62(1)	50(1)	12(1)	5(1)	0(1)
B(1)	61(1)	48(1)	44(1)	-4(1)	9(1)	-1(1)
C(1)	64(1)	124(2)	90(2)	28(2)	20(1)	-15(1)
C(2)	72(1)	104(2)	79(2)	8(1)	28(1)	16(1)
C(11)	55(1)	50(1)	42(1)	6(1)	8(1)	3(1)
C(12)	67(1)	54(1)	46(1)	5(1)	17(1)	4(1)
C(121)	86(2)	60(1)	89(2)	-12(1)	31(1)	2(1)
C(13)	70(1)	63(1)	59(1)	8(1)	28(1)	14(1)
C(14)	57(1)	77(2)	53(1)	10(1)	16(1)	4(1)
C(141)	59(1)	117(2)	88(2)	1(2)	25(1)	8(1)
C(15)	55(1)	61(1)	57(1)	2(1)	9(1)	-3(1)
C(16)	56(1)	54(1)	50(1)	4(1)	8(1)	3(1)
C(161)	69(1)	57(1)	77(2)	-7(1)	12(1)	2(1)
C(21)	53(1)	54(1)	45(1)	3(1)	8(1)	2(1)
C(22)	53(1)	63(1)	51(1)	2(1)	11(1)	7(1)
C(221)	84(1)	80(2)	53(1)	-8(1)	10(1)	-3(1)
C(23)	61(1)	81(2)	54(1)	3(1)	23(1)	6(1)
C(24)	59(1)	76(2)	68(1)	10(1)	29(1)	4(1)
C(241)	91(2)	112(2)	103(2)	17(2)	53(2)	-17(2)
C(25)	64(1)	67(1)	72(2)	-10(1)	24(1)	-13(1)
C(26)	63(1)	63(1)	52(1)	-1(1)	16(1)	-7(1)
C(261)	99(2)	95(2)	54(1)	-14(1)	18(1)	-34(1)

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

	x	y	z	U(eq)
H(1A)	2507	1036	5489	144
H(1B)	2326	986	4080	144
H(1C)	3192	347	5059	144
H(2A)	1290	-1188	3377	129
H(2B)	560	-533	2357	129
H(2C)	-219	-1067	2929	129
H(12A)	-2268	2307	4415	120
H(12B)	-3544	2810	3713	120
H(12C)	-2553	2685	3091	120
H(13)	-5427	2123	2686	76
H(14A)	-7475	1499	1803	134
H(14B)	-7490	552	1846	134
H(14C)	-7609	997	612	134
H(15)	-5562	-120	1422	75
H(16A)	-3476	-907	2273	110
H(16B)	-2221	-431	2397	110
H(16C)	-3401	-507	1080	110
H(22A)	-1356	430	926	117
H(22B)	-1775	1012	-237	117
H(22C)	-2624	953	549	117
H(23)	-596	2176	85	78
H(24A)	1681	3292	1095	147
H(24B)	1006	3955	1587	147
H(24C)	259	3576	245	147
H(25)	1117	3226	3431	82
H(26A)	107	2836	5029	131
H(26B)	1365	2314	5334	131
H(26C)	47	1895	5154	131

Table 6. Torsion angles [deg] for 1.

O(1)#1-Al(1)-O(1)-B(1)	-179.36(18)
C(1)-Al(1)-O(1)-B(1)	64.64(18)
C(2)-Al(1)-O(1)-B(1)	-71.13(17)
Al(1)#1-Al(1)-O(1)-B(1)	-179.36(18)
O(1)#1-Al(1)-O(1)-Al(1)#1	0.0
C(1)-Al(1)-O(1)-Al(1)#1	-116.00(10)
C(2)-Al(1)-O(1)-Al(1)#1	108.23(10)
Al(1)#1-O(1)-B(1)-C(21)	148.42(14)
Al(1)-O(1)-B(1)-C(21)	-32.4(2)
Al(1)#1-O(1)-B(1)-C(11)	-30.5(3)
Al(1)-O(1)-B(1)-C(11)	148.65(14)
O(1)-B(1)-C(11)-C(12)	118.5(2)
C(21)-B(1)-C(11)-C(12)	-60.4(3)
O(1)-B(1)-C(11)-C(16)	-63.7(3)
C(21)-B(1)-C(11)-C(16)	117.4(2)
C(16)-C(11)-C(12)-C(13)	1.3(3)
B(1)-C(11)-C(12)-C(13)	179.16(17)
C(16)-C(11)-C(12)-C(121)	179.84(18)
B(1)-C(11)-C(12)-C(121)	-2.2(3)
C(11)-C(12)-C(13)-C(14)	-1.4(3)
C(121)-C(12)-C(13)-C(14)	179.94(19)
C(12)-C(13)-C(14)-C(15)	0.8(3)
C(12)-C(13)-C(14)-C(141)	-179.00(19)
C(13)-C(14)-C(15)-C(16)	0.0(3)
C(141)-C(14)-C(15)-C(16)	179.75(19)
C(14)-C(15)-C(16)-C(11)	-0.1(3)
C(14)-C(15)-C(16)-C(161)	-179.13(18)
C(12)-C(11)-C(16)-C(15)	-0.5(3)
B(1)-C(11)-C(16)-C(15)	-178.41(17)
C(12)-C(11)-C(16)-C(161)	178.44(18)
B(1)-C(11)-C(16)-C(161)	0.6(3)
O(1)-B(1)-C(21)-C(26)	-65.7(2)
C(11)-B(1)-C(21)-C(26)	113.1(2)
O(1)-B(1)-C(21)-C(22)	118.5(2)
C(11)-B(1)-C(21)-C(22)	-62.6(3)
C(26)-C(21)-C(22)-C(23)	-2.2(3)
B(1)-C(21)-C(22)-C(23)	173.68(17)
C(26)-C(21)-C(22)-C(221)	175.66(18)
B(1)-C(21)-C(22)-C(221)	-8.4(3)
C(21)-C(22)-C(23)-C(24)	-0.4(3)
C(221)-C(22)-C(23)-C(24)	-178.37(18)
C(22)-C(23)-C(24)-C(25)	2.4(3)
C(22)-C(23)-C(24)-C(241)	-178.5(2)
C(23)-C(24)-C(25)-C(26)	-1.8(3)
C(241)-C(24)-C(25)-C(26)	179.1(2)
C(24)-C(25)-C(26)-C(21)	-0.9(3)
C(24)-C(25)-C(26)-C(261)	-178.5(2)
C(22)-C(21)-C(26)-C(25)	2.9(3)
B(1)-C(21)-C(26)-C(25)	-173.01(18)
C(22)-C(21)-C(26)-C(261)	-179.7(2)
B(1)-C(21)-C(26)-C(261)	4.4(3)

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

Table 1. Crystal data and structure refinement for 3.

Empirical formula	C23 H34 Al B O2
Formula weight	380.29
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 17.2070(3) A alpha = 90 deg.
	b = 8.6950(4) A beta = 90 deg.
	c = 31.413(1) A gamma = 90 deg.
Volume	4699.9(3) A^3
Z, Calculated density	8, 1.075 Mg/m^3
Absorption coefficient	0.100 mm^-1
F(000)	1648
Crystal size	0.95 x 0.32 x 0.44 mm
Theta range for data collection	2.70 to 23.81 deg.
Index ranges	-19<=h<=19, -9<=k<=9, -35<=l<=35
Reflections collected / unique	6775 / 3502 [R(int) = 0.029]
Completeness to 2theta = 23.81	97.2%
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3502 / 0 / 255
Goodness-of-fit on F^2	1.013
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1284
R indices (all data)	R1 = 0.1368, wR2 = 0.1485
Extinction coefficient	0.0031(8)
Largest diff. peak and hole	0.142 and -0.182 e.A^-3

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

	x	y	z	U(eq)
Al(1)	-314(1)	5881(1)	327(1)	53(1)
O(1)	470(1)	5969(2)	-65(1)	52(1)
O(2)	38(1)	5540(2)	827(1)	59(1)
B(1)	182(2)	6009(4)	1228(1)	52(1)
C(1)	-1124(2)	7384(4)	254(1)	81(1)
C(2)	951(2)	7276(4)	-202(1)	72(1)
C(3)	1689(3)	6631(5)	-388(2)	131(2)
C(4)	500(3)	8191(4)	-526(1)	111(2)
C(5)	1119(2)	8245(4)	191(1)	98(1)
C(11)	716(2)	4971(3)	1523(1)	51(1)
C(12)	595(2)	4853(3)	1966(1)	56(1)
C(121)	-42(2)	5707(4)	2201(1)	85(1)
C(13)	1062(2)	3892(4)	2211(1)	65(1)
C(14)	1659(2)	3044(4)	2043(1)	65(1)
C(141)	2165(2)	2003(4)	2319(1)	101(1)
C(15)	1790(2)	3174(4)	1615(1)	64(1)
C(16)	1337(2)	4108(4)	1352(1)	56(1)
C(161)	1572(2)	4176(5)	887(1)	96(1)
C(21)	-186(2)	7608(3)	1376(1)	49(1)
C(221)	-1550(2)	6465(4)	1371(1)	71(1)
C(22)	-989(2)	7807(4)	1424(1)	52(1)
C(23)	-1290(2)	9225(4)	1541(1)	61(1)
C(24)	-818(2)	10484(4)	1615(1)	59(1)
C(241)	-1155(2)	12019(4)	1753(1)	87(1)
C(25)	-29(2)	10288(4)	1566(1)	57(1)
C(26)	291(2)	8888(4)	1454(1)	52(1)
C(261)	1165(2)	8773(4)	1417(1)	82(1)

Table 3. Bond lengths [A] and angles [deg] for 3.

Al(1)-O(2)	1.709(2)
Al(1)-O(1)#1	1.826(2)
Al(1)-O(1)	1.828(2)
Al(1)-C(1)	1.924(3)
Al(1)-Al(1)#1	2.7792(18)
O(1)-C(2)	1.470(3)
O(1)-Al(1)#1	1.826(2)
O(2)-B(1)	1.348(4)
B(1)-C(11)	1.587(5)
B(1)-C(21)	1.597(5)
C(2)-C(3)	1.504(5)
C(2)-C(4)	1.507(5)
C(2)-C(5)	1.523(5)
C(11)-C(12)	1.411(4)
C(11)-C(16)	1.413(4)
C(12)-C(13)	1.391(4)
C(12)-C(121)	1.515(4)
C(13)-C(14)	1.370(4)
C(14)-C(15)	1.369(4)
C(14)-C(141)	1.526(4)
C(15)-C(16)	1.396(4)
C(16)-C(161)	1.516(4)
C(21)-C(22)	1.400(4)
C(21)-C(26)	1.403(4)
C(221)-C(22)	1.524(4)
C(22)-C(23)	1.388(4)
C(23)-C(24)	1.383(4)
C(24)-C(25)	1.377(4)
C(24)-C(241)	1.517(4)
C(25)-C(26)	1.382(4)
C(26)-C(261)	1.512(4)

O(2)-Al(1)-O(1)#1	108.24(9)
O(2)-Al(1)-O(1)	111.43(10)
O(1)#1-Al(1)-O(1)	80.97(9)
O(2)-Al(1)-C(1)	118.88(13)
O(1)#1-Al(1)-C(1)	115.96(13)
O(1)-Al(1)-C(1)	115.22(13)
O(2)-Al(1)-Al(1)#1	116.49(8)
O(1)#1-Al(1)-Al(1)#1	40.52(6)
O(1)-Al(1)-Al(1)#1	40.45(6)
C(1)-Al(1)-Al(1)#1	124.60(12)
C(2)-O(1)-Al(1)#1	129.25(19)
C(2)-O(1)-Al(1)	130.15(18)
Al(1)#1-O(1)-Al(1)	99.03(9)
B(1)-O(2)-Al(1)	150.7(2)
O(2)-B(1)-C(11)	118.8(3)
O(2)-B(1)-C(21)	117.5(3)
C(11)-B(1)-C(21)	123.7(3)
O(1)-C(2)-C(3)	107.4(3)
O(1)-C(2)-C(4)	108.4(3)
C(3)-C(2)-C(4)	111.7(4)
O(1)-C(2)-C(5)	107.3(3)
C(3)-C(2)-C(5)	111.2(3)
C(4)-C(2)-C(5)	110.7(3)
C(12)-C(11)-C(16)	116.8(3)
C(12)-C(11)-B(1)	122.1(3)

C(16)-C(11)-B(1)	121.1(3)
C(13)-C(12)-C(11)	120.2(3)
C(13)-C(12)-C(121)	116.3(3)
C(11)-C(12)-C(121)	123.5(3)
C(14)-C(13)-C(12)	122.9(3)
C(15)-C(14)-C(13)	117.2(3)
C(15)-C(14)-C(141)	120.9(4)
C(13)-C(14)-C(141)	121.9(4)
C(14)-C(15)-C(16)	122.6(3)
C(15)-C(16)-C(11)	120.3(3)
C(15)-C(16)-C(161)	116.4(3)
C(11)-C(16)-C(161)	123.3(3)
C(22)-C(21)-C(26)	117.4(3)
C(22)-C(21)-B(1)	122.0(3)
C(26)-C(21)-B(1)	120.6(3)
C(23)-C(22)-C(21)	120.4(3)
C(23)-C(22)-C(221)	118.2(3)
C(21)-C(22)-C(221)	121.3(3)
C(24)-C(23)-C(22)	121.9(3)
C(25)-C(24)-C(23)	117.5(3)
C(25)-C(24)-C(241)	121.1(3)
C(23)-C(24)-C(241)	121.4(3)
C(24)-C(25)-C(26)	122.0(3)
C(25)-C(26)-C(21)	120.7(3)
C(25)-C(26)-C(261)	118.3(3)
C(21)-C(26)-C(261)	121.0(3)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 3.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Al(1)	57(1)	59(1)	43(1)	-2(1)	-4(1)	8(1)
O(1)	57(1)	58(1)	41(1)	0(1)	0(1)	-3(1)
O(2)	68(2)	71(1)	37(2)	-7(1)	-8(1)	10(1)
B(1)	43(2)	68(3)	44(3)	1(2)	3(2)	-7(2)
C(1)	87(3)	90(2)	66(3)	5(2)	-6(2)	24(2)
C(2)	79(3)	77(2)	60(3)	-3(2)	3(2)	-25(2)
C(3)	92(4)	138(4)	164(5)	-32(3)	53(3)	-43(3)
C(4)	169(4)	92(3)	71(3)	32(2)	-20(3)	-35(3)
C(5)	133(4)	86(3)	76(3)	-7(2)	-21(3)	-39(2)
C(11)	50(2)	63(2)	40(2)	-5(2)	-2(2)	1(2)
C(12)	63(2)	62(2)	43(2)	-3(2)	-2(2)	3(2)
C(121)	110(3)	100(3)	44(2)	1(2)	12(2)	27(2)
C(13)	73(3)	78(2)	44(2)	7(2)	-3(2)	-7(2)
C(14)	63(3)	77(2)	54(3)	10(2)	-11(2)	-2(2)
C(141)	98(3)	117(3)	88(3)	35(3)	-17(2)	20(2)
C(15)	49(2)	74(2)	67(3)	-2(2)	-4(2)	4(2)
C(16)	50(2)	74(2)	45(2)	0(2)	-4(2)	2(2)
C(161)	82(3)	148(4)	57(3)	3(2)	13(2)	38(3)
C(21)	50(2)	59(2)	39(2)	-1(2)	-4(2)	-1(2)
C(221)	60(2)	80(2)	72(3)	-11(2)	8(2)	-10(2)
C(22)	50(2)	65(2)	43(2)	-2(2)	2(2)	-1(2)
C(23)	52(2)	79(3)	53(2)	-3(2)	3(2)	8(2)
C(24)	66(3)	60(2)	49(2)	-3(2)	2(2)	7(2)
C(241)	94(3)	74(3)	94(3)	-13(2)	3(2)	16(2)
C(25)	64(3)	60(2)	47(2)	-2(2)	-1(2)	-7(2)
C(26)	47(2)	69(2)	41(2)	-3(2)	-2(2)	4(2)
C(261)	63(3)	86(3)	95(3)	-16(2)	-5(2)	-5(2)

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

	x	y	z	U(eq)
H(1A)	-1612	6951	342	121
H(1B)	-1154	7677	-40	121
H(1C)	-1010	8273	424	121
H(3A)	1953	6033	-176	197
H(3B)	2018	7460	-479	197
H(3C)	1565	5989	-627	197
H(4A)	359	7537	-760	166
H(4B)	815	9024	-628	166
H(4C)	38	8595	-396	166
H(5A)	637	8570	317	147
H(5B)	1417	9132	111	147
H(5C)	1407	7645	393	147
H(12A)	-104	5276	2480	127
H(12B)	-522	5612	2047	127
H(12C)	95	6774	2225	127
H(13)	965	3822	2501	78
H(14A)	2307	2537	2574	152
H(14B)	2626	1727	2164	152
H(14C)	1880	1089	2390	152
H(15)	2196	2619	1494	76
H(16A)	2057	3648	848	144
H(16B)	1628	5230	801	144
H(16C)	1179	3693	716	144
H(22A)	-1264	5549	1304	106
H(22B)	-1907	6687	1144	106
H(22C)	-1834	6316	1630	106
H(23)	-1825	9331	1572	74
H(24A)	-1397	12510	1513	131
H(24B)	-746	12663	1860	131
H(24C)	-1534	11855	1972	131
H(25)	299	11123	1610	69
H(26A)	1378	9776	1364	123
H(26B)	1296	8101	1185	123
H(26C)	1375	8369	1677	123

Table 6. Torsion angles [deg] for 3.

O(2)-Al(1)-O(1)-C(2)	-87.4(3)
O(1)#1-Al(1)-O(1)-C(2)	166.4(3)
C(1)-Al(1)-O(1)-C(2)	51.9(3)
Al(1)#1-Al(1)-O(1)-C(2)	166.4(3)
O(2)-Al(1)-O(1)-Al(1)#1	106.15(11)
O(1)#1-Al(1)-O(1)-Al(1)#1	0.0
C(1)-Al(1)-O(1)-Al(1)#1	-114.52(14)
O(1)#1-Al(1)-O(2)-B(1)	-161.9(4)
O(1)-Al(1)-O(2)-B(1)	110.9(4)
C(1)-Al(1)-O(2)-B(1)	-26.8(5)
Al(1)#1-Al(1)-O(2)-B(1)	155.0(4)
Al(1)-O(2)-B(1)-C(11)	-169.0(3)
Al(1)-O(2)-B(1)-C(21)	10.0(6)
Al(1)#1-O(1)-C(2)-C(3)	-39.8(4)
Al(1)-O(1)-C(2)-C(3)	157.6(3)
Al(1)#1-O(1)-C(2)-C(4)	81.1(3)
Al(1)-O(1)-C(2)-C(4)	-81.5(3)
Al(1)#1-O(1)-C(2)-C(5)	-159.4(2)
Al(1)-O(1)-C(2)-C(5)	38.0(4)
O(2)-B(1)-C(11)-C(12)	-146.2(3)
C(21)-B(1)-C(11)-C(12)	34.9(4)
O(2)-B(1)-C(11)-C(16)	33.4(4)
C(21)-B(1)-C(11)-C(16)	-145.5(3)
C(16)-C(11)-C(12)-C(13)	-1.6(4)
B(1)-C(11)-C(12)-C(13)	178.0(3)
C(16)-C(11)-C(12)-C(121)	179.7(3)
B(1)-C(11)-C(12)-C(121)	-0.6(4)
C(11)-C(12)-C(13)-C(14)	1.0(5)
C(121)-C(12)-C(13)-C(14)	179.8(3)
C(12)-C(13)-C(14)-C(15)	0.2(5)
C(12)-C(13)-C(14)-C(141)	179.8(3)
C(13)-C(14)-C(15)-C(16)	-0.8(5)
C(141)-C(14)-C(15)-C(16)	179.7(3)
C(14)-C(15)-C(16)-C(11)	0.1(5)
C(14)-C(15)-C(16)-C(161)	177.9(3)
C(12)-C(11)-C(16)-C(15)	1.1(4)
B(1)-C(11)-C(16)-C(15)	-178.6(3)
C(12)-C(11)-C(16)-C(161)	-176.5(3)
B(1)-C(11)-C(16)-C(161)	3.8(5)
O(2)-B(1)-C(21)-C(22)	67.3(4)
C(11)-B(1)-C(21)-C(22)	-113.8(3)
O(2)-B(1)-C(21)-C(26)	-111.1(3)
C(11)-B(1)-C(21)-C(26)	67.8(4)
C(26)-C(21)-C(22)-C(23)	0.2(4)
B(1)-C(21)-C(22)-C(23)	-178.2(3)
C(26)-C(21)-C(22)-C(221)	-176.6(3)
B(1)-C(21)-C(22)-C(221)	5.0(4)
C(21)-C(22)-C(23)-C(24)	0.1(4)
C(221)-C(22)-C(23)-C(24)	177.1(3)
C(22)-C(23)-C(24)-C(25)	0.1(5)
C(22)-C(23)-C(24)-C(241)	-178.6(3)
C(23)-C(24)-C(25)-C(26)	-0.8(4)
C(241)-C(24)-C(25)-C(26)	178.0(3)
C(24)-C(25)-C(26)-C(21)	1.2(5)
C(24)-C(25)-C(26)-C(261)	-178.7(3)
C(22)-C(21)-C(26)-C(25)	-0.9(4)
B(1)-C(21)-C(26)-C(25)	177.5(3)

C(22)-C(21)-C(26)-C(261)	179.1(3)
B(1)-C(21)-C(26)-C(261)	-2.5(4)

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

Table 1. Crystal data and structure refinement for 4.

Empirical formula	C27 H33 B3 O3
Formula weight	437.96
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	MONOCLINIC
Space group	C2/c
Unit cell dimensions	a = 8.991(2) A alpha = 90 deg. b = 14.081(3) A beta = 101.36(3) deg. c = 20.024(4) A gamma = 90 deg.
Volume	2485.4(9) A^3
Z	4
Density (calculated)	1.170 Mg/m^3
Absorption coefficient	0.072 mm^-1
F(000)	936
Crystal size	0.72 x 0.60 x 0.45 mm
Theta range for data collection	2.73 to 30.09 deg.
Index ranges	-11<=h<=11, -19<=k<=19, 0<=l<=21
Reflections collected	6536
Independent reflections	3316 [R(int) = 0.0694]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3254 / 0 / 172
Goodness-of-fit on F^2	0.993
Final R indices [I>2sigma(I)]	R1 = 0.0681, wR2 = 0.1855
R indices (all data)	R1 = 0.1693, wR2 = 0.2669
Extinction coefficient	0.0037(12)
Largest diff. peak and hole	0.369 and -0.215 e.A^-3

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

	x	y	z	U(eq)
O(1)	-144(3)	9348(1)	1902(1)	44(1)
O(2)	0	7906(2)	2500	47(1)
B(1)	-161(4)	8369(2)	1884(2)	36(1)
B(2)	0	9849(3)	2500	35(1)
C(1)	-345(3)	7819(2)	1204(1)	33(1)
C(2)	306(3)	8156(2)	661(1)	37(1)
C(3)	189(3)	7612(2)	68(2)	43(1)
C(4)	-592(3)	6762(2)	-18(2)	42(1)
C(5)	-1263(3)	6455(2)	503(2)	41(1)
C(6)	-1161(3)	6954(2)	1108(2)	39(1)
C(7)	1164(4)	9085(2)	690(2)	54(1)
C(8)	-1966(5)	6548(3)	1641(2)	62(1)
C(9)	-726(5)	6196(3)	-669(2)	63(1)
C(10)	0	10960(2)	2500	33(1)
C(11)	1010(3)	11467(2)	2997(1)	35(1)
C(12)	991(3)	12456(2)	2983(2)	42(1)
C(13)	0	12960(3)	2500	43(1)
C(14)	2161(4)	10984(2)	3543(2)	56(1)
C(15)	0	14037(3)	2500	70(2)

Table 3. Bond lengths [A], angles [deg] and torsion angles [deg] for 4.

O(1)-B(2)	1.375(3)
O(1)-B(1)	1.380(3)
O(2)-B(1)#1	1.377(3)
O(2)-B(1)	1.377(3)
B(1)-C(1)	1.546(4)
B(2)-O(1)#1	1.375(3)
B(2)-C(10)	1.564(5)
C(1)-C(2)	1.415(4)
C(1)-C(6)	1.415(3)
C(2)-C(3)	1.399(4)
C(2)-C(7)	1.514(4)
C(3)-C(4)	1.381(4)
C(4)-C(5)	1.373(4)
C(4)-C(9)	1.513(4)
C(5)-C(6)	1.388(4)
C(6)-C(8)	1.514(4)
C(10)-C(11)#1	1.403(3)
C(10)-C(11)	1.403(3)
C(11)-C(12)	1.393(4)
C(11)-C(14)	1.511(4)
C(12)-C(13)	1.375(3)
C(13)-C(12)#1	1.375(3)
C(13)-C(15)	1.517(5)

B(2)-O(1)-B(1)	122.3(2)
B(1)#1-O(2)-B(1)	123.6(3)
O(2)-B(1)-O(1)	116.8(3)
O(2)-B(1)-C(1)	121.7(2)
O(1)-B(1)-C(1)	121.4(3)
O(1)-B(2)-O(1)#1	118.2(3)
O(1)-B(2)-C(10)	120.9(2)
O(1)#1-B(2)-C(10)	120.9(2)
C(2)-C(1)-C(6)	117.8(2)
C(2)-C(1)-B(1)	121.3(2)
C(6)-C(1)-B(1)	120.9(3)
C(3)-C(2)-C(1)	119.7(2)
C(3)-C(2)-C(7)	117.2(3)
C(1)-C(2)-C(7)	123.1(3)
C(4)-C(3)-C(2)	122.1(3)
C(5)-C(4)-C(3)	117.8(3)
C(5)-C(4)-C(9)	121.1(3)
C(3)-C(4)-C(9)	121.1(3)
C(4)-C(5)-C(6)	122.7(3)
C(5)-C(6)-C(1)	119.8(3)
C(5)-C(6)-C(8)	117.7(3)
C(1)-C(6)-C(8)	122.4(3)
C(11)#1-C(10)-C(11)	118.8(3)
C(11)#1-C(10)-B(2)	120.6(2)
C(11)-C(10)-B(2)	120.6(2)
C(12)-C(11)-C(10)	119.4(3)
C(12)-C(11)-C(14)	117.9(3)
C(10)-C(11)-C(14)	122.7(2)
C(13)-C(12)-C(11)	122.3(3)
C(12)#1-C(13)-C(12)	117.9(3)
C(12)#1-C(13)-C(15)	121.1(2)
C(12)-C(13)-C(15)	121.1(2)

B(1)#1-O(2)-B(1)-O(1)	0.5(2)
B(1)#1-O(2)-B(1)-C(1)	-179.7(3)
B(2)-O(1)-B(1)-O(2)	-1.1(4)
B(2)-O(1)-B(1)-C(1)	179.2(2)
B(1)-O(1)-B(2)-O(1)#1	0.5(2)
B(1)-O(1)-B(2)-C(10)	-179.5(2)
O(2)-B(1)-C(1)-C(2)	-143.9(3)
O(1)-B(1)-C(1)-C(2)	35.8(4)
O(2)-B(1)-C(1)-C(6)	35.4(4)
O(1)-B(1)-C(1)-C(6)	-144.9(3)
C(6)-C(1)-C(2)-C(3)	-3.0(4)
B(1)-C(1)-C(2)-C(3)	176.4(3)
C(6)-C(1)-C(2)-C(7)	178.1(3)
B(1)-C(1)-C(2)-C(7)	-2.6(4)
C(1)-C(2)-C(3)-C(4)	2.3(4)
C(7)-C(2)-C(3)-C(4)	-178.7(3)
C(2)-C(3)-C(4)-C(5)	-0.2(5)
C(2)-C(3)-C(4)-C(9)	178.9(3)
C(3)-C(4)-C(5)-C(6)	-1.1(5)
C(9)-C(4)-C(5)-C(6)	179.8(3)
C(4)-C(5)-C(6)-C(1)	0.3(5)
C(4)-C(5)-C(6)-C(8)	179.2(3)
C(2)-C(1)-C(6)-C(5)	1.8(4)
B(1)-C(1)-C(6)-C(5)	-177.6(3)
C(2)-C(1)-C(6)-C(8)	-177.1(3)
B(1)-C(1)-C(6)-C(8)	3.5(5)
O(1)-B(2)-C(10)-C(11)#1	41.3(2)
O(1)#1-B(2)-C(10)-C(11)#1	-138.7(2)
O(1)-B(2)-C(10)-C(11)	-138.7(2)
O(1)#1-B(2)-C(10)-C(11)	41.3(2)
C(11)#1-C(10)-C(11)-C(12)	-0.3(2)
B(2)-C(10)-C(11)-C(12)	179.7(2)
C(11)#1-C(10)-C(11)-C(14)	-178.7(3)
B(2)-C(10)-C(11)-C(14)	1.3(3)
C(10)-C(11)-C(12)-C(13)	0.7(4)
C(14)-C(11)-C(12)-C(13)	179.1(3)
C(11)-C(12)-C(13)-C(12)#1	-0.3(2)
C(11)-C(12)-C(13)-C(15)	179.7(2)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	75(2)	24(1)	34(1)	0(1)	9(1)	1(1)
O(2)	76(2)	25(1)	38(2)	0	12(1)	0
B(1)	47(2)	25(1)	36(2)	1(1)	7(1)	1(1)
B(2)	42(2)	27(2)	35(2)	0	8(2)	0
C(1)	39(1)	26(1)	34(2)	-2(1)	6(1)	2(1)
C(2)	42(2)	30(1)	38(2)	1(1)	3(1)	-1(1)
C(3)	48(2)	43(2)	39(2)	-2(1)	12(1)	0(1)
C(4)	43(2)	42(2)	39(2)	-11(1)	6(1)	4(1)
C(5)	44(2)	31(1)	48(2)	-10(1)	9(1)	-6(1)
C(6)	42(2)	31(1)	47(2)	-4(1)	15(1)	-1(1)
C(7)	67(2)	39(2)	55(2)	6(2)	13(2)	-16(1)
C(8)	84(3)	45(2)	66(3)	-11(2)	38(2)	-22(2)
C(9)	75(3)	64(2)	49(2)	-24(2)	13(2)	-2(2)
C(10)	35(2)	24(2)	40(2)	0	9(2)	0
C(11)	42(2)	26(1)	36(2)	1(1)	8(1)	0(1)
C(12)	50(2)	29(1)	47(2)	-6(1)	10(1)	-7(1)
C(13)	63(3)	26(2)	45(3)	0	20(2)	0
C(14)	59(2)	42(2)	56(2)	1(2)	-15(2)	1(1)
C(15)	122(5)	20(2)	64(4)	0	13(4)	0

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

	x	y	z	U(eq)
H(3)	653(3)	7829(2)	-279(2)	55(10)
H(5)	-1807(3)	5890(2)	448(2)	42(8)
H(71)	1167(4)	9391(2)	1118(2)	378(75)
H(72)	681(4)	9490(2)	325(2)	165(26)
H(73)	2190(4)	8963(2)	643(2)	223(37)
H(81)	-1808(5)	6957(3)	2032(2)	211(34)
H(82)	-1568(5)	5929(3)	1773(2)	220(37)
H(83)	-3033(5)	6501(3)	1455(2)	322(57)
H(91)	-190(5)	6517(3)	-972(2)	188(30)
H(92)	-1777(5)	6137(3)	-882(2)	206(35)
H(93)	-298(5)	5576(3)	-566(2)	117(19)
H(12)	1671(3)	12787(2)	3311(2)	45(9)
H(141)	2053(4)	10308(2)	3496(2)	192(31)
H(142)	1996(4)	11172(2)	3983(2)	236(41)
H(143)	3165(4)	11166(2)	3497(2)	240(41)
H(151)	945(64)	14265(3)	2760(60)	240(84)
H(152)	-820(98)	14265(3)	2699(66)	81(29)
H(153)	-125(161)	14265(3)	2040(6)	102(34)