

Enantioselective Synthesis of Boron-Substituted Quaternary Carbons by NHC–Cu-Catalyzed Boronate Conjugate Additions to Carboxylic Esters, Ketones or Thioesters

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SUPPORTING INFORMATION, PART II

■ Crystal data of (*S*)-Ethyl 3-(naphthalen-2-yl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate (Table 2, entry 4)

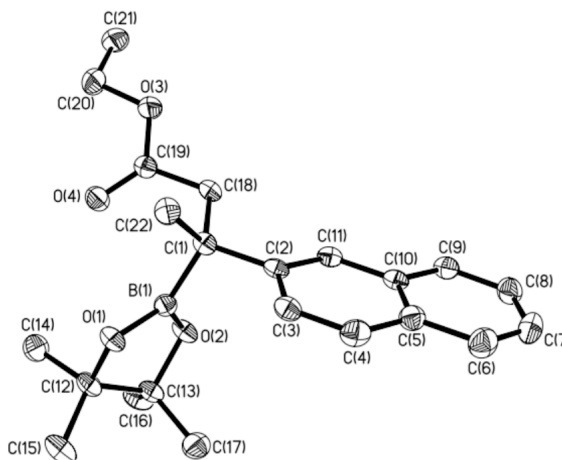
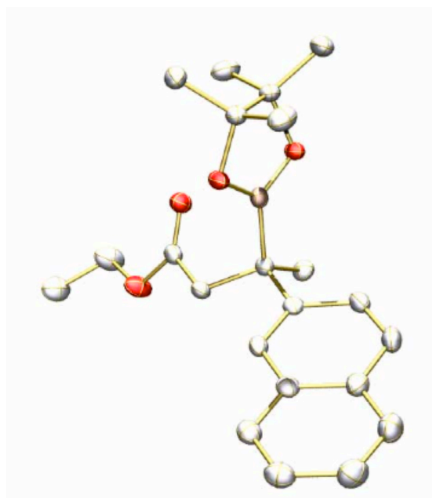


Table 1. Crystal data and structure refinement for $C_{22}H_{29}BO_4$

Identification code	$C_{22}H_{29}BO_4$	
Empirical formula	$C_{22}H_{29}BO_4$	
Formula weight	369.27	
Temperature	100(2) K	
Wavelength	1.54178 \approx	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	$a = 6.2174(3) \approx$	$a = 68.885(2)^\infty$
	$b = 9.1621(5) \approx$	$b = 72.9090(10)^\infty$
	$c = 10.3772(6) \approx$	$g = 71.408(2)^\infty$
Volume	$511.84(5) \approx^3$	
Z	1	
Density (calculated)	1.198 Mg/m^3	

Absorption coefficient	0.636 mm ⁻¹
F(000)	199
Crystal size	0.29 x 0.28 x 0.20 mm ³
Theta range for data collection	4.66 to 67.01°
Index ranges	-7<=h<=7, -10<=k<=10, -12<=l<=12
Reflections collected	9561
Independent reflections	3198 [R(int) = 0.0212]
Completeness to theta = 67.01°	93.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8807 and 0.8371
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3198 / 3 / 251
Goodness-of-fit on F ²	1.169
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0857
R indices (all data)	R1 = 0.0361, wR2 = 0.0857
Absolute structure parameter	0.08(13)
Extinction coefficient	0.102(4)
Largest diff. peak and hole	0.216 and -0.276 e. ⁻³

Table 2. Atomic coordinates (x10⁴) and equivalent isotropic displacement parameters (≈ x10³) for C₂₂H₂₉BO₄. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
B(1)	8984(3)	8341(2)	7458(2)	21(1)
O(1)	10395(2)	6868(1)	7930(1)	24(1)
O(2)	7601(2)	8361(1)	6635(1)	25(1)
O(3)	3749(2)	10751(1)	10344(1)	34(1)
O(4)	5724(2)	8372(1)	9973(1)	28(1)
C(1)	9003(2)	9946(2)	7706(1)	20(1)
C(2)	10052(2)	11011(2)	6288(1)	20(1)
C(3)	12502(2)	10645(2)	5802(2)	24(1)
C(4)	13536(2)	11573(2)	4559(2)	28(1)
C(5)	12210(3)	12929(2)	3688(2)	26(1)
C(6)	13215(3)	13908(2)	2383(2)	33(1)
C(7)	11840(3)	15178(2)	1565(2)	35(1)

C(8)	9408(3)	15523(2)	2013(2)	31(1)
C(9)	8393(3)	14611(2)	3272(2)	26(1)
C(10)	9761(2)	13283(2)	4143(1)	22(1)
C(11)	8749(2)	12309(2)	5446(1)	21(1)
C(12)	9601(2)	5709(2)	7609(2)	25(1)
C(13)	8410(2)	6809(2)	6352(2)	24(1)
C(14)	7913(3)	5031(2)	8935(2)	34(1)
C(15)	11647(3)	4372(2)	7290(2)	34(1)
C(16)	6348(3)	6322(2)	6277(2)	31(1)
C(17)	10101(3)	7031(2)	4932(2)	34(1)
C(18)	6489(2)	10815(2)	8224(2)	21(1)
C(19)	5337(2)	9822(2)	9604(2)	22(1)
C(20)	2435(3)	9945(2)	11681(2)	41(1)
C(21)	121(3)	11064(2)	11941(2)	39(1)
C(22)	10439(2)	9599(2)	8818(2)	25(1)

Table 3. Bond lengths [\approx] and angles [∞] for $C_{22}H_{29}BO_4$

B(1)-O(1)	1.361(2)
B(1)-O(2)	1.3711(19)
B(1)-C(1)	1.585(2)
O(1)-C(12)	1.4720(17)
O(2)-C(13)	1.456(2)
O(3)-C(19)	1.3329(19)
O(3)-C(20)	1.456(2)
O(4)-C(19)	1.2063(19)
C(1)-C(2)	1.5334(19)
C(1)-C(18)	1.5444(19)
C(1)-C(22)	1.5464(18)
C(2)-C(11)	1.374(2)
C(2)-C(3)	1.425(2)
C(3)-C(4)	1.368(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.420(2)
C(4)-H(4)	0.9500

C(5)-C(6)	1.419(2)
C(5)-C(10)	1.421(2)
C(6)-C(7)	1.373(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.411(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.368(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.421(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.4172(19)
C(11)-H(11)	0.9500
C(12)-C(15)	1.510(2)
C(12)-C(14)	1.527(2)
C(12)-C(13)	1.553(2)
C(13)-C(16)	1.515(2)
C(13)-C(17)	1.525(2)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.505(2)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(20)-C(21)	1.491(3)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800

C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
O(1)-B(1)-O(2)	113.62(14)
O(1)-B(1)-C(1)	125.10(12)
O(2)-B(1)-C(1)	121.13(13)
B(1)-O(1)-C(12)	106.54(11)
B(1)-O(2)-C(13)	106.56(11)
C(19)-O(3)-C(20)	117.24(13)
C(2)-C(1)-C(18)	109.94(11)
C(2)-C(1)-C(22)	109.81(11)
C(18)-C(1)-C(22)	108.65(11)
C(2)-C(1)-B(1)	107.46(11)
C(18)-C(1)-B(1)	109.15(11)
C(22)-C(1)-B(1)	111.82(12)
C(11)-C(2)-C(3)	117.67(13)
C(11)-C(2)-C(1)	123.37(12)
C(3)-C(2)-C(1)	118.96(12)
C(4)-C(3)-C(2)	121.45(13)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	121.36(13)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(6)-C(5)-C(4)	123.03(14)
C(6)-C(5)-C(10)	119.22(14)
C(4)-C(5)-C(10)	117.73(14)
C(7)-C(6)-C(5)	120.49(15)
C(7)-C(6)-H(6)	119.8
C(5)-C(6)-H(6)	119.8
C(6)-C(7)-C(8)	120.30(15)
C(6)-C(7)-H(7)	119.8
C(8)-C(7)-H(7)	119.8
C(9)-C(8)-C(7)	120.47(14)

C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(8)-C(9)-C(10)	120.74(13)
C(8)-C(9)-H(9)	119.6
C(10)-C(9)-H(9)	119.6
C(11)-C(10)-C(5)	119.42(13)
C(11)-C(10)-C(9)	121.81(12)
C(5)-C(10)-C(9)	118.77(13)
C(2)-C(11)-C(10)	122.33(12)
C(2)-C(11)-H(11)	118.8
C(10)-C(11)-H(11)	118.8
O(1)-C(12)-C(15)	109.52(11)
O(1)-C(12)-C(14)	106.11(12)
C(15)-C(12)-C(14)	109.98(14)
O(1)-C(12)-C(13)	101.66(11)
C(15)-C(12)-C(13)	115.42(14)
C(14)-C(12)-C(13)	113.38(13)
O(2)-C(13)-C(16)	108.72(12)
O(2)-C(13)-C(17)	107.12(12)
C(16)-C(13)-C(17)	110.12(13)
O(2)-C(13)-C(12)	102.55(12)
C(16)-C(13)-C(12)	114.71(13)
C(17)-C(13)-C(12)	113.01(13)
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5

C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(13)-C(17)-H(17A)	109.5
C(13)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(13)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(1)	112.78(12)
C(19)-C(18)-H(18A)	109.0
C(1)-C(18)-H(18A)	109.0
C(19)-C(18)-H(18B)	109.0
C(1)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
O(4)-C(19)-O(3)	123.95(14)
O(4)-C(19)-C(18)	124.47(13)
O(3)-C(19)-C(18)	111.50(13)
O(3)-C(20)-C(21)	107.52(14)
O(3)-C(20)-H(20A)	110.2
C(21)-C(20)-H(20A)	110.2
O(3)-C(20)-H(20B)	110.2
C(21)-C(20)-H(20B)	110.2
H(20A)-C(20)-H(20B)	108.5
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(1)-C(22)-H(22A)	109.5
C(1)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(1)-C(22)-H(22C)	109.5

H(22A)-C(22)-H(22C) 109.5

H(22B)-C(22)-H(22C) 109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx \times 10^3$) for $C_{22}H_{29}BO_4$. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^*U^{11} + \dots + 2hka^*b^*U^{12}]$

	U11	U22	U33	U23	U13	U12
B(1)	17(1)	22(1)	22(1)	-7(1)	-1(1)	-4(1)
O(1)	23(1)	18(1)	33(1)	-9(1)	-10(1)	-3(1)
O(2)	23(1)	18(1)	37(1)	-12(1)	-12(1)	-1(1)
O(3)	41(1)	25(1)	27(1)	-10(1)	4(1)	-5(1)
O(4)	27(1)	23(1)	32(1)	-8(1)	-1(1)	-5(1)
C(1)	19(1)	20(1)	25(1)	-7(1)	-7(1)	-3(1)
C(2)	21(1)	19(1)	26(1)	-12(1)	-6(1)	-4(1)
C(3)	22(1)	21(1)	30(1)	-10(1)	-8(1)	-1(1)
C(4)	18(1)	32(1)	33(1)	-13(1)	-2(1)	-4(1)
C(5)	25(1)	26(1)	27(1)	-10(1)	-3(1)	-8(1)
C(6)	27(1)	36(1)	34(1)	-10(1)	-1(1)	-9(1)
C(7)	39(1)	34(1)	27(1)	-2(1)	-1(1)	-14(1)
C(8)	39(1)	25(1)	27(1)	-5(1)	-11(1)	-5(1)
C(9)	27(1)	25(1)	27(1)	-11(1)	-6(1)	-4(1)
C(10)	25(1)	21(1)	26(1)	-12(1)	-6(1)	-4(1)
C(11)	18(1)	22(1)	25(1)	-12(1)	-4(1)	-3(1)
C(12)	23(1)	18(1)	36(1)	-10(1)	-7(1)	-6(1)
C(13)	22(1)	20(1)	34(1)	-12(1)	-6(1)	-4(1)
C(14)	45(1)	26(1)	33(1)	-8(1)	-2(1)	-17(1)
C(15)	28(1)	23(1)	54(1)	-16(1)	-13(1)	-2(1)
C(16)	23(1)	30(1)	49(1)	-21(1)	-9(1)	-4(1)
C(17)	39(1)	34(1)	33(1)	-14(1)	-3(1)	-16(1)
C(18)	21(1)	17(1)	27(1)	-8(1)	-6(1)	-2(1)
C(19)	20(1)	22(1)	25(1)	-8(1)	-8(1)	-2(1)
C(20)	50(1)	32(1)	27(1)	-6(1)	7(1)	-7(1)
C(21)	45(1)	38(1)	31(1)	-14(1)	5(1)	-11(1)

C(22) 26(1) 26(1) 26(1) -7(1) -9(1) -8(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\approx \times 10^3$) for $C_{22}H_{29}BO_4$

	x	y	z	U(eq)
H(3)	13438	9736	6353	29
H(4)	15176	11305	4272	33
H(6)	14851	13683	2073	40
H(7)	12530	15827	693	42
H(8)	8468	16396	1435	37
H(9)	6754	14867	3569	31
H(11)	7112	12562	5747	25
H(14A)	8706	4518	9732	51
H(14B)	7351	4232	8784	51
H(14C)	6599	5908	9140	51
H(15A)	12812	4833	6511	50
H(15B)	11132	3635	7021	50
H(15C)	12326	3779	8129	50
H(16A)	5154	6365	7133	47
H(16B)	6840	5223	6201	47
H(16C)	5718	7064	5450	47
H(17A)	9322	7880	4205	50
H(17B)	10635	6019	4686	50
H(17C)	11433	7338	4993	50
H(18A)	6497	11842	8333	26
H(18B)	5574	11074	7500	26
H(20A)	3251	9684	12453	49
H(20B)	2253	8930	11638	49
H(21A)	326	12126	11819	59
H(21B)	-703	10639	12905	59
H(21C)	-780	11161	11269	59
H(22A)	11998	8957	8548	37
H(22B)	9682	9002	9741	37

H(22C)	10548	10620	8870	37
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Table 6. Torsion angles [$^{\circ}$] for C₂₂H₂₉BO₄

O(2)-B(1)-O(1)-C(12)	-11.00(16)
C(1)-B(1)-O(1)-C(12)	173.50(13)
O(1)-B(1)-O(2)-C(13)	-9.30(16)
C(1)-B(1)-O(2)-C(13)	166.39(12)
O(1)-B(1)-C(1)-C(2)	108.29(15)
O(2)-B(1)-C(1)-C(2)	-66.88(16)
O(1)-B(1)-C(1)-C(18)	-132.52(14)
O(2)-B(1)-C(1)-C(18)	52.31(17)
O(1)-B(1)-C(1)-C(22)	-12.28(19)
O(2)-B(1)-C(1)-C(22)	172.55(12)
C(18)-C(1)-C(2)-C(11)	-16.66(18)
C(22)-C(1)-C(2)-C(11)	-136.14(14)
B(1)-C(1)-C(2)-C(11)	102.03(15)
C(18)-C(1)-C(2)-C(3)	163.78(12)
C(22)-C(1)-C(2)-C(3)	44.30(18)
B(1)-C(1)-C(2)-C(3)	-77.53(15)
C(11)-C(2)-C(3)-C(4)	1.7(2)
C(1)-C(2)-C(3)-C(4)	-178.68(13)
C(2)-C(3)-C(4)-C(5)	-1.0(2)
C(3)-C(4)-C(5)-C(6)	-179.12(15)
C(3)-C(4)-C(5)-C(10)	-0.7(2)
C(4)-C(5)-C(6)-C(7)	178.12(17)
C(10)-C(5)-C(6)-C(7)	-0.3(2)
C(5)-C(6)-C(7)-C(8)	-0.1(3)
C(6)-C(7)-C(8)-C(9)	0.8(3)
C(7)-C(8)-C(9)-C(10)	-1.0(2)
C(6)-C(5)-C(10)-C(11)	179.99(14)
C(4)-C(5)-C(10)-C(11)	1.5(2)
C(6)-C(5)-C(10)-C(9)	0.0(2)
C(4)-C(5)-C(10)-C(9)	-178.47(14)
C(8)-C(9)-C(10)-C(11)	-179.31(14)

C(8)-C(9)-C(10)-C(5)	0.6(2)
C(3)-C(2)-C(11)-C(10)	-0.9(2)
C(1)-C(2)-C(11)-C(10)	179.55(12)
C(5)-C(10)-C(11)-C(2)	-0.7(2)
C(9)-C(10)-C(11)-C(2)	179.25(14)
B(1)-O(1)-C(12)-C(15)	147.41(13)
B(1)-O(1)-C(12)-C(14)	-93.92(14)
B(1)-O(1)-C(12)-C(13)	24.86(14)
B(1)-O(2)-C(13)-C(16)	145.96(13)
B(1)-O(2)-C(13)-C(17)	-95.07(13)
B(1)-O(2)-C(13)-C(12)	24.11(14)
O(1)-C(12)-C(13)-O(2)	-29.49(13)
C(15)-C(12)-C(13)-O(2)	-147.90(12)
C(14)-C(12)-C(13)-O(2)	83.96(14)
O(1)-C(12)-C(13)-C(16)	-147.16(12)
C(15)-C(12)-C(13)-C(16)	94.43(16)
C(14)-C(12)-C(13)-C(16)	-33.72(19)
O(1)-C(12)-C(13)-C(17)	85.49(14)
C(15)-C(12)-C(13)-C(17)	-32.93(18)
C(14)-C(12)-C(13)-C(17)	-161.07(13)
C(2)-C(1)-C(18)-C(19)	179.09(11)
C(22)-C(1)-C(18)-C(19)	-60.72(15)
B(1)-C(1)-C(18)-C(19)	61.45(15)
C(20)-O(3)-C(19)-O(4)	0.6(2)
C(20)-O(3)-C(19)-C(18)	177.69(13)
C(1)-C(18)-C(19)-O(4)	-32.14(18)
C(1)-C(18)-C(19)-O(3)	150.81(12)
C(19)-O(3)-C(20)-C(21)	-151.11(15)

Symmetry transformations used to generate equivalent atoms:

■ **Crystal data of (*S*)-Ethyl 3-(4-bromophenyl)-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)butanoate (Table 2, entry 6)**

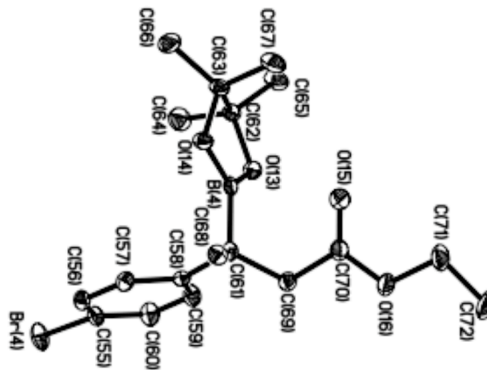
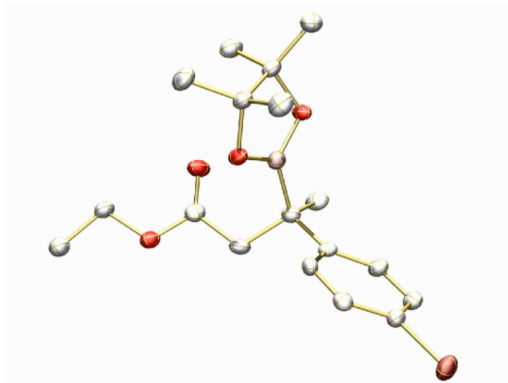


Table 1. Crystal data and structure refinement for $C_{18}H_{26}BBrO_4$.

Identification code	$C_{18}H_{26}BBrO_4$	
Empirical formula	$C_{18} H_{26} B Br O_4$	
Formula weight	397.11	
Temperature	100(2) K	
Wavelength	0.71073 \approx	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	$a = 11.0774(2) \approx$	$a = 90^\circ.$
	$b = 17.1476(3) \approx$	$b = 102.0810(10)^\circ.$
	$c = 20.9494(4) \approx$	$g = 90^\circ.$
Volume	$3891.22(12) \approx^3$	
Z	8	
Density (calculated)	1.360 Mg/m^3	
Absorption coefficient	2.131 mm^{-1}	
F(000)	1648	
Crystal size	$0.40 \times 0.18 \times 0.10 \text{ mm}^3$	
Theta range for data collection	1.55 to 27.11°	
Index ranges	$-14 \leq h \leq 14, -21 \leq k \leq 21, -26 \leq l \leq 26$	
Reflections collected	94552	
Independent reflections	17164 [R(int) = 0.0414]	
Completeness to $\theta = 27.11^\circ$	100.0 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.8152 and 0.4828
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17164 / 16 / 910
Goodness-of-fit on F^2	1.043
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0292, wR2 = 0.0695
R indices (all data)	R1 = 0.0327, wR2 = 0.0709
Absolute structure parameter	-0.019(3)
Extinction coefficient	na
Largest diff. peak and hole	0.708 and -0.212 e. \approx^{-3}

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\approx^2 \times 10^3$) for $C_{18}H_{26}BBrO_4$. $U(eq)$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	8164(1)	6176(1)	6155(1)	31(1)
O(1)	7816(2)	2206(1)	4997(1)	20(1)
O(2)	6550(2)	1944(1)	5707(1)	23(1)
O(3)	5441(2)	1748(1)	4026(1)	23(1)
O(4)	4776(2)	2534(1)	3168(1)	24(1)
B(1)	6736(3)	2382(1)	5191(1)	18(1)
C(1)	7449(2)	5241(1)	5752(1)	22(1)
C(2)	8181(2)	4710(2)	5516(1)	25(1)
C(3)	7653(2)	4018(2)	5236(1)	23(1)
C(4)	6400(2)	3847(1)	5198(1)	19(1)
C(5)	5697(2)	4406(1)	5440(1)	21(1)
C(6)	6207(2)	5101(1)	5712(1)	23(1)
C(7)	5845(2)	3076(1)	4888(1)	19(1)
C(8)	8530(2)	1697(1)	5502(1)	22(1)
C(9)	7497(2)	1328(1)	5809(1)	25(1)
C(10)	9410(2)	2225(2)	5966(1)	30(1)
C(11)	9264(2)	1123(2)	5182(1)	30(1)
C(12)	7864(3)	1158(2)	6535(1)	34(1)
C(13)	6897(3)	614(2)	5438(1)	32(1)
C(14)	4550(2)	2930(1)	5017(1)	25(1)
C(15)	5771(2)	3137(1)	4147(1)	22(1)

C(16)	5321(2)	2391(1)	3789(1)	20(1)
C(17)	4302(2)	1858(1)	2773(1)	25(1)
C(18)	3585(3)	2166(2)	2131(1)	43(1)
Br(2)	2092(1)	4031(1)	5898(1)	34(1)
O(5)	1370(2)	7900(1)	7021(1)	25(1)
O(6)	-546(2)	7625(1)	7211(1)	23(1)
O(7)	1696(2)	8135(1)	8500(1)	35(1)
O(8)	3744(2)	7950(1)	8715(1)	26(1)
B(2)	678(3)	7431(2)	7337(1)	22(1)
C(19)	1832(2)	4843(1)	6474(1)	23(1)
C(20)	2386(2)	5564(1)	6441(1)	22(1)
C(21)	2166(2)	6150(1)	6858(1)	21(1)
C(22)	1431(2)	6036(1)	7315(1)	21(1)
C(23)	909(2)	5299(1)	7339(1)	27(1)
C(24)	1095(2)	4706(1)	6918(1)	29(1)
C(25)	1237(2)	6709(1)	7772(1)	23(1)
C(26)	507(2)	8397(1)	6573(1)	25(1)
C(27)	-661(2)	8387(1)	6883(1)	23(1)
C(28)	287(3)	8004(2)	5908(1)	32(1)
C(29)	1096(3)	9192(1)	6547(2)	35(1)
C(30)	-1883(2)	8424(2)	6402(1)	30(1)
C(31)	-606(3)	9001(2)	7417(1)	30(1)
C(32)	367(3)	6485(2)	8228(1)	30(1)
C(33)	2526(2)	6925(2)	8184(1)	26(1)
C(34)	2575(2)	7730(2)	8483(1)	26(1)
C(35)	3906(2)	8750(1)	8943(1)	26(1)
C(36)	5262(2)	8861(2)	9198(1)	31(1)
Br(3)	4321(1)	4415(1)	2574(1)	30(1)
O(9)	2344(2)	8363(1)	1815(1)	21(1)
O(10)	4301(2)	8520(1)	1657(1)	35(1)
O(11)	1732(2)	8825(1)	295(1)	27(1)
O(12)	142(2)	8080(1)	-216(1)	23(1)
B(3)	3199(2)	8142(1)	1469(1)	18(1)
C(37)	3895(2)	5342(1)	2078(1)	21(1)
C(38)	4808(2)	5763(1)	1874(1)	23(1)
C(39)	4500(2)	6439(1)	1511(1)	21(1)

C(40)	3278(2)	6705(1)	1339(1)	16(1)
C(41)	2381(2)	6268(1)	1562(1)	19(1)
C(42)	2678(2)	5591(1)	1927(1)	20(1)
C(43)	2975(2)	7462(1)	944(1)	16(1)
C(44)	3013(4)	8835(2)	2356(2)	24(1)
C(45)	4083(3)	9186(2)	2066(2)	25(1)
C(46)	3457(5)	8294(2)	2930(2)	42(1)
C(47)	2141(4)	9451(3)	2519(2)	36(1)
C(48)	5255(5)	9325(4)	2569(3)	42(2)
C(49)	3721(4)	9891(2)	1637(2)	41(1)
C(44X)	2825(13)	9023(7)	2250(6)	24(1)
C(45X)	4227(9)	8818(6)	2322(3)	30(3)
C(46X)	2216(10)	9029(8)	2827(6)	35(3)
C(47X)	2538(12)	9770(6)	1851(6)	42(3)
C(48X)	4548(10)	8238(7)	2926(5)	42(2)
C(49X)	5170(20)	9499(10)	2451(12)	41(1)
C(50)	3822(2)	7560(1)	451(1)	21(1)
C(51)	1620(2)	7459(1)	575(1)	18(1)
C(52)	1207(2)	8202(1)	213(1)	20(1)
C(53)	-356(2)	8740(1)	-625(1)	26(1)
C(54)	-1689(4)	8616(3)	-863(3)	29(1)
C(54X)	-1501(12)	8416(8)	-1096(7)	29(1)
Br(4)	2556(1)	5552(1)	9892(1)	29(1)
O(13)	2943(1)	1762(1)	8970(1)	19(1)
O(14)	855(1)	1625(1)	8882(1)	20(1)
O(15)	1967(2)	1169(1)	7522(1)	28(1)
O(16)	2869(2)	1761(1)	6789(1)	27(1)
B(4)	1783(2)	1975(1)	8645(1)	17(1)
C(55)	2224(2)	4702(1)	9306(1)	19(1)
C(56)	1022(2)	4438(1)	9092(1)	20(1)
C(57)	804(2)	3790(1)	8688(1)	19(1)
C(58)	1767(2)	3394(1)	8493(1)	16(1)
C(59)	2958(2)	3676(1)	8708(1)	22(1)
C(60)	3192(2)	4329(2)	9110(1)	23(1)
C(61)	1533(2)	2630(1)	8101(1)	16(1)
C(62)	2784(2)	1311(1)	9539(1)	19(1)

C(63)	1445(2)	998(1)	9320(1)	20(1)
C(64)	2943(3)	1879(2)	10108(1)	30(1)
C(65)	3762(2)	675(1)	9675(1)	27(1)
C(66)	751(2)	892(2)	9865(1)	29(1)
C(67)	1357(2)	270(1)	8901(1)	27(1)
C(68)	202(2)	2571(1)	7704(1)	19(1)
C(69)	2432(2)	2552(1)	7634(1)	20(1)
C(70)	2377(2)	1753(1)	7319(1)	22(1)
C(71)	2913(3)	1015(2)	6464(1)	29(1)
C(72)	3464(10)	1163(4)	5874(5)	42(2)
C(72X)	3840(40)	1053(19)	6084(19)	42(2)

Table 3. Bond lengths [\approx] and angles [∞] for $C_{18}H_{26}BBrO_4$

Br(1)-C(1)	1.905(2)
O(1)-B(1)	1.375(3)
O(1)-C(8)	1.468(3)
O(2)-B(1)	1.368(3)
O(2)-C(9)	1.472(3)
O(3)-C(16)	1.205(3)
O(4)-C(16)	1.337(3)
O(4)-C(17)	1.457(3)
B(1)-C(7)	1.590(3)
C(1)-C(2)	1.378(3)
C(1)-C(6)	1.381(4)
C(2)-C(3)	1.396(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.404(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.395(3)
C(4)-C(7)	1.544(3)
C(5)-C(6)	1.390(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(14)	1.534(3)

C(7)-C(15)	1.542(3)
C(8)-C(11)	1.518(3)
C(8)-C(10)	1.522(3)
C(8)-C(9)	1.560(4)
C(9)-C(12)	1.518(3)
C(9)-C(13)	1.526(3)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-C(16)	1.514(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(17)-C(18)	1.506(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
Br(2)-C(19)	1.905(2)
O(5)-B(2)	1.373(3)
O(5)-C(26)	1.464(3)
O(6)-B(2)	1.368(3)
O(6)-C(27)	1.468(3)
O(7)-C(34)	1.203(3)

O(8)-C(34)	1.338(3)
O(8)-C(35)	1.452(3)
B(2)-C(25)	1.584(4)
C(19)-C(24)	1.380(4)
C(19)-C(20)	1.388(3)
C(20)-C(21)	1.387(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.395(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.394(3)
C(22)-C(25)	1.544(3)
C(23)-C(24)	1.389(4)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(32)	1.541(3)
C(25)-C(33)	1.550(4)
C(26)-C(29)	1.517(3)
C(26)-C(28)	1.520(4)
C(26)-C(27)	1.564(4)
C(27)-C(30)	1.511(4)
C(27)-C(31)	1.528(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800

C(33)-C(34)	1.512(3)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(35)-C(36)	1.497(4)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
Br(3)-C(37)	1.905(2)
O(9)-B(3)	1.362(3)
O(9)-C(44)	1.462(5)
O(10)-B(3)	1.365(3)
O(10)-C(45)	1.479(3)
O(11)-C(52)	1.212(3)
O(12)-C(52)	1.342(3)
O(12)-C(53)	1.457(3)
B(3)-C(43)	1.587(3)
C(37)-C(38)	1.381(3)
C(37)-C(42)	1.386(3)
C(38)-C(39)	1.389(3)
C(38)-H(38)	0.9500
C(39)-C(40)	1.403(3)
C(39)-H(39)	0.9500
C(40)-C(41)	1.401(3)
C(40)-C(43)	1.538(3)
C(41)-C(42)	1.391(3)
C(41)-H(41)	0.9500
C(42)-H(42)	0.9500
C(43)-C(51)	1.538(3)
C(43)-C(50)	1.543(3)
C(44)-C(46)	1.515(5)
C(44)-C(47)	1.518(5)
C(44)-C(45)	1.562(5)
C(45)-C(48)	1.509(6)
C(45)-C(49)	1.510(5)

C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.503(3)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(53)-C(54)	1.472(5)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
Br(4)-C(55)	1.892(2)
O(13)-B(4)	1.372(3)
O(13)-C(62)	1.461(3)
O(14)-B(4)	1.370(3)
O(14)-C(63)	1.473(3)
O(15)-C(70)	1.212(3)
O(16)-C(70)	1.336(3)
O(16)-C(71)	1.456(3)
B(4)-C(61)	1.584(3)
C(55)-C(60)	1.383(3)
C(55)-C(56)	1.389(3)
C(56)-C(57)	1.387(3)

C(56)-H(56)	0.9500
C(57)-C(58)	1.396(3)
C(57)-H(57)	0.9500
C(58)-C(59)	1.389(3)
C(58)-C(61)	1.538(3)
C(59)-C(60)	1.392(3)
C(59)-H(59)	0.9500
C(60)-H(60)	0.9500
C(61)-C(68)	1.537(3)
C(61)-C(69)	1.541(3)
C(62)-C(64)	1.521(3)
C(62)-C(65)	1.522(3)
C(62)-C(63)	1.554(3)
C(63)-C(66)	1.516(3)
C(63)-C(67)	1.518(3)
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-C(70)	1.516(3)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(71)-C(72)	1.509(7)
C(71)-H(71A)	0.9900
C(71)-H(71B)	0.9900

C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
B(1)-O(1)-C(8)	106.81(18)
B(1)-O(2)-C(9)	106.77(18)
C(16)-O(4)-C(17)	116.27(18)
O(2)-B(1)-O(1)	113.4(2)
O(2)-B(1)-C(7)	122.8(2)
O(1)-B(1)-C(7)	123.6(2)
C(2)-C(1)-C(6)	121.1(2)
C(2)-C(1)-Br(1)	119.61(19)
C(6)-C(1)-Br(1)	119.25(18)
C(1)-C(2)-C(3)	119.0(2)
C(1)-C(2)-H(2)	120.5
C(3)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	121.6(2)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(5)-C(4)-C(3)	117.1(2)
C(5)-C(4)-C(7)	122.5(2)
C(3)-C(4)-C(7)	120.4(2)
C(6)-C(5)-C(4)	121.9(2)
C(6)-C(5)-H(5)	119.1
C(4)-C(5)-H(5)	119.1
C(1)-C(6)-C(5)	119.2(2)
C(1)-C(6)-H(6)	120.4
C(5)-C(6)-H(6)	120.4
C(14)-C(7)-C(15)	109.48(19)
C(14)-C(7)-C(4)	111.77(19)
C(15)-C(7)-C(4)	107.26(18)
C(14)-C(7)-B(1)	109.54(19)
C(15)-C(7)-B(1)	110.47(19)
C(4)-C(7)-B(1)	108.30(18)
O(1)-C(8)-C(11)	109.03(19)
O(1)-C(8)-C(10)	106.42(19)
C(11)-C(8)-C(10)	109.7(2)

O(1)-C(8)-C(9)	101.94(18)
C(11)-C(8)-C(9)	115.2(2)
C(10)-C(8)-C(9)	113.8(2)
O(2)-C(9)-C(12)	108.5(2)
O(2)-C(9)-C(13)	106.27(19)
C(12)-C(9)-C(13)	110.6(2)
O(2)-C(9)-C(8)	102.20(18)
C(12)-C(9)-C(8)	115.2(2)
C(13)-C(9)-C(8)	113.2(2)
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(9)-C(13)-H(13A)	109.5
C(9)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(9)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(7)-C(14)-H(14A)	109.5
C(7)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5

C(7)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(16)-C(15)-C(7)	112.64(19)
C(16)-C(15)-H(15A)	109.1
C(7)-C(15)-H(15A)	109.1
C(16)-C(15)-H(15B)	109.1
C(7)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.8
O(3)-C(16)-O(4)	123.9(2)
O(3)-C(16)-C(15)	124.9(2)
O(4)-C(16)-C(15)	111.25(19)
O(4)-C(17)-C(18)	106.7(2)
O(4)-C(17)-H(17A)	110.4
C(18)-C(17)-H(17A)	110.4
O(4)-C(17)-H(17B)	110.4
C(18)-C(17)-H(17B)	110.4
H(17A)-C(17)-H(17B)	108.6
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
B(2)-O(5)-C(26)	107.14(19)
B(2)-O(6)-C(27)	106.95(19)
C(34)-O(8)-C(35)	115.46(19)
O(6)-B(2)-O(5)	113.3(2)
O(6)-B(2)-C(25)	123.6(2)
O(5)-B(2)-C(25)	123.0(2)
C(24)-C(19)-C(20)	121.1(2)
C(24)-C(19)-Br(2)	119.50(18)
C(20)-C(19)-Br(2)	119.45(18)
C(21)-C(20)-C(19)	118.4(2)
C(21)-C(20)-H(20)	120.8
C(19)-C(20)-H(20)	120.8

C(20)-C(21)-C(22)	122.3(2)
C(20)-C(21)-H(21)	118.8
C(22)-C(21)-H(21)	118.8
C(23)-C(22)-C(21)	117.3(2)
C(23)-C(22)-C(25)	122.9(2)
C(21)-C(22)-C(25)	119.8(2)
C(24)-C(23)-C(22)	121.5(2)
C(24)-C(23)-H(23)	119.3
C(22)-C(23)-H(23)	119.3
C(19)-C(24)-C(23)	119.4(2)
C(19)-C(24)-H(24)	120.3
C(23)-C(24)-H(24)	120.3
C(32)-C(25)-C(22)	112.6(2)
C(32)-C(25)-C(33)	109.7(2)
C(22)-C(25)-C(33)	107.00(19)
C(32)-C(25)-B(2)	109.4(2)
C(22)-C(25)-B(2)	108.49(19)
C(33)-C(25)-B(2)	109.7(2)
O(5)-C(26)-C(29)	108.5(2)
O(5)-C(26)-C(28)	106.8(2)
C(29)-C(26)-C(28)	110.6(2)
O(5)-C(26)-C(27)	102.28(18)
C(29)-C(26)-C(27)	115.1(2)
C(28)-C(26)-C(27)	112.8(2)
O(6)-C(27)-C(30)	109.11(19)
O(6)-C(27)-C(31)	106.5(2)
C(30)-C(27)-C(31)	110.6(2)
O(6)-C(27)-C(26)	101.89(18)
C(30)-C(27)-C(26)	115.2(2)
C(31)-C(27)-C(26)	112.7(2)
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5

C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(27)-C(31)-H(31A)	109.5
C(27)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(27)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(25)-C(32)-H(32A)	109.5
C(25)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(25)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(25)	113.4(2)
C(34)-C(33)-H(33A)	108.9
C(25)-C(33)-H(33A)	108.9
C(34)-C(33)-H(33B)	108.9
C(25)-C(33)-H(33B)	108.9
H(33A)-C(33)-H(33B)	107.7
O(7)-C(34)-O(8)	123.7(2)
O(7)-C(34)-C(33)	125.5(2)
O(8)-C(34)-C(33)	110.9(2)
O(8)-C(35)-C(36)	106.5(2)
O(8)-C(35)-H(35A)	110.4
C(36)-C(35)-H(35A)	110.4

O(8)-C(35)-H(35B)	110.4
C(36)-C(35)-H(35B)	110.4
H(35A)-C(35)-H(35B)	108.6
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
B(3)-O(9)-C(44)	105.7(2)
B(3)-O(10)-C(45)	106.8(2)
C(52)-O(12)-C(53)	116.36(18)
O(9)-B(3)-O(10)	113.2(2)
O(9)-B(3)-C(43)	123.3(2)
O(10)-B(3)-C(43)	123.3(2)
C(38)-C(37)-C(42)	120.6(2)
C(38)-C(37)-Br(3)	119.42(18)
C(42)-C(37)-Br(3)	119.96(18)
C(37)-C(38)-C(39)	119.6(2)
C(37)-C(38)-H(38)	120.2
C(39)-C(38)-H(38)	120.2
C(38)-C(39)-C(40)	121.7(2)
C(38)-C(39)-H(39)	119.2
C(40)-C(39)-H(39)	119.2
C(41)-C(40)-C(39)	117.0(2)
C(41)-C(40)-C(43)	122.8(2)
C(39)-C(40)-C(43)	120.20(19)
C(42)-C(41)-C(40)	121.8(2)
C(42)-C(41)-H(41)	119.1
C(40)-C(41)-H(41)	119.1
C(37)-C(42)-C(41)	119.3(2)
C(37)-C(42)-H(42)	120.4
C(41)-C(42)-H(42)	120.4
C(40)-C(43)-C(51)	110.37(17)
C(40)-C(43)-C(50)	110.96(18)
C(51)-C(43)-C(50)	109.28(19)

C(40)-C(43)-B(3)	105.25(18)
C(51)-C(43)-B(3)	110.14(18)
C(50)-C(43)-B(3)	110.79(18)
O(9)-C(44)-C(46)	107.7(3)
O(9)-C(44)-C(47)	108.5(3)
C(46)-C(44)-C(47)	111.4(4)
O(9)-C(44)-C(45)	102.4(3)
C(46)-C(44)-C(45)	113.4(4)
C(47)-C(44)-C(45)	112.9(3)
O(10)-C(45)-C(48)	107.8(4)
O(10)-C(45)-C(49)	109.2(3)
C(48)-C(45)-C(49)	111.9(4)
O(10)-C(45)-C(44)	99.0(3)
C(48)-C(45)-C(44)	113.6(4)
C(49)-C(45)-C(44)	114.3(3)
C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(44)-C(47)-H(47A)	109.5
C(44)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(44)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(45)-C(48)-H(48A)	109.5
C(45)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(45)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(45)-C(49)-H(49A)	109.5
C(45)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5

C(45)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(43)-C(50)-H(50A)	109.5
C(43)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(43)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(52)-C(51)-C(43)	114.39(18)
C(52)-C(51)-H(51A)	108.7
C(43)-C(51)-H(51A)	108.7
C(52)-C(51)-H(51B)	108.7
C(43)-C(51)-H(51B)	108.7
H(51A)-C(51)-H(51B)	107.6
O(11)-C(52)-O(12)	124.2(2)
O(11)-C(52)-C(51)	126.1(2)
O(12)-C(52)-C(51)	109.76(19)
O(12)-C(53)-C(54)	108.4(2)
O(12)-C(53)-H(53A)	110.0
C(54)-C(53)-H(53A)	110.0
O(12)-C(53)-H(53B)	110.0
C(54)-C(53)-H(53B)	110.0
H(53A)-C(53)-H(53B)	108.4
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
B(4)-O(13)-C(62)	106.57(17)
B(4)-O(14)-C(63)	105.98(17)
C(70)-O(16)-C(71)	116.05(19)
O(14)-B(4)-O(13)	113.5(2)
O(14)-B(4)-C(61)	122.7(2)
O(13)-B(4)-C(61)	123.4(2)

C(60)-C(55)-C(56)	120.3(2)
C(60)-C(55)-Br(4)	119.43(17)
C(56)-C(55)-Br(4)	120.19(17)
C(57)-C(56)-C(55)	119.3(2)
C(57)-C(56)-H(56)	120.3
C(55)-C(56)-H(56)	120.3
C(56)-C(57)-C(58)	121.5(2)
C(56)-C(57)-H(57)	119.2
C(58)-C(57)-H(57)	119.2
C(59)-C(58)-C(57)	117.8(2)
C(59)-C(58)-C(61)	120.8(2)
C(57)-C(58)-C(61)	121.1(2)
C(58)-C(59)-C(60)	121.4(2)
C(58)-C(59)-H(59)	119.3
C(60)-C(59)-H(59)	119.3
C(55)-C(60)-C(59)	119.5(2)
C(55)-C(60)-H(60)	120.2
C(59)-C(60)-H(60)	120.2
C(68)-C(61)-C(58)	112.34(18)
C(68)-C(61)-C(69)	108.99(19)
C(58)-C(61)-C(69)	110.73(18)
C(68)-C(61)-B(4)	110.26(18)
C(58)-C(61)-B(4)	103.59(17)
C(69)-C(61)-B(4)	110.87(18)
O(13)-C(62)-C(64)	106.76(18)
O(13)-C(62)-C(65)	109.23(18)
C(64)-C(62)-C(65)	110.6(2)
O(13)-C(62)-C(63)	102.22(17)
C(64)-C(62)-C(63)	113.5(2)
C(65)-C(62)-C(63)	113.90(19)
O(14)-C(63)-C(66)	109.05(18)
O(14)-C(63)-C(67)	105.92(19)
C(66)-C(63)-C(67)	110.8(2)
O(14)-C(63)-C(62)	101.79(16)
C(66)-C(63)-C(62)	115.0(2)
C(67)-C(63)-C(62)	113.42(19)

C(62)-C(64)-H(64A)	109.5
C(62)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(62)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(62)-C(65)-H(65A)	109.5
C(62)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(62)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(63)-C(66)-H(66A)	109.5
C(63)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(63)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(63)-C(67)-H(67A)	109.5
C(63)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(63)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(61)-C(68)-H(68A)	109.5
C(61)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(61)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(70)-C(69)-C(61)	112.47(19)
C(70)-C(69)-H(69A)	109.1
C(61)-C(69)-H(69A)	109.1
C(70)-C(69)-H(69B)	109.1
C(61)-C(69)-H(69B)	109.1
H(69A)-C(69)-H(69B)	107.8

O(15)-C(70)-O(16)	123.2(2)
O(15)-C(70)-C(69)	125.3(2)
O(16)-C(70)-C(69)	111.5(2)
O(16)-C(71)-C(72)	107.0(3)
O(16)-C(71)-H(71A)	110.3
C(72)-C(71)-H(71A)	110.3
O(16)-C(71)-H(71B)	110.3
C(72)-C(71)-H(71B)	110.3
H(71A)-C(71)-H(71B)	108.6
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx \times 10^3$) for $C_{18}H_{26}BBrO_4$. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + \dots + 2hka^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Br(1)	32(1)	20(1)	39(1)	-7(1)	6(1)	-7(1)
O(1)	21(1)	21(1)	17(1)	3(1)	2(1)	3(1)
O(2)	27(1)	22(1)	20(1)	4(1)	6(1)	0(1)
O(3)	28(1)	16(1)	23(1)	0(1)	1(1)	0(1)
O(4)	32(1)	20(1)	18(1)	1(1)	-1(1)	0(1)
B(1)	24(1)	14(1)	15(1)	-2(1)	1(1)	-4(1)
C(1)	30(1)	14(1)	22(1)	0(1)	1(1)	-4(1)
C(2)	21(1)	26(1)	30(1)	-1(1)	7(1)	-2(1)
C(3)	23(1)	21(1)	26(1)	-2(1)	8(1)	1(1)
C(4)	24(1)	18(1)	16(1)	1(1)	2(1)	0(1)
C(5)	18(1)	22(1)	23(1)	2(1)	3(1)	3(1)
C(6)	26(1)	19(1)	25(1)	0(1)	5(1)	4(1)
C(7)	19(1)	17(1)	21(1)	0(1)	2(1)	-1(1)

C(8)	24(1)	22(1)	17(1)	2(1)	-2(1)	4(1)
C(9)	26(1)	24(1)	23(1)	4(1)	-1(1)	3(1)
C(10)	27(1)	38(1)	23(1)	-3(1)	1(1)	-2(1)
C(11)	29(1)	30(1)	28(1)	0(1)	1(1)	9(1)
C(12)	39(2)	40(2)	23(1)	8(1)	2(1)	1(1)
C(13)	38(2)	18(1)	35(1)	3(1)	1(1)	-1(1)
C(14)	22(1)	23(1)	29(1)	-3(1)	4(1)	-3(1)
C(15)	24(1)	18(1)	22(1)	3(1)	1(1)	-1(1)
C(16)	18(1)	21(1)	20(1)	0(1)	5(1)	1(1)
C(17)	32(1)	22(1)	20(1)	-2(1)	1(1)	-4(1)
C(18)	66(2)	30(2)	24(1)	-2(1)	-11(1)	-3(1)
Br(2)	41(1)	23(1)	37(1)	-8(1)	8(1)	-2(1)
O(5)	21(1)	18(1)	36(1)	4(1)	9(1)	2(1)
O(6)	18(1)	21(1)	30(1)	6(1)	7(1)	3(1)
O(7)	27(1)	32(1)	43(1)	-8(1)	2(1)	10(1)
O(8)	26(1)	23(1)	30(1)	-2(1)	6(1)	4(1)
B(2)	23(1)	20(1)	24(1)	-3(1)	6(1)	0(1)
C(19)	23(1)	19(1)	25(1)	-1(1)	2(1)	1(1)
C(20)	20(1)	24(1)	21(1)	3(1)	4(1)	0(1)
C(21)	18(1)	18(1)	27(1)	2(1)	3(1)	-3(1)
C(22)	20(1)	18(1)	26(1)	4(1)	1(1)	5(1)
C(23)	26(1)	17(1)	38(2)	4(1)	10(1)	2(1)
C(24)	25(1)	18(1)	43(2)	5(1)	6(1)	0(1)
C(25)	21(1)	22(1)	25(1)	1(1)	6(1)	3(1)
C(26)	25(1)	18(1)	33(1)	3(1)	7(1)	2(1)
C(27)	26(1)	16(1)	29(1)	2(1)	7(1)	3(1)
C(28)	38(2)	28(1)	32(1)	2(1)	17(1)	1(1)
C(29)	38(2)	21(1)	50(2)	7(1)	15(1)	-2(1)
C(30)	26(1)	28(1)	34(1)	3(1)	3(1)	4(1)
C(31)	34(1)	25(1)	32(1)	-2(1)	7(1)	7(1)
C(32)	33(2)	26(1)	32(1)	6(1)	14(1)	6(1)
C(33)	23(1)	27(1)	29(1)	-1(1)	2(1)	8(1)
C(34)	28(1)	26(1)	23(1)	0(1)	4(1)	4(1)
C(35)	28(1)	20(1)	32(1)	-2(1)	8(1)	5(1)
C(36)	30(1)	26(1)	37(2)	-3(1)	5(1)	3(1)
Br(3)	30(1)	26(1)	31(1)	11(1)	3(1)	3(1)

O(9)	17(1)	22(1)	25(1)	-9(1)	7(1)	-2(1)
O(10)	16(1)	38(1)	54(1)	-30(1)	14(1)	-10(1)
O(11)	28(1)	17(1)	31(1)	-1(1)	-3(1)	-2(1)
O(12)	19(1)	22(1)	25(1)	3(1)	-2(1)	-1(1)
B(3)	12(1)	16(1)	25(1)	0(1)	4(1)	-3(1)
C(37)	24(1)	21(1)	16(1)	4(1)	0(1)	0(1)
C(38)	15(1)	26(1)	26(1)	2(1)	4(1)	3(1)
C(39)	14(1)	22(1)	27(1)	1(1)	6(1)	-4(1)
C(40)	15(1)	14(1)	17(1)	-3(1)	3(1)	0(1)
C(41)	14(1)	22(1)	21(1)	-1(1)	4(1)	0(1)
C(42)	19(1)	22(1)	20(1)	-1(1)	7(1)	-3(1)
C(43)	12(1)	15(1)	22(1)	0(1)	4(1)	-1(1)
C(44)	26(2)	19(2)	27(2)	-7(2)	7(2)	-3(2)
C(45)	23(2)	17(2)	35(2)	-11(2)	6(2)	-2(1)
C(46)	65(3)	37(2)	22(2)	1(2)	4(2)	-1(2)
C(47)	33(2)	34(2)	42(2)	-20(2)	12(2)	1(2)
C(48)	22(2)	56(4)	46(4)	-20(2)	4(2)	-14(2)
C(49)	65(3)	20(2)	39(2)	-7(2)	16(2)	-12(2)
C(44X)	26(2)	19(2)	27(2)	-7(2)	7(2)	-3(2)
C(45X)	12(5)	22(6)	54(8)	-15(5)	5(5)	4(4)
C(46X)	24(6)	42(7)	37(7)	-21(6)	0(5)	-3(5)
C(47X)	45(7)	26(5)	50(7)	-7(5)	-2(6)	4(5)
C(48X)	22(2)	56(4)	46(4)	-20(2)	4(2)	-14(2)
C(49X)	65(3)	20(2)	39(2)	-7(2)	16(2)	-12(2)
C(50)	20(1)	20(1)	23(1)	0(1)	8(1)	-2(1)
C(51)	17(1)	16(1)	20(1)	1(1)	2(1)	-2(1)
C(52)	19(1)	22(1)	18(1)	0(1)	3(1)	1(1)
C(53)	29(1)	23(1)	24(1)	4(1)	0(1)	2(1)
C(54)	24(2)	35(3)	26(3)	10(2)	-1(2)	0(2)
C(54X)	24(2)	35(3)	26(3)	10(2)	-1(2)	0(2)
Br(4)	21(1)	25(1)	38(1)	-15(1)	4(1)	-1(1)
O(13)	14(1)	20(1)	25(1)	2(1)	6(1)	1(1)
O(14)	15(1)	18(1)	27(1)	6(1)	6(1)	2(1)
O(15)	37(1)	21(1)	30(1)	-2(1)	15(1)	-2(1)
O(16)	34(1)	24(1)	27(1)	-7(1)	17(1)	-4(1)
B(4)	15(1)	15(1)	22(1)	-4(1)	8(1)	1(1)

C(55)	20(1)	16(1)	21(1)	-4(1)	4(1)	0(1)
C(56)	17(1)	20(1)	23(1)	-1(1)	7(1)	4(1)
C(57)	13(1)	23(1)	21(1)	0(1)	5(1)	-1(1)
C(58)	18(1)	16(1)	14(1)	2(1)	4(1)	1(1)
C(59)	15(1)	23(1)	28(1)	-3(1)	4(1)	2(1)
C(60)	14(1)	26(1)	28(1)	-6(1)	2(1)	-2(1)
C(61)	14(1)	17(1)	18(1)	-2(1)	4(1)	0(1)
C(62)	18(1)	16(1)	23(1)	2(1)	6(1)	1(1)
C(63)	15(1)	16(1)	29(1)	6(1)	6(1)	3(1)
C(64)	36(2)	28(1)	27(1)	-3(1)	4(1)	-1(1)
C(65)	20(1)	23(1)	38(1)	8(1)	3(1)	5(1)
C(66)	24(1)	30(1)	38(2)	12(1)	16(1)	6(1)
C(67)	24(1)	18(1)	39(2)	3(1)	5(1)	-2(1)
C(68)	20(1)	18(1)	19(1)	-2(1)	2(1)	-1(1)
C(69)	20(1)	19(1)	24(1)	-2(1)	10(1)	-3(1)
C(70)	22(1)	22(1)	22(1)	-2(1)	6(1)	3(1)
C(71)	34(1)	26(1)	31(1)	-13(1)	13(1)	-4(1)
C(72)	59(4)	45(2)	27(4)	-17(3)	25(3)	-14(3)
C(72X)	59(4)	45(2)	27(4)	-17(3)	25(3)	-14(3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\approx \times 10^3$) for $C_{18}H_{26}BBrO_4$

	x	y	z	U(eq)
H(2)	9033	4813	5543	31
H(3)	8153	3655	5068	28
H(5)	4845	4309	5417	26
H(6)	5708	5476	5869	28
H(10A)	10032	2436	5742	44
H(10B)	9819	1925	6348	44
H(10C)	8944	2656	6106	44
H(11A)	9887	1405	5003	44
H(11B)	8706	848	4829	44
H(11C)	9673	746	5508	44

H(12A)	7160	930	6684	52
H(12B)	8111	1644	6772	52
H(12C)	8556	790	6616	52
H(13A)	6259	409	5654	47
H(13B)	7525	212	5435	47
H(13C)	6521	762	4989	47
H(14A)	4000	3357	4829	37
H(14B)	4594	2905	5489	37
H(14C)	4229	2436	4816	37
H(15A)	5204	3567	3969	26
H(15B)	6598	3266	4069	26
H(17A)	3759	1544	2993	30
H(17B)	4991	1524	2702	30
H(18A)	3246	1728	1849	64
H(18B)	4134	2473	1918	64
H(18C)	2909	2496	2209	64
H(20)	2903	5653	6139	26
H(21)	2530	6648	6831	25
H(23)	416	5200	7651	32
H(24)	718	4211	6936	34
H(28A)	1045	8027	5736	47
H(28B)	-379	8275	5608	47
H(28C)	54	7459	5951	47
H(29A)	1814	9143	6345	53
H(29B)	1360	9397	6991	53
H(29C)	495	9549	6289	53
H(30A)	-2557	8417	6639	45
H(30B)	-1960	7974	6108	45
H(30C)	-1925	8906	6147	45
H(31A)	-1355	8969	7595	45
H(31B)	-547	9521	7231	45
H(31C)	119	8907	7766	45
H(32A)	711	6038	8497	44
H(32B)	-445	6347	7966	44
H(32C)	283	6928	8511	44
H(33A)	2762	6536	8537	32

H(33B)	3140	6896	7902	32
H(35A)	3445	8844	9293	32
H(35B)	3601	9117	8580	32
H(36A)	5418	9397	9356	47
H(36B)	5705	8763	8848	47
H(36C)	5549	8496	9558	47
H(38)	5641	5592	1982	27
H(39)	5134	6728	1376	25
H(41)	1547	6439	1462	23
H(42)	2053	5301	2070	24
H(46A)	4018	7904	2810	63
H(46B)	2747	8031	3045	63
H(46C)	3893	8597	3304	63
H(47A)	1874	9793	2141	53
H(47B)	2568	9762	2891	53
H(47C)	1420	9198	2630	53
H(48A)	5469	8852	2832	62
H(48B)	5130	9758	2854	62
H(48C)	5927	9454	2349	62
H(49A)	2945	9785	1326	61
H(49B)	4371	10006	1397	61
H(49C)	3611	10340	1909	61
H(46D)	2398	8539	3070	53
H(46E)	1321	9082	2675	53
H(46F)	2531	9468	3113	53
H(47D)	2929	9749	1473	63
H(47E)	2857	10220	2124	63
H(47F)	1642	9822	1701	63
H(48D)	3985	7791	2851	62
H(48E)	4457	8511	3324	62
H(48F)	5401	8056	2975	62
H(49D)	4969	9884	2099	61
H(49E)	6006	9294	2466	61
H(49F)	5144	9747	2869	61
H(50A)	3666	7136	130	31
H(50B)	4687	7545	683	31

H(50C)	3649	8062	226	31
H(51A)	1497	7022	260	21
H(51B)	1087	7362	892	21
H(53A)	59	8785	-998	31
H(53B)	-213	9229	-369	31
H(54A)	-2039	9056	-1139	44
H(54B)	-2093	8577	-490	44
H(54C)	-1822	8133	-1118	44
H(54D)	-1889	8833	-1389	44
H(54E)	-2091	8219	-846	44
H(54F)	-1253	7991	-1354	44
H(56)	355	4698	9222	24
H(57)	-19	3613	8540	22
H(59)	3627	3418	8579	26
H(60)	4012	4518	9248	28
H(64A)	3804	2052	10224	46
H(64B)	2722	1619	10485	46
H(64C)	2404	2331	9984	46
H(65A)	4579	913	9811	41
H(65B)	3735	367	9278	41
H(65C)	3600	334	10023	41
H(66A)	-81	696	9683	44
H(66B)	693	1394	10080	44
H(66C)	1191	517	10183	44
H(67A)	493	104	8778	40
H(67B)	1850	-147	9148	40
H(67C)	1669	383	8506	40
H(68A)	57	2981	7370	29
H(68B)	-377	2636	7996	29
H(68C)	75	2059	7493	29
H(69A)	2231	2953	7288	24
H(69B)	3284	2650	7880	24
H(71A)	2072	795	6328	35
H(71B)	3429	640	6762	35
H(72A)	3510	672	5642	62
H(72B)	4296	1380	6015	62

H(72C)	2945	1534	5583	62
H(72D)	3881	553	5863	62
H(72E)	4640	1165	6370	62
H(72F)	3633	1468	5758	62

Table 6. Torsion angles [$^{\circ}$] for $C_{18}H_{26}BBrO_4$

C(9)-O(2)-B(1)-O(1)	-9.4(3)
C(9)-O(2)-B(1)-C(7)	175.5(2)
C(8)-O(1)-B(1)-O(2)	-10.7(3)
C(8)-O(1)-B(1)-C(7)	164.3(2)
C(6)-C(1)-C(2)-C(3)	-0.4(4)
Br(1)-C(1)-C(2)-C(3)	178.45(18)
C(1)-C(2)-C(3)-C(4)	-0.9(4)
C(2)-C(3)-C(4)-C(5)	1.3(3)
C(2)-C(3)-C(4)-C(7)	-179.7(2)
C(3)-C(4)-C(5)-C(6)	-0.5(3)
C(7)-C(4)-C(5)-C(6)	-179.5(2)
C(2)-C(1)-C(6)-C(5)	1.1(4)
Br(1)-C(1)-C(6)-C(5)	-177.67(17)
C(4)-C(5)-C(6)-C(1)	-0.7(4)
C(5)-C(4)-C(7)-C(14)	-12.4(3)
C(3)-C(4)-C(7)-C(14)	168.6(2)
C(5)-C(4)-C(7)-C(15)	107.6(2)
C(3)-C(4)-C(7)-C(15)	-71.4(3)
C(5)-C(4)-C(7)-B(1)	-133.1(2)
C(3)-C(4)-C(7)-B(1)	47.8(3)
O(2)-B(1)-C(7)-C(14)	-26.2(3)
O(1)-B(1)-C(7)-C(14)	159.3(2)
O(2)-B(1)-C(7)-C(15)	-146.8(2)
O(1)-B(1)-C(7)-C(15)	38.6(3)
O(2)-B(1)-C(7)-C(4)	96.0(3)
O(1)-B(1)-C(7)-C(4)	-78.6(3)
B(1)-O(1)-C(8)-C(11)	146.8(2)
B(1)-O(1)-C(8)-C(10)	-94.9(2)

B(1)-O(1)-C(8)-C(9)	24.6(2)
B(1)-O(2)-C(9)-C(12)	146.0(2)
B(1)-O(2)-C(9)-C(13)	-95.0(2)
B(1)-O(2)-C(9)-C(8)	23.9(2)
O(1)-C(8)-C(9)-O(2)	-29.1(2)
C(11)-C(8)-C(9)-O(2)	-147.02(19)
C(10)-C(8)-C(9)-O(2)	85.0(2)
O(1)-C(8)-C(9)-C(12)	-146.6(2)
C(11)-C(8)-C(9)-C(12)	95.6(3)
C(10)-C(8)-C(9)-C(12)	-32.4(3)
O(1)-C(8)-C(9)-C(13)	84.7(2)
C(11)-C(8)-C(9)-C(13)	-33.1(3)
C(10)-C(8)-C(9)-C(13)	-161.1(2)
C(14)-C(7)-C(15)-C(16)	-62.6(3)
C(4)-C(7)-C(15)-C(16)	175.98(19)
B(1)-C(7)-C(15)-C(16)	58.1(3)
C(17)-O(4)-C(16)-O(3)	0.5(3)
C(17)-O(4)-C(16)-C(15)	-179.9(2)
C(7)-C(15)-C(16)-O(3)	-26.8(3)
C(7)-C(15)-C(16)-O(4)	153.6(2)
C(16)-O(4)-C(17)-C(18)	172.4(2)
C(27)-O(6)-B(2)-O(5)	-12.0(3)
C(27)-O(6)-B(2)-C(25)	171.4(2)
C(26)-O(5)-B(2)-O(6)	-7.7(3)
C(26)-O(5)-B(2)-C(25)	168.9(2)
C(24)-C(19)-C(20)-C(21)	-1.0(4)
Br(2)-C(19)-C(20)-C(21)	178.91(17)
C(19)-C(20)-C(21)-C(22)	1.2(3)
C(20)-C(21)-C(22)-C(23)	-0.1(3)
C(20)-C(21)-C(22)-C(25)	179.2(2)
C(21)-C(22)-C(23)-C(24)	-1.1(4)
C(25)-C(22)-C(23)-C(24)	179.6(2)
C(20)-C(19)-C(24)-C(23)	-0.2(4)
Br(2)-C(19)-C(24)-C(23)	179.87(19)
C(22)-C(23)-C(24)-C(19)	1.3(4)
C(23)-C(22)-C(25)-C(32)	-2.6(3)

C(21)-C(22)-C(25)-C(32)	178.2(2)
C(23)-C(22)-C(25)-C(33)	118.0(3)
C(21)-C(22)-C(25)-C(33)	-61.3(3)
C(23)-C(22)-C(25)-B(2)	-123.7(2)
C(21)-C(22)-C(25)-B(2)	57.0(3)
O(6)-B(2)-C(25)-C(32)	-22.4(3)
O(5)-B(2)-C(25)-C(32)	161.2(2)
O(6)-B(2)-C(25)-C(22)	100.7(3)
O(5)-B(2)-C(25)-C(22)	-75.6(3)
O(6)-B(2)-C(25)-C(33)	-142.7(2)
O(5)-B(2)-C(25)-C(33)	40.9(3)
B(2)-O(5)-C(26)-C(29)	144.5(2)
B(2)-O(5)-C(26)-C(28)	-96.2(2)
B(2)-O(5)-C(26)-C(27)	22.5(2)
B(2)-O(6)-C(27)-C(30)	147.1(2)
B(2)-O(6)-C(27)-C(31)	-93.5(2)
B(2)-O(6)-C(27)-C(26)	24.8(2)
O(5)-C(26)-C(27)-O(6)	-28.4(2)
C(29)-C(26)-C(27)-O(6)	-145.8(2)
C(28)-C(26)-C(27)-O(6)	86.0(2)
O(5)-C(26)-C(27)-C(30)	-146.3(2)
C(29)-C(26)-C(27)-C(30)	96.2(3)
C(28)-C(26)-C(27)-C(30)	-32.0(3)
O(5)-C(26)-C(27)-C(31)	85.5(2)
C(29)-C(26)-C(27)-C(31)	-32.0(3)
C(28)-C(26)-C(27)-C(31)	-160.2(2)
C(32)-C(25)-C(33)-C(34)	-77.2(3)
C(22)-C(25)-C(33)-C(34)	160.4(2)
B(2)-C(25)-C(33)-C(34)	42.9(3)
C(35)-O(8)-C(34)-O(7)	-5.3(4)
C(35)-O(8)-C(34)-C(33)	172.9(2)
C(25)-C(33)-C(34)-O(7)	11.0(4)
C(25)-C(33)-C(34)-O(8)	-167.1(2)
C(34)-O(8)-C(35)-C(36)	178.1(2)
C(44)-O(9)-B(3)-O(10)	-10.2(3)
C(44)-O(9)-B(3)-C(43)	164.6(2)

C(45)-O(10)-B(3)-O(9)	-14.0(3)
C(45)-O(10)-B(3)-C(43)	171.2(3)
C(42)-C(37)-C(38)-C(39)	-0.4(4)
Br(3)-C(37)-C(38)-C(39)	179.82(18)
C(37)-C(38)-C(39)-C(40)	-0.6(4)
C(38)-C(39)-C(40)-C(41)	1.4(3)
C(38)-C(39)-C(40)-C(43)	179.2(2)
C(39)-C(40)-C(41)-C(42)	-1.4(3)
C(43)-C(40)-C(41)-C(42)	-179.1(2)
C(38)-C(37)-C(42)-C(41)	0.4(3)
Br(3)-C(37)-C(42)-C(41)	-179.78(17)
C(40)-C(41)-C(42)-C(37)	0.5(3)
C(41)-C(40)-C(43)-C(51)	-26.1(3)
C(39)-C(40)-C(43)-C(51)	156.3(2)
C(41)-C(40)-C(43)-C(50)	-147.4(2)
C(39)-C(40)-C(43)-C(50)	35.0(3)
C(41)-C(40)-C(43)-B(3)	92.7(2)
C(39)-C(40)-C(43)-B(3)	-84.9(2)
O(9)-B(3)-C(43)-C(40)	-82.9(3)
O(10)-B(3)-C(43)-C(40)	91.3(3)
O(9)-B(3)-C(43)-C(51)	36.0(3)
O(10)-B(3)-C(43)-C(51)	-149.7(2)
O(9)-B(3)-C(43)-C(50)	157.1(2)
O(10)-B(3)-C(43)-C(50)	-28.7(3)
B(3)-O(9)-C(44)-C(46)	-91.5(3)
B(3)-O(9)-C(44)-C(47)	147.9(3)
B(3)-O(9)-C(44)-C(45)	28.3(3)
B(3)-O(10)-C(45)-C(48)	148.2(3)
B(3)-O(10)-C(45)-C(49)	-90.1(3)
B(3)-O(10)-C(45)-C(44)	29.7(3)
O(9)-C(44)-C(45)-O(10)	-34.7(3)
C(46)-C(44)-C(45)-O(10)	81.0(4)
C(47)-C(44)-C(45)-O(10)	-151.1(3)
O(9)-C(44)-C(45)-C(48)	-148.7(4)
C(46)-C(44)-C(45)-C(48)	-33.0(5)
C(47)-C(44)-C(45)-C(48)	94.9(5)

O(9)-C(44)-C(45)-C(49)	81.2(3)
C(46)-C(44)-C(45)-C(49)	-163.0(3)
C(47)-C(44)-C(45)-C(49)	-35.2(5)
C(40)-C(43)-C(51)-C(52)	175.74(18)
C(50)-C(43)-C(51)-C(52)	-62.0(2)
B(3)-C(43)-C(51)-C(52)	60.0(2)
C(53)-O(12)-C(52)-O(11)	3.4(3)
C(53)-O(12)-C(52)-C(51)	-177.77(19)
C(43)-C(51)-C(52)-O(11)	-16.5(3)
C(43)-C(51)-C(52)-O(12)	164.65(19)
C(52)-O(12)-C(53)-C(54)	-158.1(3)
C(63)-O(14)-B(4)-O(13)	-12.4(2)
C(63)-O(14)-B(4)-C(61)	173.93(19)
C(62)-O(13)-B(4)-O(14)	-8.7(2)
C(62)-O(13)-B(4)-C(61)	164.9(2)
C(60)-C(55)-C(56)-C(57)	0.8(3)
Br(4)-C(55)-C(56)-C(57)	-176.91(17)
C(55)-C(56)-C(57)-C(58)	0.4(3)
C(56)-C(57)-C(58)-C(59)	-1.1(3)
C(56)-C(57)-C(58)-C(61)	173.9(2)
C(57)-C(58)-C(59)-C(60)	0.5(3)
C(61)-C(58)-C(59)-C(60)	-174.5(2)
C(56)-C(55)-C(60)-C(59)	-1.4(4)
Br(4)-C(55)-C(60)-C(59)	176.34(18)
C(58)-C(59)-C(60)-C(55)	0.8(4)
C(59)-C(58)-C(61)-C(68)	-159.2(2)
C(57)-C(58)-C(61)-C(68)	26.0(3)
C(59)-C(58)-C(61)-C(69)	-37.1(3)
C(57)-C(58)-C(61)-C(69)	148.2(2)
C(59)-C(58)-C(61)-B(4)	81.8(2)
C(57)-C(58)-C(61)-B(4)	-92.9(2)
O(14)-B(4)-C(61)-C(68)	-22.9(3)
O(13)-B(4)-C(61)-C(68)	164.1(2)
O(14)-B(4)-C(61)-C(58)	97.5(2)
O(13)-B(4)-C(61)-C(58)	-75.5(3)
O(14)-B(4)-C(61)-C(69)	-143.7(2)

O(13)-B(4)-C(61)-C(69)	43.3(3)
B(4)-O(13)-C(62)-C(64)	-94.9(2)
B(4)-O(13)-C(62)-C(65)	145.52(19)
B(4)-O(13)-C(62)-C(63)	24.5(2)
B(4)-O(14)-C(63)-C(66)	148.4(2)
B(4)-O(14)-C(63)-C(67)	-92.3(2)
B(4)-O(14)-C(63)-C(62)	26.5(2)
O(13)-C(62)-C(63)-O(14)	-30.8(2)
C(64)-C(62)-C(63)-O(14)	83.8(2)
C(65)-C(62)-C(63)-O(14)	-148.48(19)
O(13)-C(62)-C(63)-C(66)	-148.52(19)
C(64)-C(62)-C(63)-C(66)	-33.9(3)
C(65)-C(62)-C(63)-C(66)	93.8(2)
O(13)-C(62)-C(63)-C(67)	82.5(2)
C(64)-C(62)-C(63)-C(67)	-162.9(2)
C(65)-C(62)-C(63)-C(67)	-35.2(3)
C(68)-C(61)-C(69)-C(70)	-65.2(2)
C(58)-C(61)-C(69)-C(70)	170.71(19)
B(4)-C(61)-C(69)-C(70)	56.3(3)
C(71)-O(16)-C(70)-O(15)	-1.2(4)
C(71)-O(16)-C(70)-C(69)	177.4(2)
C(61)-C(69)-C(70)-O(15)	-19.6(4)
C(61)-C(69)-C(70)-O(16)	161.9(2)
C(70)-O(16)-C(71)-C(72)	178.5(6)

Symmetry transformations used to generate equivalent atoms: