Compound 2

Table 1. Crystal data and structure refinement for 2.

Identification code	2	
Empirical formula	$C_9 H_{14} O_2$	
Formula weight	154.20	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P 2_1$	
Unit cell dimensions	a = 6.1182(3) Å	α= 90°.
	b = 6.6921(4) Å	β= 94.019(3)°.
	c = 10.1810(5) Å	γ = 90°.
Volume	415.82(4) $Å^3$	
Z	2	
Density (calculated)	1.232 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	168	
Crystal size	0.25 x 0.18 x 0.08 mm^3	
Theta range for data collection	3.34 to 30.02°.	
Index ranges	-8<=h<=8, -9<=k<=9, -14<=l<=14	
Reflections collected	4157	
Independent reflections (Pt Gp 2/m)	1316 [R(int) = 0.036]	
Independent reflections (Pt Gp 2)	2340	
Completeness to theta = 30.02°	99.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2340 / 1 / 108	
Goodness-of-fit on F^2	1.042	
R indices [2043 I>2sigma(I)]	R1 = 0.0425, wR2 = 0.0878	
R indices (all data)	R1 = 0.0541, wR2 = 0.0929	
Absolute structure parameter	-0.2(11)	
Largest diff. peak and hole	0.26 and -0.18 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	3583(2)	9663(2)	6318(1)	14(1)
C(2)	2837(2)	7801(2)	7003(1)	14(1)
C(3)	1649(2)	8475(2)	8200(1)	16(1)
C(4)	1847(2)	10774(2)	8066(1)	16(1)
C(5)	369(2)	11540(2)	6887(1)	18(1)
C(6)	1461(2)	10642(2)	5694(1)	16(1)
C(7)	4121(2)	11026(2)	7516(1)	16(1)
C(8)	2909(3)	7702(3)	9457(1)	22(1)
C(9)	-685(2)	7639(2)	8138(1)	20(1)
O(1)	5203(2)	9183(2)	5465(1)	20(1)
O(2)	3147(2)	6092(2)	6677(1)	22(1)
H(4)	1673	11520	8903	22(2)
H(5A)	360	13018	6853	22(2)
H(5B)	-1153	11052	6926	22(2)
H(6A)	1805	11697	5059	22(2)
H(6B)	499	9634	5236	22(2)
H(7A)	4429	12422	7265	22(2)
H(7B)	5328	10501	8117	22(2)
H(8A)	2991	6240	9426	29(2)
H(8B)	2145	8111	10227	29(2)
H(8C)	4393	8260	9519	29(2)
H(9A)	-1439	7973	7285	29(2)
H(9B)	-1480	8225	8846	29(2)
H(9C)	-629	6184	8242	29(2)
H(1)	5380(40)	10140(40)	4970(30)	45(7)

Table 3. Bond lengths [Å] and angles [°] for 2.

C(1)-O(1)	1.4002(17)	C(5)-H(5A)	0.9900
C(1)-C(2)	1.514(2)	C(5)-H(5B)	0.9900
C(1)-C(7)	1.539(2)	C(6)-H(6A)	0.9900
C(1)-C(6)	1.5503(19)	C(6)-H(6B)	0.9900
C(2)-O(2)	1.2099(19)	C(7)-H(7A)	0.9900
C(2)-C(3)	1.530(2)	C(7)-H(7B)	0.9900
C(3)-C(9)	1.531(2)	C(8)-H(8A)	0.9800
C(3)-C(8)	1.536(2)	C(8)-H(8B)	0.9800
C(3)-C(4)	1.550(2)	C(8)-H(8C)	0.9800
C(4)-C(5)	1.539(2)	C(9)-H(9A)	0.9800
C(4)-C(7)	1.5450(19)	C(9)-H(9B)	0.9800
C(4)-H(4)	1.0000	C(9)-H(9C)	0.9800
C(5)-C(6)	1.5483(19)	O(1)-H(1)	0.82(3)
O(1)-C(1)-C(2)	110.24(12)	C(9)-C(3)-C(8)	108.88(12)
O(1)-C(1)-C(7)	120.40(12)	C(2)-C(3)-C(4)	100.25(11)
C(2)-C(1)-C(7)	100.21(10)	C(9)-C(3)-C(4)	115.92(12)
O(1)-C(1)-C(6)	116.84(11)	C(8)-C(3)-C(4)	111.70(13)
C(2)-C(1)-C(6)	105.40(11)	C(5)-C(4)-C(7)	100.11(11)
C(7)-C(1)-C(6)	101.60(11)	C(5)-C(4)-C(3)	110.73(12)
O(2)-C(2)-C(1)	126.45(13)	C(7)-C(4)-C(3)	102.58(11)
O(2)-C(2)-C(3)	126.10(13)	C(4)-C(5)-C(6)	102.75(11)
C(1)-C(2)-C(3)	107.45(12)	C(5)-C(6)-C(1)	103.71(11)
C(2)-C(3)-C(9)	110.69(12)	C(1)-C(7)-C(4)	94.29(11)
C(2)-C(3)-C(8)	109.01(12)	C(1)-O(1)-H(1)	109.4(17)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2. 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}
C(1)	16(1)	13(1)	13(1)	1(1)	4(1)	0(1)
C(2)	15(1)	15(1)	14(1)	0(1)	2(1)	1(1)
C(3)	16(1)	16(1)	15(1)	2(1)	4(1)	2(1)
C(4)	19(1)	15(1)	14(1)	-2(1)	1(1)	2(1)
C(5)	18(1)	16(1)	20(1)	2(1)	3(1)	4(1)
C(6)	17(1)	15(1)	16(1)	2(1)	-1(1)	0(1)
C(7)	18(1)	14(1)	16(1)	0(1)	1(1)	-1(1)
C(8)	25(1)	26(1)	17(1)	5(1)	3(1)	4(1)
C(9)	21(1)	20(1)	21(1)	4(1)	6(1)	-1(1)
O(1)	24(1)	19(1)	19(1)	4(1)	11(1)	4(1)
O(2)	29(1)	14(1)	24(1)	0(1)	10(1)	2(1)

Table 5. Torsion angles [°] for 2.

O(1)-C(1)-C(2)-O(2)	-16.4(2)
C(7)-C(1)-C(2)-O(2)	-144.31(15)
C(6)-C(1)-C(2)-O(2)	110.52(16)
O(1)-C(1)-C(2)-C(3)	162.66(12)
C(7)-C(1)-C(2)-C(3)	34.75(13)
C(6)-C(1)-C(2)-C(3)	-70.41(13)
O(2)-C(2)-C(3)-C(9)	-57.9(2)
C(1)-C(2)-C(3)-C(9)	123.00(13)
O(2)-C(2)-C(3)-C(8)	61.80(19)
C(1)-C(2)-C(3)-C(8)	-117.27(13)
O(2)-C(2)-C(3)-C(4)	179.17(14)
C(1)-C(2)-C(3)-C(4)	0.11(14)
C(2)-C(3)-C(4)-C(5)	70.96(14)
C(9)-C(3)-C(4)-C(5)	-48.19(17)
C(8)-C(3)-C(4)-C(5)	-173.68(11)
C(2)-C(3)-C(4)-C(7)	-35.11(14)
C(9)-C(3)-C(4)-C(7)	-154.26(11)
C(8)-C(3)-C(4)-C(7)	80.25(14)
C(7)-C(4)-C(5)-C(6)	40.51(13)
C(3)-C(4)-C(5)-C(6)	-67.18(14)
C(4)-C(5)-C(6)-C(1)	-6.10(14)
O(1)-C(1)-C(6)-C(5)	-163.67(12)
C(2)-C(1)-C(6)-C(5)	73.53(13)
C(7)-C(1)-C(6)-C(5)	-30.61(13)
O(1)-C(1)-C(7)-C(4)	-174.78(12)
C(2)-C(1)-C(7)-C(4)	-53.90(12)
C(6)-C(1)-C(7)-C(4)	54.31(12)
C(5)-C(4)-C(7)-C(1)	-58.36(12)
C(3)-C(4)-C(7)-C(1)	55.73(12)

Table 6. Hydrogen bonds for 2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#1	0.82(3)	2.06(3)	2.7780(14)	145(2)

Symmetry transformations used to generate equivalent atoms:

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

(a) Compound 3

Table 1. Crystal data and structure refinement for 3.

Identification code	3	
Empirical formula	$C_{10}H_{16}O$	
Formula weight	152.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 5.9714(1) Å	α= 90°.
	b = 20.5466(5) Å	β= 90°.
	c = 22.5632(6) Å	γ = 90°.
Volume	2768.32(11) $Å^3$	
Z	12	
Density (calculated)	1.096 Mg/m^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	1008	
Crystal size	0.75 x 0.06 x 0.04 mm^3	
Theta range for data collection	2.06 to 25.20°.	
Index ranges	0<=h<=7, 0<=k<=23, 0<=l<=27	
Reflections collected	15934	
Independent reflections	2845 [R(int) = 0.069]	
Completeness to theta = 25.20°	98.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2845 / 0 / 304	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0508, wR2 = 0.0996	
R indices (all data)	R1 = 0.0671, wR2 = 0.1081	
Absolute structure parameter	Not determined	
Largest diff. peak and hole	0.21 and -0.21 e.$Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	3698(5)	7151(1)	3229(1)	21(1)
C(2)	3011(5)	6533(1)	3549(1)	20(1)
C(3)	4188(6)	6559(2)	4153(1)	27(1)
C(4)	5351(6)	7234(2)	4117(1)	27(1)
C(5)	3618(7)	7787(2)	4123(2)	39(1)
C(6)	2426(6)	7719(1)	3510(1)	28(1)
C(7)	6072(5)	7259(2)	3466(1)	24(1)
C(8)	1681(6)	6075(1)	3344(2)	30(1)
C(9)	5930(7)	6013(2)	4204(2)	36(1)
C(10)	2531(8)	6493(2)	4672(2)	45(1)
C(11)	-3176(5)	5686(1)	1939(1)	20(1)
C(12)	-4005(5)	5697(1)	1301(1)	21(1)
C(13)	-2978(6)	5104(1)	996(1)	22(1)
C(14)	-1796(6)	4770(1)	1531(1)	22(1)
C(15)	-3525(6)	4515(1)	1981(1)	27(1)
C(16)	-4481(6)	5148(1)	2266(1)	24(1)
C(17)	-877(6)	5364(2)	1873(1)	23(1)
C(18)	-5392(6)	6130(1)	1075(2)	28(1)
C(19)	-1234(7)	5314(2)	532(1)	32(1)
C(20)	-4737(7)	4685(2)	688(2)	33(1)
C(21)	-239(5)	7676(1)	1434(1)	20(1)
C(22)	-1091(6)	8332(1)	1639(1)	22(1)

C(23)	-358(5)	8825(1)	1162(1)	20(1)
C(24)	867(6)	8366(1)	717(1)	22(1)
C(25)	-820(6)	7924(1)	396(1)	25(1)
C(26)	-1645(6)	7459(1)	894(1)	24(1)
C(27)	1972(5)	7869(1)	1135(1)	22(1)
C(28)	-2257(7)	8449(2)	2122(2)	43(1)
C(29)	1268(6)	9326(1)	1415(2)	31(1)
C(30)	-2361(6)	9192(2)	899(2)	32(1)
O(1)	3413(4)	7136(1)	2602(1)	26(1)
O(2)	-3299(4)	6287(1)	2244(1)	23(1)
O(3)	-200(4)	7176(1)	1867(1)	27(1)

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

C(1)-O(1)	1.424(3)	C(13)-C(14)	1.557(4)
C(1)-C(2)	1.517(4)	C(14)-C(15)	1.541(4)
C(1)-C(7)	1.531(4)	C(14)-C(17)	1.545(4)
C(1)-C(6)	1.530(4)	C(15)-C(16)	1.559(4)
C(2)-C(8)	1.317(4)	C(21)-O(3)	1.418(3)
C(2)-C(3)	1.534(4)	C(21)-C(22)	1.514(4)
C(3)-C(9)	1.534(5)	C(21)-C(27)	1.534(4)
C(3)-C(10)	1.539(5)	C(21)-C(26)	1.545(4)
C(3)-C(4)	1.554(4)	C(22)-C(28)	1.315(5)
C(4)-C(7)	1.532(4)	C(22)-C(23)	1.540(4)
C(4)-C(5)	1.537(5)	C(23)-C(29)	1.526(4)
C(5)-C(6)	1.561(5)	C(23)-C(30)	1.534(5)
C(11)-O(2)	1.415(3)	C(23)-C(24)	1.559(4)
C(11)-C(12)	1.524(4)	C(24)-C(27)	1.539(4)
C(11)-C(17)	1.531(4)	C(24)-C(25)	1.539(4)
C(11)-C(16)	1.540(4)	C(25)-C(26)	1.554(4)
C(12)-C(18)	1.318(4)	O(1)-O(3)	2.723(3)
C(12)-C(13)	1.526(4)	O(1)-O(2)#1	2.749(3)
C(13)-C(20)	1.527(5)	O(2)-O(3)	2.736(3)
C(13)-C(19)	1.539(5)	O(2)-O(1)#2	2.749(3)

O(1)-C(1)-C(2)	115.0(2)	C(12)-C(11)-C(16)	107.3(2)
O(1)-C(1)-C(7)	117.4(3)	C(17)-C(11)-C(16)	100.9(2)
C(2)-C(1)-C(7)	101.8(3)	C(18)-C(12)-C(11)	125.3(3)
O(1)-C(1)-C(6)	111.6(2)	C(18)-C(12)-C(13)	128.2(3)
C(2)-C(1)-C(6)	107.9(2)	C(11)-C(12)-C(13)	106.5(2)
C(7)-C(1)-C(6)	101.8(2)	C(12)-C(13)-C(20)	112.3(3)
C(8)-C(2)-C(1)	126.4(3)	C(12)-C(13)-C(19)	110.7(2)
C(8)-C(2)-C(3)	127.9(3)	C(20)-C(13)-C(19)	108.3(3)
C(1)-C(2)-C(3)	105.7(2)	C(12)-C(13)-C(14)	100.7(2)
C(9)-C(3)-C(2)	110.6(3)	C(20)-C(13)-C(14)	114.6(2)
C(9)-C(3)-C(10)	108.4(3)	C(19)-C(13)-C(14)	110.1(3)
C(2)-C(3)-C(10)	112.2(3)	C(15)-C(14)-C(17)	100.2(2)
C(9)-C(3)-C(4)	110.7(3)	C(15)-C(14)-C(13)	110.9(3)
C(2)-C(3)-C(4)	100.9(2)	C(17)-C(14)-C(13)	101.6(2)
C(10)-C(3)-C(4)	114.0(3)	C(14)-C(15)-C(16)	103.5(2)
C(7)-C(4)-C(5)	100.0(3)	C(11)-C(16)-C(15)	102.5(2)
C(7)-C(4)-C(3)	101.9(2)	C(11)-C(17)-C(14)	94.1(2)
C(5)-C(4)-C(3)	111.0(3)	O(3)-C(21)-C(22)	116.0(2)
C(4)-C(5)-C(6)	103.5(3)	O(3)-C(21)-C(27)	118.4(3)
C(1)-C(6)-C(5)	102.0(3)	C(22)-C(21)-C(27)	101.1(2)
C(1)-C(7)-C(4)	94.0(2)	O(3)-C(21)-C(26)	110.2(2)
O(2)-C(11)-C(12)	115.5(2)	C(22)-C(21)-C(26)	108.4(3)
O(2)-C(11)-C(17)	118.1(2)	C(27)-C(21)-C(26)	101.3(2)
C(12)-C(11)-C(17)	101.8(2)	C(28)-C(22)-C(21)	126.5(3)
O(2)-C(11)-C(16)	111.6(2)	C(28)-C(22)-C(23)	127.5(3)

C(21)-C(22)-C(23)	106.0(2)	C(21)-C(26)-C(25)	102.8(2)
C(29)-C(23)-C(30)	108.0(2)	C(21)-C(27)-C(24)	94.1(2)
C(29)-C(23)-C(22)	111.3(3)	C(1)-O(1)-O(3)	134.33(19)
C(30)-C(23)-C(22)	111.8(3)	C(1)-O(1)-O(2)#1	102.73(17)
C(29)-C(23)-C(24)	110.5(3)	O(3)-O(1)-O(2)#1	113.94(9)
C(30)-C(23)-C(24)	114.4(3)	C(11)-O(2)-O(3)	113.36(17)
C(22)-C(23)-C(24)	100.7(2)	C(11)-O(2)-O(1)#2	137.21(19)
C(27)-C(24)-C(25)	100.2(2)	O(3)-O(2)-O(1)#2	98.68(9)
C(27)-C(24)-C(23)	101.9(2)	C(21)-O(3)-O(1)	117.08(18)
C(25)-C(24)-C(23)	110.7(3)	C(21)-O(3)-O(2)	133.36(19)
C(24)-C(25)-C(26)	103.3(2)	O(1)-O(3)-O(2)	109.05(9)

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 3. 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}
C(1)	26(2)	19(2)	17(2)	0(1)	-2(1)	2(2)
C(2)	21(2)	15(1)	25(2)	-3(1)	5(2)	4(1)
C(3)	34(2)	26(2)	20(2)	3(1)	3(2)	-2(2)
C(4)	34(2)	30(2)	16(2)	-2(1)	-4(2)	-5(2)
C(5)	61(3)	26(2)	29(2)	-6(2)	3(2)	-8(2)
C(6)	31(2)	21(2)	30(2)	-2(1)	2(2)	1(2)
C(7)	26(2)	25(2)	21(2)	5(1)	0(2)	-6(2)
C(8)	34(2)	22(2)	34(2)	-3(1)	3(2)	-2(2)
C(9)	39(2)	33(2)	37(2)	12(2)	-5(2)	0(2)
C(10)	58(3)	51(2)	24(2)	4(2)	10(2)	-9(2)
C(11)	18(2)	18(2)	24(2)	1(1)	-3(2)	-2(1)
C(12)	24(2)	17(1)	22(2)	3(1)	0(2)	-4(1)
C(13)	30(2)	18(1)	19(2)	0(1)	-4(2)	-1(2)
C(14)	27(2)	19(2)	20(2)	-2(1)	-1(2)	5(1)
C(15)	33(2)	23(2)	25(2)	3(1)	-3(2)	-2(2)
C(16)	26(2)	24(2)	22(2)	3(1)	2(2)	-1(2)
C(17)	23(2)	26(2)	21(2)	1(1)	-1(2)	1(2)
C(18)	34(2)	22(2)	27(2)	4(1)	-6(2)	-2(2)
C(19)	45(2)	30(2)	20(2)	-1(1)	3(2)	2(2)
C(20)	46(2)	25(2)	28(2)	-2(1)	-12(2)	-2(2)
C(21)	22(2)	19(2)	21(2)	5(1)	-1(2)	0(1)
C(22)	24(2)	24(2)	18(2)	0(1)	-3(2)	0(2)
C(23)	23(2)	17(1)	20(2)	0(1)	2(2)	-2(1)
C(24)	21(2)	26(2)	18(2)	1(1)	2(1)	-1(2)
C(25)	29(2)	27(2)	18(2)	-2(1)	2(2)	1(2)
C(26)	23(2)	22(2)	26(2)	1(1)	-6(2)	-2(2)
C(27)	21(2)	20(1)	26(2)	-2(1)	0(2)	3(2)
C(28)	60(3)	38(2)	32(2)	5(2)	22(2)	10(2)
C(29)	40(2)	22(2)	32(2)	-2(1)	-2(2)	-3(2)
C(30)	36(2)	29(2)	31(2)	5(2)	2(2)	7(2)
O(1)	32(1)	32(1)	16(1)	-1(1)	-5(1)	5(1)
O(2)	26(1)	20(1)	24(1)	-3(1)	4(1)	-4(1)
O(3)	28(1)	24(1)	28(1)	12(1)	-10(1)	-6(1)

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

	x	y	z	U(eq)
H(4)	6607	7294	4405	32

H(5A)	4356	8216	4161	47
H(5B)	2542	7732	4452	47
H(6A)	817	7616	3558	33
H(6B)	2581	8121	3272	33
H(7A)	6705	7685	3350	29
H(7B)	7114	6903	3357	29
H(8A)	1050	6114	2959	36
H(8B)	1352	5704	3581	36
H(9A)	7011	6051	3879	55
H(9B)	5177	5590	4181	55
H(9C)	6715	6050	4584	55
H(10A)	1978	6045	4691	67
H(10B)	1268	6791	4611	67
H(10C)	3291	6602	5044	67
H(14)	-629	4445	1416	27
H(15A)	-2803	4236	2283	32
H(15B)	-4720	4264	1781	32
H(16A)	-6112	5188	2196	29
H(16B)	-4189	5161	2697	29
H(17A)	-197	5245	2259	28
H(17B)	183	5628	1636	28
H(18A)	-5957	6471	1317	33
H(18B)	-5826	6101	671	33
H(19A)	-1986	5545	208	48
H(19B)	-474	4928	375	48
H(19C)	-132	5603	718	48
H(20A)	-5350	4922	347	50
H(20B)	-5946	4583	966	50
H(20C)	-4045	4279	551	50
H(24)	1940	8594	447	26
H(25A)	-88	7678	72	30
H(25B)	-2076	8180	230	30
H(26A)	-3267	7516	969	28
H(26B)	-1349	6999	791	28
H(27A)	2688	7504	921	27
H(27B)	3048	8071	1414	27
H(28A)	-2641	8102	2381	52
H(28B)	-2715	8881	2212	52
H(29A)	2584	9103	1577	47
H(29B)	527	9572	1731	47
H(29C)	1737	9625	1100	47
H(30A)	-2964	9494	1195	48
H(30B)	-3524	8880	784	48
H(30C)	-1874	9436	549	48
H(1)	4204	6838	2457	40
H(2A)	-2394	6552	2092	35
H(3)	937	7221	2083	40

Table 6. Torsion angles [°] for 3.

O(1)-C(1)-C(2)-C(8)	-19.3(5)	C(8)-C(2)-C(3)-C(4)	-177.1(3)
C(7)-C(1)-C(2)-C(8)	-147.4(3)	C(1)-C(2)-C(3)-C(4)	3.0(3)
C(6)-C(1)-C(2)-C(8)	105.9(4)	C(9)-C(3)-C(4)-C(7)	79.4(3)
O(1)-C(1)-C(2)-C(3)	160.6(3)	C(2)-C(3)-C(4)-C(7)	-37.6(3)
C(7)-C(1)-C(2)-C(3)	32.5(3)	C(10)-C(3)-C(4)-C(7)	-158.1(3)
C(6)-C(1)-C(2)-C(3)	-74.2(3)	C(9)-C(3)-C(4)-C(5)	-174.9(3)
C(8)-C(2)-C(3)-C(9)	65.7(4)	C(2)-C(3)-C(4)-C(5)	68.0(3)
C(1)-C(2)-C(3)-C(9)	-114.2(3)	C(10)-C(3)-C(4)-C(5)	-52.4(4)
C(8)-C(2)-C(3)-C(10)	-55.4(4)	C(7)-C(4)-C(5)-C(6)	37.6(3)
C(1)-C(2)-C(3)-C(10)	124.7(3)	C(3)-C(4)-C(5)-C(6)	-69.3(3)

O(1)-C(1)-C(6)-C(5)	-160.7(3)
C(2)-C(1)-C(6)-C(5)	72.0(3)
C(7)-C(1)-C(6)-C(5)	-34.7(3)
C(4)-C(5)-C(6)-C(1)	-1.9(3)
O(1)-C(1)-C(7)-C(4)	179.5(2)
C(2)-C(1)-C(7)-C(4)	-54.0(3)
C(6)-C(1)-C(7)-C(4)	57.4(3)
C(5)-C(4)-C(7)-C(1)	-57.6(3)
C(3)-C(4)-C(7)-C(1)	56.5(3)
O(2)-C(11)-C(12)-C(18)	-21.9(5)
C(17)-C(11)-C(12)-C(18)	-151.1(3)
C(16)-C(11)-C(12)-C(18)	103.3(3)
O(2)-C(11)-C(12)-C(13)	160.0(3)
C(17)-C(11)-C(12)-C(13)	30.7(3)
C(16)-C(11)-C(12)-C(13)	-74.9(3)
C(18)-C(12)-C(13)-C(20)	-50.6(4)
C(11)-C(12)-C(13)-C(20)	127.4(3)
C(18)-C(12)-C(13)-C(19)	70.5(4)
C(11)-C(12)-C(13)-C(19)	-111.4(3)
C(18)-C(12)-C(13)-C(14)	-173.0(3)
C(11)-C(12)-C(13)-C(14)	5.1(3)
C(12)-C(13)-C(14)-C(15)	66.9(3)
C(20)-C(13)-C(14)-C(15)	-53.8(3)
C(19)-C(13)-C(14)-C(15)	-176.2(2)
C(12)-C(13)-C(14)-C(17)	-38.9(3)
C(20)-C(13)-C(14)-C(17)	-159.6(3)
C(19)-C(13)-C(14)-C(17)	78.0(3)
C(17)-C(14)-C(15)-C(16)	35.8(3)
C(13)-C(14)-C(15)-C(16)	-70.9(3)
O(2)-C(11)-C(16)-C(15)	-162.8(3)
C(12)-C(11)-C(16)-C(15)	69.7(3)
C(17)-C(11)-C(16)-C(15)	-36.5(3)
C(14)-C(15)-C(16)-C(11)	0.1(3)
O(2)-C(11)-C(17)-C(14)	179.7(2)
C(12)-C(11)-C(17)-C(14)	-52.7(2)
C(16)-C(11)-C(17)-C(14)	57.9(3)
C(15)-C(14)-C(17)-C(11)	-57.3(3)
C(13)-C(14)-C(17)-C(11)	56.7(3)
O(3)-C(21)-C(22)-C(28)	-16.9(5)
C(27)-C(21)-C(22)-C(28)	-146.3(4)
C(26)-C(21)-C(22)-C(28)	107.6(4)
O(3)-C(21)-C(22)-C(23)	164.3(3)
C(27)-C(21)-C(22)-C(23)	34.8(3)
C(26)-C(21)-C(22)-C(23)	-71.2(3)
C(28)-C(22)-C(23)-C(29)	64.5(5)
C(21)-C(22)-C(23)-C(29)	-116.6(3)
C(28)-C(22)-C(23)-C(30)	-56.4(5)
C(21)-C(22)-C(23)-C(30)	122.4(3)
C(28)-C(22)-C(23)-C(24)	-178.3(4)
C(21)-C(22)-C(23)-C(24)	0.5(3)
C(29)-C(23)-C(24)-C(27)	82.1(3)
C(30)-C(23)-C(24)-C(27)	-155.8(3)
C(22)-C(23)-C(24)-C(27)	-35.7(3)
C(29)-C(23)-C(24)-C(25)	-172.0(2)
C(30)-C(23)-C(24)-C(25)	-49.9(3)
C(22)-C(23)-C(24)-C(25)	70.2(3)
C(27)-C(24)-C(25)-C(26)	37.9(3)
C(23)-C(24)-C(25)-C(26)	-69.1(3)
O(3)-C(21)-C(26)-C(25)	-160.2(2)
C(22)-C(21)-C(26)-C(25)	71.8(3)
C(27)-C(21)-C(26)-C(25)	-34.0(3)
C(24)-C(25)-C(26)-C(21)	-2.5(3)
O(3)-C(21)-C(27)-C(24)	177.0(2)
C(22)-C(21)-C(27)-C(24)	-55.0(3)
C(26)-C(21)-C(27)-C(24)	56.5(3)
C(25)-C(24)-C(27)-C(21)	-57.8(3)
C(23)-C(24)-C(27)-C(21)	56.1(3)
C(2)-C(1)-O(1)-O(3)	72.6(3)
C(7)-C(1)-O(1)-O(3)	-167.69(19)
C(6)-C(1)-O(1)-O(3)	-50.7(4)
C(2)-C(1)-O(1)-O(2)#1	-70.8(3)
C(7)-C(1)-O(1)-O(2)#1	49.0(3)
C(6)-C(1)-O(1)-O(2)#1	165.9(2)
C(12)-C(11)-O(2)-O(3)	-72.1(3)
C(17)-C(11)-O(2)-O(3)	48.7(3)
C(16)-C(11)-O(2)-O(3)	164.9(2)
C(12)-C(11)-O(2)-O(1)#2	63.0(3)
C(17)-C(11)-O(2)-O(1)#2	-176.20(19)
C(16)-C(11)-O(2)-O(1)#2	-59.9(3)
C(22)-C(21)-O(3)-O(1)	-83.3(3)
C(27)-C(21)-O(3)-O(1)	37.2(3)
C(26)-C(21)-O(3)-O(1)	153.1(2)
C(22)-C(21)-O(3)-O(2)	87.4(3)
C(27)-C(21)-O(3)-O(2)	-152.0(2)
C(26)-C(21)-O(3)-O(2)	-36.1(4)
C(1)-O(1)-O(3)-C(21)	123.7(3)
O(2)#1-O(1)-O(3)-C(21)	-95.9(2)
C(1)-O(1)-O(3)-O(2)	-49.2(3)
O(2)#1-O(1)-O(3)-O(2)	91.22(11)
C(11)-O(2)-O(3)-C(21)	92.1(3)
O(1)#2-O(2)-O(3)-C(21)	-58.8(3)
C(11)-O(2)-O(3)-O(1)	-96.59(19)
O(1)#2-O(2)-O(3)-O(1)	112.43(10)

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

Table 7. Hydrogen bonds for 3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#1	0.84	1.93	2.749(3)	163.3
O(2)-H(2A)...O(3)	0.84	1.90	2.736(3)	171.4
O(3)-H(3)...O(1)	0.84	1.90	2.723(3)	168.2

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

(b) Compound 4

Table 1. Crystal data and structure refinement for km5101.

Identification code	km5101
Empirical formula	$C_{10} H_{16} O$
Formula weight	152.23
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P 4_1 2_1 2
Unit cell dimensions	a = 10.7633(1) Å
	c = 31.3398(5) Å
Volume	3630.67(8) $Å^3$
Z	16
Density (calculated)	1.114 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	1344
Crystal size	0.38 x 0.33 x 0.15 mm^3
Theta range for data collection	2.00 to 33.14°.
Index ranges	-16<=h<=16, -11<=k<=11, -48<=l<=44
Reflections collected	22563
Independent reflections	4009 [R(int) = 0.0324]
Completeness to theta = 33.14°	99.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4009 / 0 / 234
Goodness-of-fit on F^2	1.046
R indices [3345 I>2σ(I)]	R1 = 0.0482, wR2 = 0.1244
R indices (all data)	R1 = 0.0606, wR2 = 0.1320
Absolute structure parameter	Not determined
Largest diff. peak and hole	0.24 and -0.19 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for km5101. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9615(1)	2151(1)	106(1)	30(1)
C(1)*	8262(2)	3979(3)	56(1)	22(1)
C(2)*	9562(2)	3439(1)	16(1)	20(1)
C(3)*	10084(2)	3845(2)	-422(1)	26(1)
C(4)*	10267(2)	5265(2)	-362(1)	33(1)
C(5)	9833(2)	5488(1)	114(1)	34(1)
C(6)	8409(2)	5352(1)	110(1)	32(1)
C(7)*	10291(2)	4285(2)	333(1)	25(1)
C(8)*	11698(2)	4075(2)	328(1)	37(1)
C(9)*	9843(2)	4156(2)	795(1)	34(1)
C(10)	7199(2)	3314(2)	26(1)	32(1)
O(2)	10774(1)	382(1)	567(1)	32(1)
C(11)	10703(1)	534(2)	1352(1)	28(1)
C(12)	10377(1)	-184(1)	949(1)	25(1)
C(13)	10970(2)	-1471(2)	1006(1)	37(1)
C(14)	10144(2)	-2074(2)	1355(1)	45(1)
C(15)	9189(2)	-1055(2)	1453(1)	33(1)
C(16)	9907(2)	-35(2)	1702(1)	36(1)

C(17)	8971(1)	-435(2)	1014(1)	28(1)
C(18)	8409(2)	-1298(2)	679(1)	46(1)
C(19)	8195(2)	759(2)	1033(1)	34(1)
C(20)	11523(2)	1452(2)	1381(1)	39(1)
C(1A)**	8050(20)	3830(20)	51(8)	35(1)
C(2A)**	9405(11)	3451(11)	209(4)	35(1)
C(3A)**	9644(11)	3779(11)	682(4)	35(1)
C(4A)**	9873(10)	5208(9)	667(3)	35(1)
C(7A)**	10274(10)	4332(10)	-42(3)	35(1)
C(8A)**	10056(11)	4331(12)	-512(4)	35(1)
C(9A)**	11673(10)	4114(11)	74(4)	35(1)

* Disordered: SOF $\alpha = 0.833(3)$. ** Minor disorder sites SOF = 1 - α.

Table 3. Bond lengths [Å] and angles [°] for km5101.

O(1)-C(2)	1.4162(18)	C(11)-C(20)	1.328(2)
O(1)-C(2A)	1.453(12)	C(11)-C(12)	1.520(2)
C(1)-C(10)	1.353(2)	C(11)-C(16)	1.521(2)
C(1)-C(6)	1.496(3)	C(12)-C(13)	1.536(2)
C(1)-C(2)	1.520(3)	C(12)-C(17)	1.551(2)
C(2)-C(3)	1.546(2)	C(13)-C(14)	1.552(3)
C(2)-C(7)	1.559(2)	C(14)-C(15)	1.534(3)
C(3)-C(4)	1.552(3)	C(15)-C(17)	1.548(2)
C(4)-C(5)	1.582(3)	C(15)-C(16)	1.553(2)
C(5)-C(7A)	1.418(11)	C(17)-C(18)	1.527(2)
C(5)-C(6)	1.540(2)	C(17)-C(19)	1.534(2)
C(5)-C(7)	1.545(2)	C(1A)-C(2A)	1.59(3)
C(5)-C(4A)	1.759(10)	C(2A)-C(7A)	1.547(16)
C(6)-C(1A)	1.69(2)	C(2A)-C(3A)	1.546(17)
C(7)-C(8)	1.532(3)	C(3A)-C(4A)	1.558(15)
C(7)-C(9)	1.534(3)	C(7A)-C(8A)	1.494(15)
C(10)-C(1A)	1.079(19)	C(7A)-C(9A)	1.567(15)
O(2)-C(12)	1.4105(16)		

C(2)-O(1)-C(2A)	25.3(5)	C(4)-C(5)-C(4A)	153.6(4)
C(10)-C(1)-C(6)	128.3(2)	C(1)-C(6)-C(5)	101.53(15)
C(10)-C(1)-C(2)	124.8(2)	C(1)-C(6)-C(1A)	7.0(8)
C(6)-C(1)-C(2)	106.88(14)	C(5)-C(6)-C(1A)	108.5(8)
O(1)-C(2)-C(1)	113.25(15)	C(8)-C(7)-C(9)	107.80(16)
O(1)-C(2)-C(3)	116.15(14)	C(8)-C(7)-C(5)	115.81(16)
C(1)-C(2)-C(3)	107.41(17)	C(9)-C(7)-C(5)	113.23(15)
O(1)-C(2)-C(7)	115.07(14)	C(8)-C(7)-C(2)	113.91(15)
C(1)-C(2)-C(7)	100.77(14)	C(9)-C(7)-C(2)	113.02(15)
C(3)-C(2)-C(7)	102.55(13)	C(5)-C(7)-C(2)	92.68(12)
C(2)-C(3)-C(4)	102.51(13)	C(1A)-C(10)-C(1)	0.9(15)
C(3)-C(4)-C(5)	103.11(13)	C(20)-C(11)-C(12)	126.12(13)
C(7A)-C(5)-C(6)	104.3(4)	C(20)-C(11)-C(16)	128.58(14)
C(7A)-C(5)-C(7)	46.4(4)	C(12)-C(11)-C(16)	105.29(12)
C(6)-C(5)-C(7)	103.98(13)	O(2)-C(12)-C(11)	114.51(12)
C(7A)-C(5)-C(4)	56.2(4)	O(2)-C(12)-C(13)	111.18(12)
C(6)-C(5)-C(4)	105.77(15)	C(11)-C(12)-C(13)	105.49(12)
C(7)-C(5)-C(4)	101.31(13)	O(2)-C(12)-C(17)	118.85(12)
C(7A)-C(5)-C(4A)	100.4(5)	C(11)-C(12)-C(17)	101.84(11)
C(6)-C(5)-C(4A)	91.0(4)	C(13)-C(12)-C(17)	103.53(12)
C(7)-C(5)-C(4A)	54.0(3)	C(12)-C(13)-C(14)	102.68(13)

C(15)-C(14)-C(13)	103.17(13)	O(1)-C(2A)-C(7A)	112.6(9)
C(14)-C(15)-C(17)	103.33(13)	O(1)-C(2A)-C(3A)	114.0(9)
C(14)-C(15)-C(16)	105.84(15)	C(7A)-C(2A)-C(3A)	104.3(9)
C(17)-C(15)-C(16)	102.48(13)	O(1)-C(2A)-C(1A)	108.7(10)
C(11)-C(16)-C(15)	101.75(12)	C(7A)-C(2A)-C(1A)	103.7(11)
C(18)-C(17)-C(19)	108.71(14)	C(3A)-C(2A)-C(1A)	113.1(13)
C(18)-C(17)-C(15)	114.17(14)	C(2A)-C(3A)-C(4A)	102.8(9)
C(19)-C(17)-C(15)	114.18(13)	C(3A)-C(4A)-C(5)	101.3(7)
C(18)-C(17)-C(12)	113.69(14)	C(5)-C(7A)-C(8A)	106.8(9)
C(19)-C(17)-C(12)	113.00(13)	C(5)-C(7A)-C(2A)	99.2(7)
C(15)-C(17)-C(12)	92.50(11)	C(8A)-C(7A)-C(2A)	114.0(9)
C(10)-C(1A)-C(2A)	132(2)	C(5)-C(7A)-C(9A)	112.0(8)
C(10)-C(1A)-C(6)	134(2)	C(8A)-C(7A)-C(9A)	112.3(9)
C(2A)-C(1A)-C(6)	90.5(10)	C(2A)-C(7A)-C(9A)	111.8(9)

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for km5101. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	16(1)	28(1)	0(1)	5(1)	1(1)
C(1)	23(1)	21(1)	23(1)	0(1)	-1(1)	-4(1)
C(2)	26(1)	14(1)	21(1)	-1(1)	3(1)	-1(1)
C(3)	34(1)	21(1)	24(1)	-1(1)	9(1)	-2(1)
C(4)	41(1)	20(1)	37(1)	2(1)	10(1)	-4(1)
C(5)	38(1)	18(1)	48(1)	-6(1)	5(1)	-4(1)
C(6)	34(1)	23(1)	41(1)	-1(1)	8(1)	5(1)
C(7)	24(1)	24(1)	28(1)	-7(1)	2(1)	-3(1)
C(8)	25(1)	45(1)	42(1)	-7(1)	-1(1)	-2(1)
C(9)	36(1)	39(1)	26(1)	-9(1)	0(1)	-4(1)
C(10)	30(1)	41(1)	25(1)	-1(1)	0(1)	-6(1)
O(2)	36(1)	41(1)	20(1)	8(1)	7(1)	9(1)
C(11)	25(1)	38(1)	21(1)	4(1)	1(1)	-3(1)
C(12)	28(1)	27(1)	20(1)	4(1)	3(1)	3(1)
C(13)	36(1)	33(1)	41(1)	9(1)	4(1)	10(1)
C(14)	40(1)	36(1)	58(1)	20(1)	2(1)	1(1)
C(15)	29(1)	37(1)	31(1)	10(1)	1(1)	-6(1)
C(16)	33(1)	55(1)	21(1)	6(1)	2(1)	-11(1)
C(17)	27(1)	32(1)	26(1)	-1(1)	-2(1)	-1(1)
C(18)	48(1)	44(1)	45(1)	-11(1)	-12(1)	-3(1)
C(19)	26(1)	38(1)	37(1)	2(1)	2(1)	5(1)
C(20)	39(1)	49(1)	30(1)	1(1)	0(1)	-15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for km5101.

	x	y	z	U(eq)
H(1)	9790(30)	1850(20)	-97(7)	53(7)
H(3A)	9487	3667	-655	32
H(3B)	10882	3426	-485	32
H(4A)	9749	5742	-565	39
H(4B)	11149	5502	-401	39
H(5)	10145	6274	246	41
H(6A)	8036	5642	381	39

H(6B)	8033	5813	-131	39
H(8A)	12096	4646	530	56
H(8B)	12020	4227	40	56
H(8C)	11879	3216	411	56
H(9A)	10121	3357	911	51
H(9B)	8934	4196	803	51
H(9C)	10189	4833	967	51
H(10A)	6418	3724	39	38
H(10B)	7233	2438	-8	38
H(2)	10370(20)	970(20)	507(6)	38(6)
H(13A)	11844	-1402	1101	44
H(13B)	10941	-1954	737	44
H(14A)	9733	-2834	1247	54
H(14B)	10637	-2285	1611	54
H(15)	8417	-1357	1598	39
H(16A)	9334	586	1827	44
H(16B)	10425	-398	1931	44
H(18A)	7542	-1475	752	69
H(18B)	8881	-2076	670	69
H(18C)	8443	-896	398	69
H(19A)	8141	1125	747	51
H(19B)	8590	1352	1228	51
H(19C)	7358	564	1136	51
H(20A)	11968	1714	1135	47
H(20B)	11664	1846	1648	47
H(3A1)	10381	3334	794	42
H(3A2)	8914	3575	862	42
H(4A1)	10689	5430	791	42
H(4A2)	9210	5670	818	42
H(8A1)	9388	3746	-581	53
H(8A2)	10819	4079	-660	53
H(8A3)	9818	5167	-605	53
H(9A1)	12198	4633	-109	53
H(9A2)	11883	3237	29	53
H(9A3)	11814	4334	373	53

Table 6. Torsion angles [°] for km5101.

C(2A)-O(1)-C(2)-C(1)	-63.9(11)	C(2)-C(1)-C(6)-C(5)	-2.2(2)
C(2A)-O(1)-C(2)-C(3)	171.0(11)	C(10)-C(1)-C(6)-C(1A)	2(8)
C(2A)-O(1)-C(2)-C(7)	51.3(11)	C(2)-C(1)-C(6)-C(1A)	179(100)
C(10)-C(1)-C(2)-O(1)	-22.9(3)	C(7A)-C(5)-C(6)-C(1)	14.4(5)
C(6)-C(1)-C(2)-O(1)	159.86(17)	C(7)-C(5)-C(6)-C(1)	-33.6(2)
C(10)-C(1)-C(2)-C(3)	106.7(3)	C(4)-C(5)-C(6)-C(1)	72.72(19)
C(6)-C(1)-C(2)-C(3)	-70.5(2)	C(4A)-C(5)-C(6)-C(1)	-86.6(4)
C(10)-C(1)-C(2)-C(7)	-146.4(3)	C(7A)-C(5)-C(6)-C(1A)	14.6(10)
C(6)-C(1)-C(2)-C(7)	36.4(2)	C(7)-C(5)-C(6)-C(1A)	-33.4(9)
O(1)-C(2)-C(3)-C(4)	-163.08(16)	C(4)-C(5)-C(6)-C(1A)	72.9(9)
C(1)-C(2)-C(3)-C(4)	68.97(18)	C(4A)-C(5)-C(6)-C(1A)	-86.4(9)
C(7)-C(2)-C(3)-C(4)	-36.72(17)	C(7A)-C(5)-C(7)-C(8)	75.4(6)
C(2)-C(3)-C(4)-C(5)	0.64(19)	C(6)-C(5)-C(7)-C(8)	171.99(15)
C(3)-C(4)-C(5)-C(7A)	24.4(5)	C(4)-C(5)-C(7)-C(8)	62.39(19)
C(3)-C(4)-C(5)-C(6)	-72.41(17)	C(4A)-C(5)-C(7)-C(8)	-107.2(5)
C(3)-C(4)-C(5)-C(7)	35.80(18)	C(7A)-C(5)-C(7)-C(9)	-159.3(6)
C(3)-C(4)-C(5)-C(4A)	55.0(8)	C(6)-C(5)-C(7)-C(9)	-62.76(18)
C(10)-C(1)-C(6)-C(5)	-179.2(3)	C(4)-C(5)-C(7)-C(9)	-172.36(15)

C(4A)-C(5)-C(7)-C(9)	18.1(4)	C(13)-C(12)-C(17)-C(15)	54.44(13)
C(7A)-C(5)-C(7)-C(2)	-42.8(6)	C(1)-C(10)-C(1A)-C(2A)	179(100)
C(6)-C(5)-C(7)-C(2)	53.74(15)	C(1)-C(10)-C(1A)-C(6)	24(99)
C(4)-C(5)-C(7)-C(2)	-55.86(14)	C(1)-C(6)-C(1A)-C(10)	-177(100)
C(4A)-C(5)-C(7)-C(2)	134.6(5)	C(5)-C(6)-C(1A)-C(10)	-179(2)
O(1)-C(2)-C(7)-C(8)	64.7(2)	C(1)-C(6)-C(1A)-C(2A)	21(7)
C(1)-C(2)-C(7)-C(8)	-173.15(18)	C(5)-C(6)-C(1A)-C(2A)	19.8(13)
C(3)-C(2)-C(7)-C(8)	-62.39(19)	C(2)-O(1)-C(2A)-C(7A)	-33.0(7)
O(1)-C(2)-C(7)-C(9)	-58.8(2)	C(2)-O(1)-C(2A)-C(3A)	-151.5(17)
C(1)-C(2)-C(7)-C(9)	63.4(2)	C(2)-O(1)-C(2A)-C(1A)	81.3(14)
C(3)-C(2)-C(7)-C(9)	174.13(15)	C(10)-C(1A)-C(2A)-O(1)	32(3)
O(1)-C(2)-C(7)-C(5)	-175.50(14)	C(6)-C(1A)-C(2A)-O(1)	-165.8(9)
C(1)-C(2)-C(7)-C(5)	-53.31(16)	C(10)-C(1A)-C(2A)-C(7A)	152(2)
C(3)-C(2)-C(7)-C(5)	57.45(14)	C(6)-C(1A)-C(2A)-C(7A)	-45.8(12)
C(6)-C(1)-C(10)-C(1A)	-155(100)	C(10)-C(1A)-C(2A)-C(3A)	-96(3)
C(2)-C(1)-C(10)-C(1A)	28(100)	C(6)-C(1A)-C(2A)-C(3A)	66.6(13)
C(20)-C(11)-C(12)-O(2)	-15.4(2)	O(1)-C(2A)-C(3A)-C(4A)	158.4(8)
C(16)-C(11)-C(12)-O(2)	165.08(13)	C(7A)-C(2A)-C(3A)-C(4A)	35.3(11)
C(20)-C(11)-C(12)-C(13)	107.15(19)	C(1A)-C(2A)-C(3A)-C(4A)	-76.7(13)
C(16)-C(11)-C(12)-C(13)	-72.35(15)	C(2A)-C(3A)-C(4A)-C(5)	-4.5(10)
C(20)-C(11)-C(12)-C(17)	-145.02(18)	C(7A)-C(5)-C(4A)-C(3A)	-29.7(8)
C(16)-C(11)-C(12)-C(17)	35.49(15)	C(6)-C(5)-C(4A)-C(3A)	75.0(7)
O(2)-C(12)-C(13)-C(14)	-163.82(14)	C(7)-C(5)-C(4A)-C(3A)	-31.7(5)
C(11)-C(12)-C(13)-C(14)	71.49(16)	C(4)-C(5)-C(4A)-C(3A)	-55.1(12)
C(17)-C(12)-C(13)-C(14)	-35.11(16)	C(6)-C(5)-C(7A)-C(8A)	75.3(8)
C(12)-C(13)-C(14)-C(15)	-0.12(19)	C(7)-C(5)-C(7A)-C(8A)	171.1(11)
C(13)-C(14)-C(15)-C(17)	35.36(18)	C(4)-C(5)-C(7A)-C(8A)	-24.3(6)
C(13)-C(14)-C(15)-C(16)	-71.98(17)	C(4A)-C(5)-C(7A)-C(8A)	168.9(8)
C(20)-C(11)-C(16)-C(15)	-179.30(18)	C(6)-C(5)-C(7A)-C(2A)	-43.4(7)
C(12)-C(11)-C(16)-C(15)	0.18(17)	C(7)-C(5)-C(7A)-C(2A)	52.5(6)
C(14)-C(15)-C(16)-C(11)	71.99(16)	C(4)-C(5)-C(7A)-C(2A)	-143.0(8)
C(17)-C(15)-C(16)-C(11)	-35.97(16)	C(4A)-C(5)-C(7A)-C(2A)	50.3(8)
C(14)-C(15)-C(17)-C(18)	63.04(18)	C(6)-C(5)-C(7A)-C(9A)	-161.5(6)
C(16)-C(15)-C(17)-C(18)	172.90(15)	C(7)-C(5)-C(7A)-C(9A)	-65.6(7)
C(14)-C(15)-C(17)-C(19)	-171.01(14)	C(4)-C(5)-C(7A)-C(9A)	98.9(8)
C(16)-C(15)-C(17)-C(19)	-61.15(17)	C(4A)-C(5)-C(7A)-C(9A)	-67.8(8)
C(14)-C(15)-C(17)-C(12)	-54.37(15)	O(1)-C(2A)-C(7A)-C(5)	178.5(7)
C(16)-C(15)-C(17)-C(12)	55.48(14)	C(3A)-C(2A)-C(7A)-C(5)	-57.5(9)
O(2)-C(12)-C(17)-C(18)	60.45(19)	C(1A)-C(2A)-C(7A)-C(5)	61.1(12)
C(11)-C(12)-C(17)-C(18)	-172.72(14)	O(1)-C(2A)-C(7A)-C(8A)	65.4(12)
C(13)-C(12)-C(17)-C(18)	-63.39(16)	C(3A)-C(2A)-C(7A)-C(8A)	-170.6(9)
O(2)-C(12)-C(17)-C(19)	-64.07(17)	C(1A)-C(2A)-C(7A)-C(8A)	-52.0(15)
C(11)-C(12)-C(17)-C(19)	62.75(14)	O(1)-C(2A)-C(7A)-C(9A)	-63.3(11)
C(13)-C(12)-C(17)-C(19)	172.09(12)	C(3A)-C(2A)-C(7A)-C(9A)	60.8(11)
O(2)-C(12)-C(17)-C(15)	178.28(13)	C(1A)-C(2A)-C(7A)-C(9A)	179.4(12)
C(11)-C(12)-C(17)-C(15)	-54.90(13)		

Table 7. Hydrogen bonds for km5101 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)#1	0.74(2)	1.97(3)	2.7076(15)	169(3)
O(2)-H(2)...O(1)	0.79(2)	1.96(2)	2.6956(16)	154(2)

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

Bibliography for Group (C) Crystal structures of monotertiary alcohols containing a Csp^3-COH fragment

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ADAMOL
1-Adamantanol
1-Hydroxyadamantane
C10 H16 O1
J.P.Amoureux,M.Bee,C.Gors,V.Warin,F.Baert
Cryst.Struct.Commun., 8, 449,1979

AFRICO10
Africanol
absolute configuration.
C15 H26 O1
R.Karlsson
Acta Crystallogr.,Sect.B, 32, 2609,1976

BAFWUA
1-Phenylcyclohexanol
C12 H16 O1
F.R.Ahmed,C.P.Huber
Acta Crystallogr.,Sect.B, 37, 1874,1981

BAJKEC
trans,cis,trans-(1beta,4alpha,7beta,8alpha)-4,10,10-
Trimethyltricyclo(6.2.1.0$5,
11!)undecan-4beta-ol
12-nor-8alpha-Presilphiperfolan-9beta-ol
at 198 K.
C14 H24 O1
S.Shankar,R.M.Coates
J.Org.Chem., 63, 9177,1998

BAJNAB
1,4,4,11-Tetramethyltricyclo(5.3.1.0$3,8!)undecan-3-ol
at 198 K.
C15 H26 O1
R.M.Coates,J.Z.Ho,M.Klobus,Lijuan Zhu
J.Org.Chem., 63, 9166,1998

BELFAZ
(+)-2-((3R,6S,10R)-6,10-Dimethylbicyclo(4.4.0)dec-1-en-3-yl)-propan-2-
ol
Rosifoliol
C15 H26 O1
B.Beagley,R.G.Pritchard,R.Ramage,I.A.Southwell
Acta Crystallogr.,Sect.B, 38, 1391,1982

BETXAZ
(Z)-Ethynyl-tricyclo(3.3.1.1$3,7!)decan-2-ol
2-Ethynyl-2-adamantanol
C12 H16 O1
S.Y.Lin,Y.Okaya,D.M.Chiou,W.J.Le Noble
Acta Crystallogr.,Sect.B, 38, 1669,1982
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BETXAZ01
(Z)-Ethynyl-tricyclo(3.3.1.1$3,7!)decan-2-ol
2-Ethynyl-2-adamantanol
at 100 K; neutron radiation.
C12 H16 O1
F.H.Allen,J.A.K.Howard,V.J.Hoy,G.R.Desiraju,D.S.Reddy,C.C.Wilson
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CIHYEX
4-Hydroxy-10-epi-eudesm-11-ene
C15 H26 O1
R.Baker,A.J.Organ,S.A.Walmsley,M.Webster,A.M.R.Galas
J.Chem.Res., 138, 1401,1984
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CINVEA10
1,1-Diphenyl-ethanol
C14 H14 O1
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CUWVAR
2-Hydroxy-tetracyclo(6.2.1.1$3,6!.0$2,7!)dodecane
C12 H18 O1
L.A.Paquette,G.DeLucca,K.Ohkata,J.C.Gallucci
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FELWEY
2-Phenyltricyclo(3.3.1.1$3,7!)decan-2-ol
2-Phenyladamantan-2-ol
C16 H20 O1
F.A.Singelenberg,B.P.van Eijck
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FESMEV
2-Methyl-4-phenyl-3-butyn-2-ol
C11 H12 O1
F.A.J.Singelenberg,B.P.van Eijck
Acta Crystallogr.,Sect.C(Cr.Str.Comm.), 43, 693,1987
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FICCUP
1Z,2R,4R,7S,11S-3,3,7,11-Tetramethyltricyclo(6.3.0.0$2,4!)undec-1(8)-
en-4-ol
C15 H24 O1

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FOZWEW
1-Hydroxy-2,3-diphenylbicyclo(3.3.0)oct-2-ene
C20 H20 O1
S.K.Chowdhury,K.K.D.Amarasinghe,M.J.Heeg,J.Montgomery
J.Am.Chem.Soc., 122, 6775,2000
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GEBSUB
alpha,alpha-Dicyclohexyl-cyclohexylmethanol
C19 H34 O1
P.Sgarabotto,F.Ugozzoli,S.Sorriso,Z.Malarski
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GEPWON
7-(2-Isopropenylcyclopentenyl)bicyclo(2.2.1)hept-2-en-7-ol
C15 H20 O1
L.A.Paquette,D.T.DeRussy,R.D.Rogers
Tetrahedron, 44, 3139,1988
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GOXMAH
11b,3,3,7a-Tetramethyl-7b-hydroxy-1aH,2bH,4bH,8bH-
tricyclo(6.3.0.0$2,4!)undecane

(+)-Globulol
C15 H26 O1
E.Yu.Vinogradov,E.E.Shults,I.Yu.Bagryanskaya,Yu.V.Gatilov,G.A.Tolstikov
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HAVGAM
endo-13-syn-Methyltricyclo(8.2.1.0$2,9!)trideca-5,11-dien-13-anti-ol
C14 H20 O1
J.G.Garcia,G.Morales,F.R.Fronczek,M.L.McLaughlin
Acta Crystallogr.,Sect.C(Cr.Str.Comm.), 50, 317,1994
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HIBLAF
1-(4,6,8-Trimethylazulen-2-yl)cyclopropanol
at -100 deg.C.
C16 H18 O1
R.-A.Fallahpour,H.-J.Hansen
Helv.Chim.Acta, 77, 2297,1994
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LAFKAE
9-Methylfluoren-9-ol
C14 H12 O1
I.Csoregh,M.Czugler,E.Weber
J.Phys.Org.Chem., 6, 171,1993
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NAMLAO
2-Buta-1,3-diynyl-2-adamantanol
C14 H16 O1
M.B.Keller,H.S.Rzepa,A.J.P.White,D.J.Williams
First Electr.Conf.Trends in Org.Chem., , 50,1995
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NOXJIT
1,1-Dimethyl-3-t-butylprop-2-yn-1-ol
at 183K.
C9 H16 O1
D.Braga,F.Grepioni,D.Walther,K.Heubach,A.Schmidt,W.Imhof,H.Gorls,T.Klet
tke
Organometallics, 16, 4910,1997
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NOXJOZ
1,1-Diethyl-3-t-butylprop-2-yn-1-ol
at 183K.
C11 H20 O1
D.Braga,F.Grepioni,D.Walther,K.Heubach,A.Schmidt,W.Imhof,H.Gorls,T.Klet
tke
Organometallics, 16, 4910,1997
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NOXJUF
1-(2-t-Butylethynyl)cyclohexanol
at 173K.
C12 H20 O1
D.Braga,F.Grepioni,D.Walther,K.Heubach,A.Schmidt,W.Imhof,H.Gorls,T.Klet
tke
Organometallics, 16, 4910,1997
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NUJHUV
trans-1,2-Diphenylcyclo-octanol
C20 H24 O1
S.M.Moosavi,R.S.Beddoes,C.I.F.Watt
J.Chem.Soc.,Perkin Trans.2, , 1585,1997
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NUJJAD
trans-1,2-Diphenylcycloheptanol
C19 H22 O1
S.M.Moosavi,R.S.Beddoes,C.I.F.Watt
J.Chem.Soc.,Perkin Trans.2, , 1585,1997
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NUJJIL
trans-1,2-Diphenylcyclopentanol
C17 H18 O1
S.M.Moosavi,R.S.Beddoes,C.I.F.Watt
J.Chem.Soc.,Perkin Trans.2, , 1585,1997
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PEWVOC
1,2-Diphenylcyclopentanol

at 213 K.
2(C17 H18 O1)
T.Studemann,M.Ibrahim-Ouali,G.Cahiez,P.Knochel
Synlett, , 143,1998
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PEZQEQ
cis-1,3-Dimethylindan-1-ol
at -73 deg.C.
C11 H14 O1
J.K.MacLeod,A.Ward,A.C.Willis
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Ledol
C15 H26 O1
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QAZQAJ
1,7,7-Trimethyltricyclo(2.2.1.0$2,6!)heptan-4-ol
4-Tricyclanol
at 150 K; synchrotron radiation.
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QEBBII
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Str.,D-35032 M
      arburg, Germany.
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QEJKIZ
1-Hydroxy-9-methylenetricyclo(8.4.0.0$2,7!)tetradecane
at 237 K.
C15 H24 O1
J.M.Warrington,G.P.A.Yap,L.Barriault
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(1RS,2SR,9SR)-Tricyclo(7.5.0.0$2,8!)tetradec-7-ene-1-ol
C14 H22 O1
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VEXMAM
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C10 H20 O1
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C26 H26 O1
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XAYDIK
rac-1,2-Diphenylbut-3-yn-2-ol
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C20 H34 O1
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YUHHEO
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ZEHFUN
(+-)-3-Phenyl-but-1-yn-3-ol
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C12 H20 O1
W.Thielemann,H.J.Schafer,S.Kotila
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Z-2-Ethynyl-5-phenyl-2-adamantanol
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