(A) Crystal Structure Analysis of Compound 5:

km1802 $C_{11}H_{18}O_3$

Table 1. Crystal data and structure refinement for **5**.

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

Table 3. Bond lengths [Å] and angles [°] for **5**.

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for **5**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

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

Table 6. Torsion angles [°] for **5**.

Table 7. Hydrogen bonds for **5** [Å and °].

Figure 1 The heavy atom skeleton of the two disordered molecules.

Figure 2 The main structure showing hydrogen positions and 20% ellipsoids.

Table 1. Crystal data and structure refinement for 5.

Identification code	km1802	
Empirical formula	$C_{11}H_{18}O_3$	
Formula weight	198.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 7.1247(2) Å	a= 90°.
	b = 12.6181(3) Å	b= 95.189(1)°.
	c = 11.4236(4) Å	g= 90°.
Volume	1022.77(5) $Å^3$	
Z	4	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	432	
Crystal size	0.45 x 0.30 x 0.05 mm^3	
Theta range for data collection	2.41 to 30.07°.	
Index ranges	-10<=h<=9, 0<=k<=17, 0<=l<=16	
Reflections collected	12328	
Independent reflections	2967 [R(int) = 0.0254]	
Completeness to theta = 30.07°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9954 and 0.9598	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2967 / 0 / 186	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0387, wR2 = 0.1008	
R indices (all data)	R1 = 0.0421, wR2 = 0.1036	
Largest diff. peak and hole	0.36 and -0.20 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)*	6316(1)	2619(1)	-840(1)	13(1)
C(2)	7731(1)	3560(1)	-703(1)	17(1)
C(3)*	7698(2)	3879(1)	623(1)	19(1)
C(4)*	6645(1)	3005(1)	1242(1)	17(1)
C(5)*	6548(1)	2052(1)	376(1)	13(1)
C(6)	8223(1)	1291(1)	633(1)	20(1)
C(7)	7534(1)	541(1)	1542(1)	20(1)
C(8)	4910(1)	1330(1)	611(1)	16(1)
C(9)*	6551(2)	1905(1)	-1892(1)	19(1)
C(10)	7105(1)	4487(1)	-1516(1)	23(1)
C(11)*	9722(1)	3256(1)	-965(1)	21(1)
O(1)	4476(1)	3097(1)	-971(1)	21(1)
O(2)	5497(1)	497(1)	1275(1)	19(1)
O(3)	3247(1)	1456(1)	310(1)	22(1)
C(1')**	6390(20)	3051(12)	-104(13)	26(2)
C(3')**	8090(20)	2399(12)	-1724(13)	26(2)
C(4')**	6970(20)	1464(12)	-1213(13)	26(2)
C(5')**	6710(30)	1843(15)	73(17)	26(2)
C(9')**	6500(20)	3656(13)	1036(13)	26(2)
C(11')**	9820(20)	3622(12)	-232(13)	26(2)

* Occupancy a = 0.924(2). ** Occupancy 1-a. Single U_{iso} refined for these disordered atoms.

Table 3. Bond lengths [Å] and angles [°] for 5.

C(1)-O(1)	1.4391(11)	C(7)-H(71)	0.990(14)
C(1)-C(9)	1.5236(13)	C(7)-H(72)	0.938(15)
C(1)-C(2)	1.5563(12)	C(8)-O(3)	1.2142(11)
C(1)-C(5)	1.5570(13)	C(8)-O(2)	1.3406(11)
C(2)-C(1')	1.383(15)	C(8)-C(5')	1.61(2)
C(2)-C(11)	1.5247(13)	C(9)-H(9A)	0.9800
C(2)-C(10)	1.5345(13)	C(9)-H(9B)	0.9800
C(2)-C(11')	1.538(15)	C(9)-H(9C)	0.9800
C(2)-C(3)	1.5695(14)	C(10)-H(10A)	0.9800
C(2)-C(3')	1.903(15)	C(10)-H(10B)	0.9800
C(3)-C(4)	1.5409(14)	C(10)-H(10C)	0.9800
C(3)-H(31)	1.017(16)	C(11)-H(11A)	0.9800
C(3)-H(32)	0.952(16)	C(11)-H(11B)	0.9800
C(4)-C(5)	1.5542(14)	C(11)-H(11C)	0.9800
C(4)-H(41)	0.988(15)	O(1)-C(1')	1.612(14)
C(4)-H(42)	0.970(15)	O(1)-H(1)	0.823(18)
C(5)-C(8)	1.5240(13)	C(1')-C(9')	1.50(2)
C(5)-C(6)	1.5395(14)	C(1')-C(5')	1.55(2)
C(6)-C(5')	1.388(19)	C(3')-C(4')	1.56(2)
C(6)-C(7)	1.5181(13)	C(4')-C(5')	1.57(2)
C(6)-H(61)	1.027(15)	C(9')-H(31)	1.27(2)
C(6)-H(62)	0.970(14)	C(9')-H(41)	1.03(2)
C(7)-O(2)	1.4573(11)		

O(1)-C(1)-C(9)	109.25(7)	C(6)-C(5)-C(1)	118.32(8)
O(1)-C(1)-C(2)	105.44(7)	C(4)-C(5)-C(1)	101.99(8)
C(9)-C(1)-C(2)	114.45(8)	C(5')-C(6)-C(7)	110.1(8)
O(1)-C(1)-C(5)	107.89(7)	C(5')-C(6)-C(5)	17.1(8)
C(9)-C(1)-C(5)	114.98(8)	C(7)-C(6)-C(5)	103.10(8)
C(2)-C(1)-C(5)	104.22(7)	C(5')-C(6)-H(61)	94.6(11)
C(1')-C(2)-C(11)	132.6(6)	C(7)-C(6)-H(61)	107.7(8)
C(1')-C(2)-C(10)	118.5(6)	C(5)-C(6)-H(61)	111.7(8)
C(11)-C(2)-C(10)	107.34(8)	C(5')-C(6)-H(62)	122.9(12)
C(1')-C(2)-C(11')	122.7(8)	C(7)-C(6)-H(62)	111.7(8)
C(11)-C(2)-C(11')	36.3(6)	C(5)-C(6)-H(62)	114.9(8)
C(10)-C(2)-C(11')	113.1(5)	H(61)-C(6)-H(62)	107.6(11)
C(1')-C(2)-C(1)	39.2(6)	O(2)-C(7)-C(6)	104.94(7)
C(11)-C(2)-C(1)	113.19(8)	O(2)-C(7)-H(71)	107.6(8)
C(10)-C(2)-C(1)	111.81(7)	C(6)-C(7)-H(71)	112.6(9)
C(11')-C(2)-C(1)	132.2(5)	O(2)-C(7)-H(72)	107.0(9)
C(1')-C(2)-C(3)	64.5(6)	C(6)-C(7)-H(72)	113.3(9)
C(11)-C(2)-C(3)	110.41(8)	H(71)-C(7)-H(72)	110.9(12)
C(10)-C(2)-C(3)	111.05(8)	O(3)-C(8)-O(2)	120.62(8)
C(11')-C(2)-C(3)	75.4(6)	O(3)-C(8)-C(5)	127.97(8)
C(1)-C(2)-C(3)	103.06(7)	O(2)-C(8)-C(5)	111.35(8)
C(1')-C(2)-C(3')	94.8(7)	O(3)-C(8)-C(5')	129.2(7)
C(11)-C(2)-C(3')	60.5(4)	O(2)-C(8)-C(5')	108.2(7)
C(10)-C(2)-C(3')	105.3(4)	C(5)-C(8)-C(5')	16.6(7)
C(11')-C(2)-C(3')	94.3(7)	C(2)-C(10)-H(10A)	109.5
C(1)-C(2)-C(3')	58.2(4)	C(2)-C(10)-H(10B)	109.5
C(3)-C(2)-C(3')	143.4(4)	H(10A)-C(10)-H(10B)	109.5
C(4)-C(3)-C(2)	108.07(8)	C(2)-C(10)-H(10C)	109.5
C(4)-C(3)-H(31)	107.5(9)	H(10A)-C(10)-H(10C)	109.5
C(2)-C(3)-H(31)	111.8(9)	H(10B)-C(10)-H(10C)	109.5
C(4)-C(3)-H(32)	110.6(10)	C(2)-C(11)-H(11A)	109.5
C(2)-C(3)-H(32)	109.0(10)	C(2)-C(11)-H(11B)	109.5
H(31)-C(3)-H(32)	109.9(13)	C(2)-C(11)-H(11C)	109.5
C(3)-C(4)-C(5)	104.87(8)	C(1)-O(1)-C(1')	37.7(5)
C(3)-C(4)-H(41)	107.9(9)	C(1)-O(1)-H(1)	105.0(12)
C(5)-C(4)-H(41)	111.5(9)	C(1')-O(1)-H(1)	104.8(13)
C(3)-C(4)-H(42)	111.5(9)	C(8)-O(2)-C(7)	110.00(7)
C(5)-C(4)-H(42)	111.4(9)	C(2)-C(1')-C(9')	102.0(11)
H(41)-C(4)-H(42)	109.5(12)	C(2)-C(1')-C(5')	114.8(12)
C(8)-C(5)-C(6)	100.68(8)	C(9')-C(1')-C(5')	112.9(13)
C(8)-C(5)-C(4)	109.98(8)	C(2)-C(1')-O(1)	105.3(9)
C(6)-C(5)-C(4)	111.87(8)	C(9')-C(1')-O(1)	119.3(11)
C(8)-C(5)-C(1)	114.22(8)	C(5')-C(1')-O(1)	102.9(11)

C(4')-C(3')-C(2)	104.6(9)	C(1')-C(5')-C(8)	109.3(13)
C(3')-C(4')-C(5')	103.1(12)	C(4')-C(5')-C(8)	113.6(13)
C(6)-C(5')-C(1')	130.8(15)	C(1')-C(9')-H(31)	101.9(13)
C(6)-C(5')-C(4')	97.2(12)	C(1')-C(9')-H(41)	95.5(15)
C(1')-C(5')-C(4')	101.9(14)	H(31)-C(9')-H(41)	140.4(19)
C(6)-C(5')-C(8)	103.5(12)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 5. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	12(1)	14(1)	14(1)	2(1)	0(1)	0(1)
C(2)	14(1)	17(1)	20(1)	4(1)	0(1)	-2(1)
C(3)	23(1)	17(1)	18(1)	-2(1)	3(1)	-6(1)
C(4)	21(1)	16(1)	14(1)	-1(1)	4(1)	-2(1)
C(5)	12(1)	14(1)	14(1)	2(1)	1(1)	-1(1)
C(6)	16(1)	20(1)	23(1)	6(1)	2(1)	2(1)
C(7)	20(1)	19(1)	20(1)	5(1)	-3(1)	-1(1)
C(8)	17(1)	16(1)	16(1)	1(1)	3(1)	-2(1)
C(9)	24(1)	19(1)	14(1)	0(1)	1(1)	-2(1)
C(10)	22(1)	19(1)	27(1)	9(1)	-1(1)	-3(1)
C(11)	14(1)	21(1)	29(1)	3(1)	7(1)	-1(1)
O(1)	12(1)	22(1)	29(1)	9(1)	1(1)	1(1)
O(2)	20(1)	17(1)	19(1)	4(1)	1(1)	-3(1)
O(3)	15(1)	24(1)	28(1)	3(1)	3(1)	-2(1)

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

	x	y	z	U(eq)
H(9A)	5590	1347	-1930	28
H(9B)	7807	1582	-1808	28
H(9C)	6407	2326	-2615	28
H(10A)	8020	5066	-1399	34
H(10B)	5863	4737	-1331	34
H(10C)	7033	4251	-2336	34
H(11A)	9728	3081	-1800	31
H(11B)	10141	2639	-489	31
H(11C)	10576	3852	-773	31
H(1)	3770(20)	2660(14)	-700(15)	39(4)
H(31)	6990(20)	4570(13)	715(13)	34(4)
H(32)	8960(20)	3943(13)	968(14)	37(4)
H(41)	5370(20)	3275(12)	1363(13)	29(4)
H(42)	7300(20)	2817(12)	1994(13)	29(4)
H(61)	8470(20)	849(12)	-93(13)	28(3)
H(62)	9400(20)	1629(11)	915(12)	25(3)
H(71)	7790(20)	813(12)	2355(13)	28(3)
H(72)	7990(20)	-152(12)	1482(12)	25(3)

Table 6. Torsion angles [°] for 5.

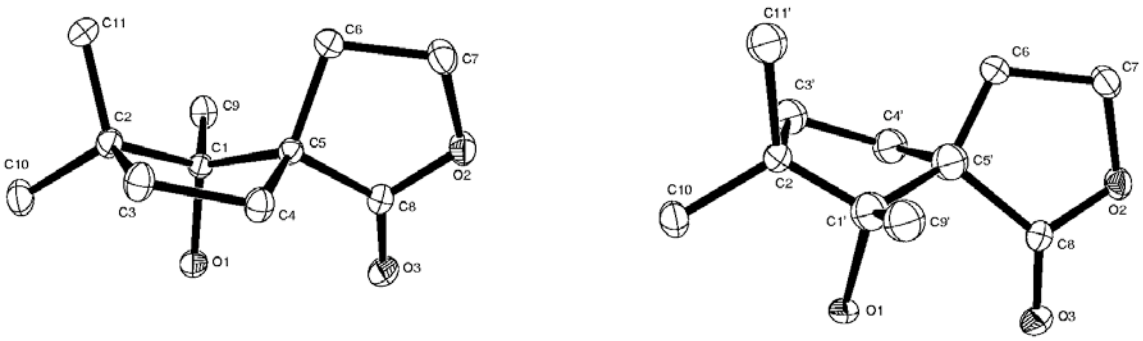
O(1)-C(1)-C(2)-C(1')	69.7(9)	C(5)-C(1)-C(2)-C(3')	112.3(5)
C(9)-C(1)-C(2)-C(1')	-170.3(9)	C(1')-C(2)-C(3)-C(4)	18.7(7)
C(5)-C(1)-C(2)-C(1')	-43.8(9)	C(11)-C(2)-C(3)-C(4)	-109.80(9)
O(1)-C(1)-C(2)-C(11)	-160.56(8)	C(10)-C(2)-C(3)-C(4)	131.25(8)
C(9)-C(1)-C(2)-C(11)	-40.47(11)	C(11')-C(2)-C(3)-C(4)	-119.3(6)
C(5)-C(1)-C(2)-C(11)	85.94(9)	C(1)-C(2)-C(3)-C(4)	11.38(10)
O(1)-C(1)-C(2)-C(10)	-39.17(10)	C(3')-C(2)-C(3)-C(4)	-42.1(7)
C(9)-C(1)-C(2)-C(10)	80.91(10)	C(2)-C(3)-C(4)-C(5)	14.82(10)
C(5)-C(1)-C(2)-C(10)	-152.67(8)	C(3)-C(4)-C(5)-C(8)	-156.59(8)
O(1)-C(1)-C(2)-C(11')	162.1(7)	C(3)-C(4)-C(5)-C(6)	92.40(9)
C(9)-C(1)-C(2)-C(11')	-77.8(8)	C(3)-C(4)-C(5)-C(1)	-35.03(9)
C(5)-C(1)-C(2)-C(11')	48.6(8)	O(1)-C(1)-C(5)-C(8)	49.64(11)
O(1)-C(1)-C(2)-C(3)	80.17(8)	C(9)-C(1)-C(5)-C(8)	-72.55(11)
C(9)-C(1)-C(2)-C(3)	-159.74(8)	C(2)-C(1)-C(5)-C(8)	161.37(8)
C(5)-C(1)-C(2)-C(3)	-33.33(9)	O(1)-C(1)-C(5)-C(6)	167.89(8)
O(1)-C(1)-C(2)-C(3')	-134.2(5)	C(9)-C(1)-C(5)-C(6)	45.70(12)
C(9)-C(1)-C(2)-C(3')	-14.1(5)	C(2)-C(1)-C(5)-C(6)	-80.38(10)

O(1)-C(1)-C(5)-C(4)	-68.95(9)	C(11')-C(2)-C(1')-O(1)	-175.1(7)
C(9)-C(1)-C(5)-C(4)	168.87(8)	C(1)-C(2)-C(1')-O(1)	-56.8(7)
C(2)-C(1)-C(5)-C(4)	42.78(9)	C(3)-C(2)-C(1')-O(1)	134.6(9)
C(8)-C(5)-C(6)-C(5')	87(3)	C(3')-C(2)-C(1')-O(1)	-76.9(8)
C(4)-C(5)-C(6)-C(5')	-156(3)	C(1)-O(1)-C(1')-C(2)	69.2(8)
C(1)-C(5)-C(6)-C(5')	-38(3)	C(1)-O(1)-C(1')-C(9')	-177.2(17)
C(8)-C(5)-C(6)-C(7)	-29.28(9)	C(1)-O(1)-C(1')-C(5')	-51.3(9)
C(4)-C(5)-C(6)-C(7)	87.48(9)	C(1')-C(2)-C(3')-C(4')	-9.1(11)
C(1)-C(5)-C(6)-C(7)	-154.45(8)	C(11)-C(2)-C(3')-C(4')	128.1(10)
C(5')-C(6)-C(7)-O(2)	13.8(8)	C(10)-C(2)-C(3')-C(4')	-130.4(8)
C(5)-C(6)-C(7)-O(2)	30.09(10)	C(11')-C(2)-C(3')-C(4')	114.3(10)
C(6)-C(5)-C(8)-O(3)	-163.20(9)	C(1)-C(2)-C(3')-C(4')	-23.9(7)
C(4)-C(5)-C(8)-O(3)	78.64(12)	C(3)-C(2)-C(3')-C(4')	43.2(13)
C(1)-C(5)-C(8)-O(3)	-35.31(14)	C(2)-C(3')-C(4')-C(5')	-18.0(13)
C(6)-C(5)-C(8)-O(2)	19.74(10)	C(7)-C(6)-C(5')-C(1')	126.5(17)
C(4)-C(5)-C(8)-O(2)	-98.42(9)	C(5)-C(6)-C(5')-C(1')	58(2)
C(1)-C(5)-C(8)-O(2)	147.63(8)	C(7)-C(6)-C(5')-C(4')	-121.0(9)
C(6)-C(5)-C(8)-C(5')	-62(2)	C(5)-C(6)-C(5')-C(4')	171(4)
C(4)-C(5)-C(8)-C(5')	180(3)	C(7)-C(6)-C(5')-C(8)	-4.5(12)
C(1)-C(5)-C(8)-C(5')	66(2)	C(5)-C(6)-C(5')-C(8)	-73(3)
C(9)-C(1)-O(1)-C(1')	-179.7(9)	C(2)-C(1')-C(5')-C(6)	59(2)
C(2)-C(1)-O(1)-C(1')	-56.2(8)	C(9')-C(1')-C(5')-C(6)	-57(2)
C(5)-C(1)-O(1)-C(1')	54.7(8)	O(1)-C(1')-C(5')-C(6)	172.8(15)
O(3)-C(8)-O(2)-C(7)	-178.35(8)	C(2)-C(1')-C(5')-C(4')	-51.5(16)
C(5)-C(8)-O(2)-C(7)	-1.04(10)	C(9')-C(1')-C(5')-C(4')	-167.9(12)
C(5')-C(8)-O(2)-C(7)	16.2(7)	O(1)-C(1')-C(5')-C(4')	62.3(13)
C(6)-C(7)-O(2)-C(8)	-18.71(10)	C(2)-C(1')-C(5')-C(8)	-171.9(10)
C(11)-C(2)-C(1')-C(9')	104.3(10)	C(9')-C(1')-C(5')-C(8)	71.7(15)
C(10)-C(2)-C(1')-C(9')	-91.8(10)	O(1)-C(1')-C(5')-C(8)	-58.2(13)
C(11')-C(2)-C(1')-C(9')	59.7(13)	C(3')-C(4')-C(5')-C(6)	-97.4(12)
C(1)-C(2)-C(1')-C(9')	178.0(15)	C(3')-C(4')-C(5')-C(1')	37.0(15)
C(3)-C(2)-C(1')-C(9')	9.4(7)	C(3')-C(4')-C(5')-C(8)	154.4(12)
C(3')-C(2)-C(1')-C(9')	157.9(10)	O(3)-C(8)-C(5')-C(6)	-170.9(4)
C(11)-C(2)-C(1')-C(5')	-18.1(16)	O(2)-C(8)-C(5')-C(6)	-7.1(12)
C(10)-C(2)-C(1')-C(5')	145.7(10)	C(5)-C(8)-C(5')-C(6)	97(3)
C(11')-C(2)-C(1')-C(5')	-62.8(15)	O(3)-C(8)-C(5')-C(1')	46.4(16)
C(1)-C(2)-C(1')-C(5')	55.6(11)	O(2)-C(8)-C(5')-C(1')	-149.9(10)
C(3)-C(2)-C(1')-C(5')	-113.1(13)	C(5)-C(8)-C(5')-C(1')	-46.0(19)
C(3')-C(2)-C(1')-C(5')	35.4(13)	O(3)-C(8)-C(5')-C(4')	-66.6(15)
C(11)-C(2)-C(1')-O(1)	-130.4(5)	O(2)-C(8)-C(5')-C(4')	97.2(12)
C(10)-C(2)-C(1')-O(1)	33.4(10)	C(5)-C(8)-C(5')-C(4')	-159(3)

Table 7. Hydrogen bonds for 5 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(3)	0.823(18)	1.964(18)	2.7250(10)	153.3(16)

Figure 1 The heavy atom skeletons of the two disordered molecules. (a) The main structure. (b) The minor component of the disordered structure. Only C1', C3' – C5', C9' and C11' are separately resolved; these sites have 7.6(2)% occupancy and their positions are subject to systematic error which seems most serious for C3' [C(2)-C(3') = 1.90(2) Å].



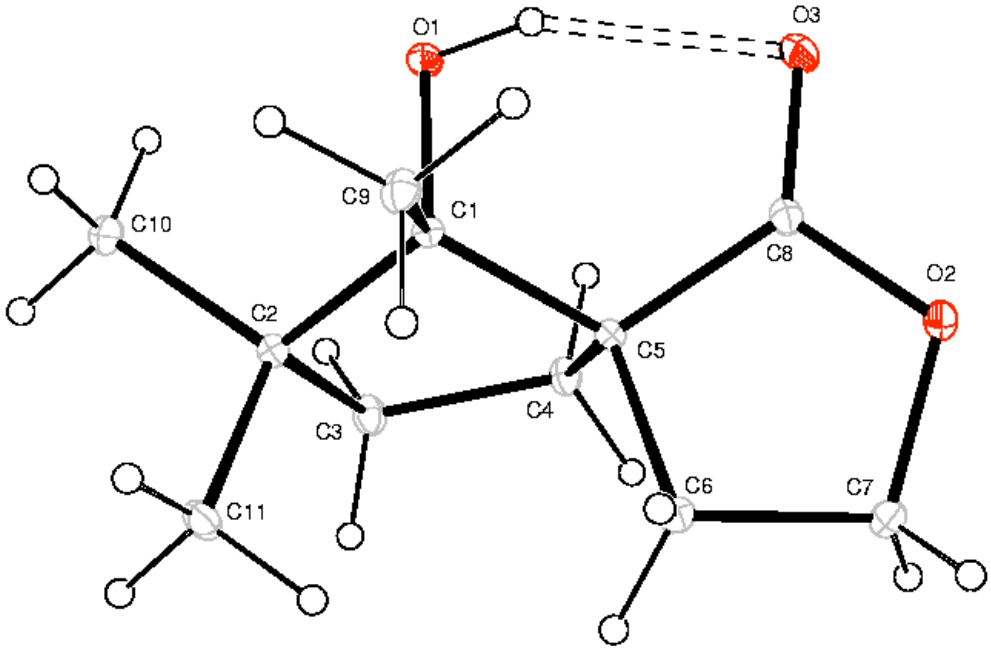


Figure 2. The main structure showing hydrogen positions and 20% probability ellipsoids. The intramolecular hydrogen bond is indicated by broken lines.

(B) Crystal Structure Analysis of Compound 15:

km0603 $C_{11}H_{16}O_3$

Table 8. Crystal data and structure refinement for **15**.

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table 10. Bond lengths [Å] and angles [°] for **15**.

Table 11. Anisotropic displacement parameters ($Å^2$x 10^3)for 15. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)for **15**.

Table 13. Torsion angles [°] for **15**.

Table 14. Hydrogen bonds for **15** [Å and °].

Figure 3 A view of the molecule showing 20% ellipsoids.

Table 8. Crystal data and structure refinement for 15.

Identification code	km0603	
Empirical formula	$C_{11}H_{16}O_3$	
Formula weight	196.24	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 12.1695(2) Å	a= 90°.
	b = 7.45440(10) Å	b= 92.9850(10)°.
	c = 21.8995(5) Å	g= 90°.
Volume	1983.95(6) $Å^3$	
Z	8	
Density (calculated)	1.314 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	848	
Crystal size	0.40 x 0.35 x 0.33 mm^3	
Theta range for data collection	3.3 to 30.0°.	
Index ranges	-17<=h<=17, 0<=k<=10, 0<=l<=30	
Reflections collected	9018	
Independent reflections	2846 [R(int) = 0.0248]	
Completeness to theta = 30.04°	98.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2846 / 0 / 127	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0951	
R indices (all data)	R1 = 0.0415, wR2 = 0.0987	
Largest diff. peak and hole	0.39 and -0.19 $e.Å^{-3}$	

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	5984(1)	2095(1)	5856(1)	18(1)
O(2)	7239(1)	-311(1)	4959(1)	21(1)
O(3)	5670(1)	-1790(1)	5079(1)	21(1)
C(1)	7425(1)	2881(1)	6860(1)	20(1)
C(2)	6304(1)	3021(1)	7122(1)	21(1)
C(3)	6672(1)	1275(1)	6850(1)	16(1)
C(4)	6122(1)	600(1)	6256(1)	14(1)
C(5)	5036(1)	-361(1)	6379(1)	19(1)
C(6)	5375(1)	-2253(2)	6590(1)	29(1)
C(7)	6510(1)	-2629(1)	6338(1)	19(1)
C(8)	6831(1)	-947(1)	5982(1)	14(1)
C(9)	8066(1)	-588(1)	5955(1)	18(1)
C(10)	8147(1)	410(1)	5352(1)	22(1)
C(11)	6492(1)	-1090(1)	5306(1)	16(1)

Table 10. Bond lengths [Å] and angles [°] for 15.

O(1)-C(4)	1.4236(10)	C(5)-C(6)	1.5340(14)
O(1)-H(1)	0.8400	C(5)-H(5A)	0.9900
O(2)-C(11)	1.3463(11)	C(5)-H(5B)	0.9900
O(2)-C(10)	1.4666(11)	C(6)-C(7)	1.5398(14)
O(3)-C(11)	1.2117(11)	C(6)-H(6A)	0.9900
C(1)-C(3)	1.5071(12)	C(6)-H(6B)	0.9900
C(1)-C(2)	1.5116(13)	C(7)-C(8)	1.5382(12)
C(1)-H(1A)	0.9900	C(7)-H(7A)	0.9900
C(1)-H(1B)	0.9900	C(7)-H(7B)	0.9900
C(2)-C(3)	1.5084(13)	C(8)-C(11)	1.5186(12)
C(2)-H(2A)	0.9900	C(8)-C(9)	1.5310(12)
C(2)-H(2B)	0.9900	C(9)-C(10)	1.5237(13)
C(3)-C(4)	1.5175(11)	C(9)-H(9A)	0.9900
C(3)-H(3)	1.0000	C(9)-H(9B)	0.9900
C(4)-C(5)	1.5385(12)	C(10)-H(10A)	0.9900
C(4)-C(8)	1.5784(12)	C(10)-H(10B)	0.9900
C(4)-O(1)-H(1)	109.5	C(5)-C(6)-H(6A)	110.3
C(11)-O(2)-C(10)	109.72(7)	C(7)-C(6)-H(6A)	110.3
C(3)-C(1)-C(2)	59.96(6)	C(5)-C(6)-H(6B)	110.3
C(3)-C(1)-H(1A)	117.8	C(7)-C(6)-H(6B)	110.3
C(2)-C(1)-H(1A)	117.8	H(6A)-C(6)-H(6B)	108.6
C(3)-C(1)-H(1B)	117.8	C(8)-C(7)-C(6)	106.88(7)
C(2)-C(1)-H(1B)	117.8	C(8)-C(7)-H(7A)	110.3
H(1A)-C(1)-H(1B)	114.9	C(6)-C(7)-H(7A)	110.3
C(3)-C(2)-C(1)	59.87(6)	C(8)-C(7)-H(7B)	110.3
C(3)-C(2)-H(2A)	117.8	C(6)-C(7)-H(7B)	110.3
C(1)-C(2)-H(2A)	117.8	H(7A)-C(7)-H(7B)	108.6
C(3)-C(2)-H(2B)	117.8	C(11)-C(8)-C(9)	101.11(7)
C(1)-C(2)-H(2B)	117.8	C(11)-C(8)-C(7)	111.94(7)
H(2A)-C(2)-H(2B)	114.9	C(9)-C(8)-C(7)	115.96(7)
C(1)-C(3)-C(2)	60.17(6)	C(11)-C(8)-C(4)	107.26(7)
C(1)-C(3)-C(4)	121.08(7)	C(9)-C(8)-C(4)	116.39(7)
C(2)-C(3)-C(4)	119.78(7)	C(7)-C(8)-C(4)	104.09(7)
C(1)-C(3)-H(3)	115.0	C(10)-C(9)-C(8)	103.07(7)
C(2)-C(3)-H(3)	115.0	C(10)-C(9)-H(9A)	111.1
C(4)-C(3)-H(3)	115.0	C(8)-C(9)-H(9A)	111.1
O(1)-C(4)-C(3)	107.53(7)	C(10)-C(9)-H(9B)	111.1
O(1)-C(4)-C(5)	113.42(7)	C(8)-C(9)-H(9B)	111.1
C(3)-C(4)-C(5)	110.50(7)	H(9A)-C(9)-H(9B)	109.1
O(1)-C(4)-C(8)	112.70(7)	O(2)-C(10)-C(9)	104.41(7)
C(3)-C(4)-C(8)	110.08(7)	O(2)-C(10)-H(10A)	110.9
C(5)-C(4)-C(8)	102.58(7)	C(9)-C(10)-H(10A)	110.9
C(6)-C(5)-C(4)	105.14(7)	O(2)-C(10)-H(10B)	110.9
C(6)-C(5)-H(5A)	110.7	C(9)-C(10)-H(10B)	110.9
C(4)-C(5)-H(5A)	110.7	H(10A)-C(10)-H(10B)	108.9
C(6)-C(5)-H(5B)	110.7	O(3)-C(11)-O(2)	121.44(8)
C(4)-C(5)-H(5B)	110.7	O(3)-C(11)-C(8)	127.31(8)
H(5A)-C(5)-H(5B)	108.8	O(2)-C(11)-C(8)	111.25(7)
C(5)-C(6)-C(7)	106.90(8)		

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 15. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	19(1)	15(1)	18(1)	3(1)	-4(1)	0(1)
O(2)	27(1)	22(1)	16(1)	1(1)	2(1)	-1(1)
O(3)	22(1)	21(1)	20(1)	-4(1)	-7(1)	2(1)
C(1)	18(1)	20(1)	22(1)	-6(1)	0(1)	-3(1)
C(2)	21(1)	21(1)	22(1)	-6(1)	2(1)	1(1)
C(3)	17(1)	16(1)	14(1)	-1(1)	-1(1)	-1(1)
C(4)	15(1)	14(1)	14(1)	1(1)	-1(1)	-1(1)
C(5)	14(1)	20(1)	22(1)	0(1)	1(1)	-3(1)
C(6)	21(1)	24(1)	41(1)	11(1)	5(1)	-4(1)
C(7)	23(1)	15(1)	19(1)	3(1)	-1(1)	-1(1)
C(8)	15(1)	14(1)	14(1)	0(1)	-2(1)	0(1)
C(9)	15(1)	19(1)	20(1)	-2(1)	0(1)	0(1)
C(10)	21(1)	20(1)	24(1)	0(1)	4(1)	-3(1)
C(11)	20(1)	14(1)	15(1)	0(1)	-2(1)	3(1)

Table 12. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for 15.

	x	y	z	U(eq)
H(1)	5453	1903	5604	26
H(1A)	7537	3494	6467	24
H(1B)	8077	2867	7150	24
H(2A)	6271	3091	7572	26
H(2B)	5731	3719	6889	26
H(3)	6883	321	7155	19
H(5A)	4643	269	6700	23
H(5B)	4551	-415	6002	23
H(6A)	4830	-3147	6431	34
H(6B)	5418	-2320	7042	34
H(7A)	7060	-2868	6677	23
H(7B)	6472	-3687	6064	23
H(9A)	8340	160	6304	21
H(9B)	8488	-1723	5955	21
H(10A)	8062	1718	5410	26
H(10B)	8864	177	5173	26

Table 13. Torsion angles [°] for 15.

C(2)-C(1)-C(3)-C(4)	108.84(9)
C(1)-C(2)-C(3)-C(4)	-110.95(9)
C(1)-C(3)-C(4)-O(1)	-28.57(10)
C(2)-C(3)-C(4)-O(1)	42.51(10)
C(1)-C(3)-C(4)-C(5)	-152.85(8)
C(2)-C(3)-C(4)-C(5)	-81.77(10)
C(1)-C(3)-C(4)-C(8)	94.55(9)
C(2)-C(3)-C(4)-C(8)	165.63(8)
O(1)-C(4)-C(5)-C(6)	158.37(8)
C(3)-C(4)-C(5)-C(6)	-80.80(9)
C(8)-C(4)-C(5)-C(6)	36.53(9)
C(4)-C(5)-C(6)-C(7)	-23.32(10)
C(5)-C(6)-C(7)-C(8)	0.20(11)
C(6)-C(7)-C(8)-C(11)	-93.26(9)
C(6)-C(7)-C(8)-C(9)	151.44(8)
C(6)-C(7)-C(8)-C(4)	22.25(9)
O(1)-C(4)-C(8)-C(11)	-39.72(9)
C(3)-C(4)-C(8)-C(11)	-159.76(7)
C(5)-C(4)-C(8)-C(11)	82.62(8)
O(1)-C(4)-C(8)-C(9)	72.58(9)
C(3)-C(4)-C(8)-C(9)	-47.46(10)
C(5)-C(4)-C(8)-C(9)	-165.08(7)
O(1)-C(4)-C(8)-C(7)	-158.49(7)
C(3)-C(4)-C(8)-C(7)	81.47(8)
C(5)-C(4)-C(8)-C(7)	-36.16(8)
C(11)-C(8)-C(9)-C(10)	30.04(8)
C(7)-C(8)-C(9)-C(10)	151.32(8)
C(4)-C(8)-C(9)-C(10)	-85.74(9)
C(11)-O(2)-C(10)-C(9)	19.43(9)
C(8)-C(9)-C(10)-O(2)	-30.89(9)
C(10)-O(2)-C(11)-O(3)	-179.57(8)
C(10)-O(2)-C(11)-C(8)	0.55(10)
C(9)-C(8)-C(11)-O(3)	160.20(9)
C(7)-C(8)-C(11)-O(3)	36.14(12)
C(4)-C(8)-C(11)-O(3)	-77.43(11)
C(9)-C(8)-C(11)-O(2)	-19.93(9)
C(7)-C(8)-C(11)-O(2)	-143.99(7)
C(4)-C(8)-C(11)-O(2)	102.44(8)

Symmetry transformations used to generate equivalent atoms:

Table 14. Hydrogen bonds for 15 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(3)#1	0.84	1.97	2.8040(9)	169.5

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

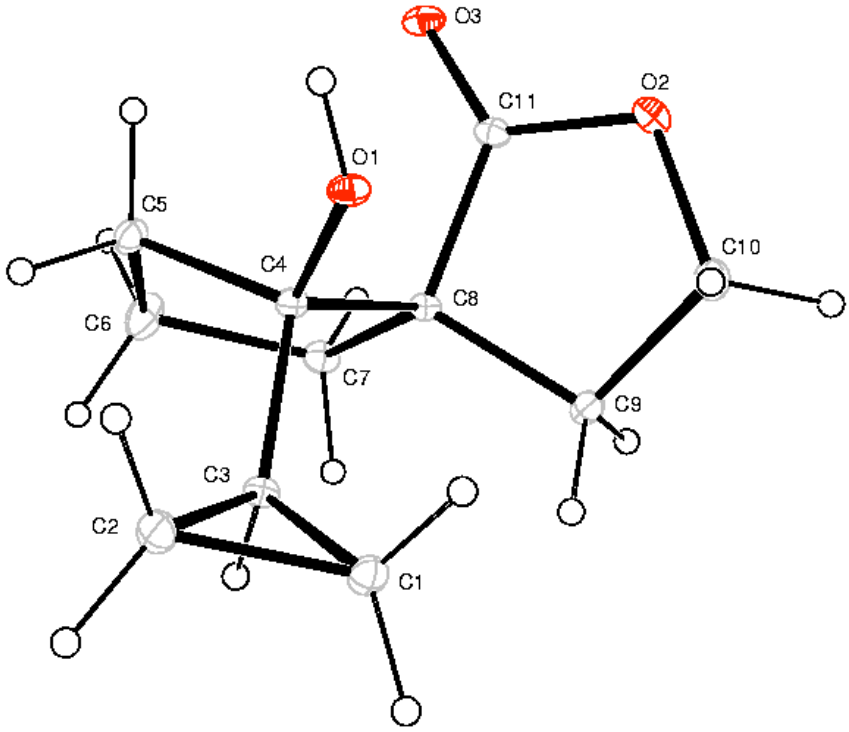


Figure 3 Aview of the molecule showing 20% ellipsoids.

(C) Crystal Structure Analysis of Compound 35:

km1003 $C_{11}H_{16}O_3$

Table 15. Crystal data and structure refinement for **35**.

Table 16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **35**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table 17. Bond lengths [Å] and angles [°] for **35**.

Table 18. Anisotropic displacement parameters ($Å^2$x 10^3)for **35**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table 19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)for **35**.

Table 20. Torsion angles [°] for **35**.

Figure 4 A view of the molecule showing 20% ellipsoids.

Table 15. Crystal data and structure refinement for 35.

Identification code	km1003/TH5-37-2	
Empirical formula	$C_{16} H_{17} N O_6$	
Formula weight	319.31	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 24.8813(5) Å	a= 90°.
	b = 6.9879(2) Å	b= 119.580(1)°.
	c = 19.7369(6) Å	g= 90°.
Volume	2984.36(14) $Å^3$	
Z	8	
Density (calculated)	1.421 Mg/m^3	
Absorption coefficient	0.110 mm^{-1}	
F(000)	1344	
Crystal size	0.4 x 0.2 x 0.08 mm^3	
Theta range for data collection	1.88 to 25.76°.	
Index ranges	-29<=h<=26, 0<=k<=8, 0<=l<=24	
Reflections collected	13054	
Independent reflections	2787 [R(int) = 0.0750]	
Completeness to theta = 25.76°	97.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.091 and 0.916	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2787 / 0 / 209	
Goodness-of-fit on F^2	1.176	
Final R indices [I>2sigma(I)]	R1 = 0.0707, wR2 = 0.1561	
R indices (all data)	R1 = 0.0978, wR2 = 0.1682	
Largest diff. peak and hole	0.421 and -0.263 $e.Å^{-3}$	

Table 16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for 35. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1382(1)	5915(5)	2812(2)	34(1)
C(2)	1696(1)	3967(5)	2927(2)	37(1)
C(3)	2149(2)	4597(5)	3778(2)	42(1)
C(4)	1929(1)	6689(4)	3563(2)	34(1)
C(5)	2298(2)	7881(4)	3272(2)	34(1)
C(6)	1825(1)	8256(5)	2424(2)	33(1)
C(7)	748(2)	5908(5)	2741(2)	45(1)
C(8)	2601(2)	9684(4)	3733(2)	38(1)
C(9)	3176(1)	9277(5)	4493(2)	41(1)
C(10)	4206(2)	8234(4)	4940(2)	36(1)
C(11)	4661(1)	7618(4)	4698(2)	34(1)
C(12)	4485(2)	7230(5)	3923(2)	39(1)
C(13)	4911(2)	6660(5)	3717(2)	38(1)
C(14)	5524(1)	6466(4)	4296(2)	34(1)
C(15)	5713(2)	6811(4)	5075(2)	36(1)
C(16)	5278(2)	7396(4)	5273(2)	35(1)
N(1)	5984(1)	5894(4)	4075(2)	41(1)
O(1)	1344(1)	7067(3)	2174(1)	37(1)
O(2)	1861(1)	9399(4)	1991(1)	44(1)
O(3)	3648(1)	8614(3)	4323(1)	40(1)
O(4)	4321(1)	8391(4)	5604(1)	47(1)
O(5)	5819(1)	5693(4)	3379(1)	53(1)
O(6)	6519(1)	5642(4)	4593(1)	56(1)

Table 17. Bond lengths [Å] and angles [°] for 35.

C(1)-O(1)	1.457(4)	C(8)-H(8A)	0.9700
C(1)-C(7)	1.513(4)	C(8)-H(8B)	0.9700
C(1)-C(2)	1.530(5)	C(9)-O(3)	1.448(4)
C(1)-C(4)	1.533(4)	C(9)-H(9A)	0.9700
C(2)-C(3)	1.554(4)	C(9)-H(9B)	0.9700
C(2)-H(2A)	0.9700	C(10)-O(4)	1.199(4)
C(2)-H(2B)	0.9700	C(10)-O(3)	1.347(4)
C(3)-C(4)	1.545(5)	C(10)-C(11)	1.491(5)
C(3)-H(3A)	0.9700	C(11)-C(12)	1.396(4)
C(3)-H(3B)	0.9700	C(11)-C(16)	1.396(4)
C(4)-C(5)	1.544(4)	C(12)-C(13)	1.368(5)
C(4)-H(4)	0.9800	C(12)-H(12)	0.9300
C(5)-C(6)	1.519(4)	C(13)-C(14)	1.389(4)
C(5)-C(8)	1.519(4)	C(13)-H(13)	0.9300
C(5)-H(5)	0.9800	C(14)-C(15)	1.390(4)
C(6)-O(2)	1.205(4)	C(14)-N(1)	1.468(4)
C(6)-O(1)	1.337(4)	C(15)-C(16)	1.382(5)
C(7)-H(7A)	0.9600	C(15)-H(15)	0.9300
C(7)-H(7B)	0.9600	C(16)-H(16)	0.9300
C(7)-H(7C)	0.9600	N(1)-O(6)	1.227(3)
C(8)-C(9)	1.503(4)	N(1)-O(5)	1.231(3)

O(1)-C(1)-C(7)	107.5(3)	C(1)-C(7)-H(7C)	109.5
O(1)-C(1)-C(2)	115.5(2)	H(7A)-C(7)-H(7C)	109.5
C(7)-C(1)-C(2)	116.4(3)	H(7B)-C(7)-H(7C)	109.5
O(1)-C(1)-C(4)	106.7(2)	C(9)-C(8)-C(5)	112.8(3)
C(7)-C(1)-C(4)	118.6(3)	C(9)-C(8)-H(8A)	109.0
C(2)-C(1)-C(4)	91.4(2)	C(5)-C(8)-H(8A)	109.0
C(1)-C(2)-C(3)	87.3(2)	C(9)-C(8)-H(8B)	109.0
C(1)-C(2)-H(2A)	114.1	C(5)-C(8)-H(8B)	109.0
C(3)-C(2)-H(2A)	114.1	H(8A)-C(8)-H(8B)	107.8
C(1)-C(2)-H(2B)	114.1	O(3)-C(9)-C(8)	108.0(3)
C(3)-C(2)-H(2B)	114.1	O(3)-C(9)-H(9A)	110.1
H(2A)-C(2)-H(2B)	111.3	C(8)-C(9)-H(9A)	110.1
C(4)-C(3)-C(2)	90.1(2)	O(3)-C(9)-H(9B)	110.1
C(4)-C(3)-H(3A)	113.6	C(8)-C(9)-H(9B)	110.1
C(2)-C(3)-H(3A)	113.6	H(9A)-C(9)-H(9B)	108.4
C(4)-C(3)-H(3B)	113.6	O(4)-C(10)-O(3)	123.6(3)
C(2)-C(3)-H(3B)	113.6	O(4)-C(10)-C(11)	124.5(3)
H(3A)-C(3)-H(3B)	110.9	O(3)-C(10)-C(11)	111.9(3)
C(1)-C(4)-C(5)	103.8(2)	C(12)-C(11)-C(16)	119.5(3)
C(1)-C(4)-C(3)	87.6(2)	C(12)-C(11)-C(10)	122.0(3)
C(5)-C(4)-C(3)	114.7(3)	C(16)-C(11)-C(10)	118.4(3)
C(1)-C(4)-H(4)	115.6	C(13)-C(12)-C(11)	120.9(3)
C(5)-C(4)-H(4)	115.6	C(13)-C(12)-H(12)	119.6
C(3)-C(4)-H(4)	115.6	C(11)-C(12)-H(12)	119.6
C(6)-C(5)-C(8)	113.7(3)	C(12)-C(13)-C(14)	118.7(3)
C(6)-C(5)-C(4)	102.9(2)	C(12)-C(13)-H(13)	120.6
C(8)-C(5)-C(4)	115.9(3)	C(14)-C(13)-H(13)	120.6
C(6)-C(5)-H(5)	108.0	C(13)-C(14)-C(15)	121.9(3)
C(8)-C(5)-H(5)	108.0	C(13)-C(14)-N(1)	118.9(3)
C(4)-C(5)-H(5)	108.0	C(15)-C(14)-N(1)	119.2(3)
O(2)-C(6)-O(1)	121.1(3)	C(16)-C(15)-C(14)	118.6(3)
O(2)-C(6)-C(5)	127.5(3)	C(16)-C(15)-H(15)	120.7
O(1)-C(6)-C(5)	111.4(3)	C(14)-C(15)-H(15)	120.7
C(1)-C(7)-H(7A)	109.5	C(15)-C(16)-C(11)	120.3(3)
C(1)-C(7)-H(7B)	109.5	C(15)-C(16)-H(16)	119.9
H(7A)-C(7)-H(7B)	109.5	C(11)-C(16)-H(16)	119.9

O(6)-N(1)-O(5)	122.7(3)
O(6)-N(1)-C(14)	118.4(3)
O(5)-N(1)-C(14)	118.9(3)
C(6)-O(1)-C(1)	111.1(2)
C(10)-O(3)-C(9)	116.5(2)

Table 18. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 35. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	37(2)	36(2)	28(2)	-3(1)	17(1)	-9(1)
C(2)	36(2)	43(2)	31(2)	-6(1)	16(1)	-4(2)
C(3)	43(2)	42(2)	35(2)	2(2)	16(2)	-1(2)
C(4)	42(2)	32(2)	26(2)	-4(1)	16(1)	-8(1)
C(5)	40(2)	30(2)	28(2)	-1(1)	13(1)	-1(1)
C(6)	32(2)	39(2)	27(2)	3(1)	14(1)	1(1)
C(7)	43(2)	44(2)	53(2)	-5(2)	27(2)	-7(2)
C(8)	46(2)	31(2)	39(2)	-1(1)	23(2)	-5(1)
C(9)	39(2)	44(2)	35(2)	-6(2)	15(2)	-10(2)
C(10)	42(2)	24(2)	28(2)	0(1)	7(1)	-9(1)
C(11)	39(2)	24(2)	26(2)	1(1)	6(1)	-7(1)
C(12)	38(2)	40(2)	24(2)	2(1)	4(1)	-2(2)
C(13)	42(2)	39(2)	21(2)	2(1)	5(1)	-5(2)
C(14)	39(2)	26(2)	32(2)	3(1)	13(1)	-6(1)
C(15)	35(2)	27(2)	27(2)	4(1)	2(1)	-7(1)
C(16)	43(2)	24(2)	21(2)	0(1)	5(1)	-8(1)
N(1)	42(2)	36(2)	37(2)	5(1)	13(1)	-8(1)
O(1)	35(1)	43(1)	29(1)	0(1)	11(1)	-10(1)
O(2)	42(1)	54(2)	34(1)	12(1)	17(1)	-3(1)
O(3)	37(1)	44(1)	26(1)	-5(1)	6(1)	-5(1)
O(4)	54(2)	50(2)	26(1)	0(1)	12(1)	-2(1)
O(5)	62(2)	61(2)	35(1)	7(1)	22(1)	0(1)
O(6)	40(1)	68(2)	47(2)	-4(1)	12(1)	-5(1)

Table 19. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for 35.

	x	y	z	U(eq)
H(2A)	1891	3777	2611	44
H(2B)	1437	2888	2886	44
H(3A)	2055	4045	4158	50
H(3B)	2581	4410	3933	50
H(4)	1822	7349	3918	41
H(5)	2622	7062	3285	41
H(7A)	624	7198	2761	68
H(7B)	761	5184	3162	68
H(7C)	456	5336	2254	68
H(8A)	2706	10514	3421	45
H(8B)	2309	10360	3836	45
H(9A)	3314	10429	4808	49
H(9B)	3093	8306	4780	49
H(12)	4073	7361	3541	47
H(13)	4792	6407	3199	46
H(15)	6124	6651	5456	43
H(16)	5397	7644	5791	41

Table 20. Torsion angles [°] for 35.

O(1)-C(1)-C(2)-C(3)	123.7(3)
C(7)-C(1)-C(2)-C(3)	-108.8(3)
C(4)-C(1)-C(2)-C(3)	14.4(2)
C(1)-C(2)-C(3)-C(4)	-14.3(2)
O(1)-C(1)-C(4)-C(5)	-16.8(3)
C(7)-C(1)-C(4)-C(5)	-138.3(3)
C(2)-C(1)-C(4)-C(5)	100.4(3)
O(1)-C(1)-C(4)-C(3)	-131.7(3)
C(7)-C(1)-C(4)-C(3)	106.8(3)
C(2)-C(1)-C(4)-C(3)	-14.5(2)
C(2)-C(3)-C(4)-C(1)	14.3(2)
C(2)-C(3)-C(4)-C(5)	-89.8(3)
C(1)-C(4)-C(5)-C(6)	19.5(3)
C(3)-C(4)-C(5)-C(6)	113.2(3)
C(1)-C(4)-C(5)-C(8)	144.3(3)
C(3)-C(4)-C(5)-C(8)	-122.0(3)
C(8)-C(5)-C(6)-O(2)	39.8(5)
C(4)-C(5)-C(6)-O(2)	166.0(3)
C(8)-C(5)-C(6)-O(1)	-143.0(3)
C(4)-C(5)-C(6)-O(1)	-16.8(3)
C(6)-C(5)-C(8)-C(9)	-164.7(3)
C(4)-C(5)-C(8)-C(9)	76.4(4)
C(5)-C(8)-C(9)-O(3)	69.7(3)
O(4)-C(10)-C(11)-C(12)	171.9(3)
O(3)-C(10)-C(11)-C(12)	-8.7(4)
O(4)-C(10)-C(11)-C(16)	-7.0(5)
O(3)-C(10)-C(11)-C(16)	172.4(3)
C(16)-C(11)-C(12)-C(13)	-0.9(5)
C(10)-C(11)-C(12)-C(13)	-179.7(3)
C(11)-C(12)-C(13)-C(14)	0.2(5)
C(12)-C(13)-C(14)-C(15)	0.8(5)
C(12)-C(13)-C(14)-N(1)	-178.7(3)
C(13)-C(14)-C(15)-C(16)	-1.2(5)
N(1)-C(14)-C(15)-C(16)	178.4(3)
C(14)-C(15)-C(16)-C(11)	0.5(4)
C(12)-C(11)-C(16)-C(15)	0.5(4)
C(10)-C(11)-C(16)-C(15)	179.4(3)
C(13)-C(14)-N(1)-O(6)	-176.7(3)
C(15)-C(14)-N(1)-O(6)	3.7(4)
C(13)-C(14)-N(1)-O(5)	3.6(4)
C(15)-C(14)-N(1)-O(5)	-176.0(3)
O(2)-C(6)-O(1)-C(1)	-176.1(3)
C(5)-C(6)-O(1)-C(1)	6.5(3)
C(7)-C(1)-O(1)-C(6)	135.2(3)
C(2)-C(1)-O(1)-C(6)	-92.9(3)
C(4)-C(1)-O(1)-C(6)	6.9(3)
O(4)-C(10)-O(3)-C(9)	1.1(4)
C(11)-C(10)-O(3)-C(9)	-178.3(3)
C(8)-C(9)-O(3)-C(10)	178.0(3)

Figure 4. A view of the molecule showing 20% probability ellipsoids.