C(13)	0.6993 (4)	0.2065 (3)	0.1483 (3)	4.8
C(14)	0.5540 (4)	0.2337 (4)	0.0978 (4)	5.5
C(15)	0.4045 (4)	0.2148 (3)	0.1388 (3)	4.8
C(16)	0.4058 (4)	0.1667 (4)	0.2311 (4)	5.4
C(17)	0.5518 (4)	0.1385 (3)	0.2828 (3)	4.6
C(18)	0.2444 (4)	0.2440 (4)	0.0794 (4)	7.2

Table 2. *Selected geometric parameters (Å, °)*

S(1)—N(1)	1.648 (3)	C(4)—C(9)	1.407 (4)
S(1)—O(3)	1.428 (2)	C(5)—C(6)	1.378 (5)
S(1)—O(4)	1.433 (3)	C(6)—C(7)	1.390 (6)
S(1)—C(12)	1.758 (3)	C(7)—C(8)	1.390 (5)
N(1)—C(3)	1.413 (4)	C(8)—C(9)	1.362 (5)
N(2)—N(3)	1.401 (4)	C(10)—C(11)	1.502 (4)
N(2)—C(10)	1.284 (5)	C(12)—C(13)	1.387 (4)
O(1)—C(2)	1.379 (4)	C(12)—C(17)	1.370 (4)
O(1)—C(5)	1.372 (4)	C(13)—C(14)	1.369 (5)
C(2)—C(3)	1.366 (4)	C(14)—C(15)	1.387 (5)
C(2)—C(10)	1.453 (4)	C(15)—C(16)	1.381 (5)
C(3)—C(4)	1.438 (4)	C(15)—C(18)	1.510 (5)
C(4)—C(5)	1.392 (4)	C(16)—C(17)	1.386 (4)
O(3)—S(1)—N(1)	107.7 (1)	C(6)—C(5)—O(1)	124.8 (3)
O(4)—S(1)—N(1)	104.5 (1)	C(6)—C(5)—C(4)	123.7 (3)
O(4)—S(1)—O(3)	119.9 (1)	C(7)—C(6)—C(5)	116.3 (3)
C(12)—S(1)—N(1)	108.2 (1)	C(8)—C(7)—C(6)	121.0 (4)
C(12)—S(1)—O(3)	107.8 (1)	C(9)—C(8)—C(7)	122.3 (3)
C(12)—S(1)—O(4)	108.2 (1)	C(8)—C(9)—C(4)	118.1 (3)
C(3)—N(1)—S(1)	121.6 (2)	C(2)—C(10)—N(2)	115.1 (3)
C(10)—N(2)—N(3)	117.1 (3)	C(11)—C(10)—N(2)	125.8 (3)
C(5)—O(1)—C(2)	106.0 (2)	C(11)—C(10)—C(2)	119.1 (3)
C(3)—C(2)—O(1)	110.5 (2)	C(13)—C(12)—S(1)	119.7 (2)
C(10)—C(2)—O(1)	117.4 (2)	C(17)—C(12)—S(1)	120.1 (2)
C(10)—C(2)—C(3)	132.0 (3)	C(17)—C(12)—C(13)	120.2 (3)
C(2)—C(3)—N(1)	122.8 (3)	C(14)—C(13)—C(12)	119.6 (3)
C(4)—C(3)—N(1)	129.2 (2)	C(15)—C(14)—C(13)	121.5 (3)
C(4)—C(3)—C(2)	107.6 (3)	C(16)—C(15)—C(14)	117.9 (3)
C(5)—C(4)—C(3)	104.4 (2)	C(18)—C(15)—C(14)	121.1 (3)
C(9)—C(4)—C(3)	136.9 (3)	C(18)—C(15)—C(16)	121.0 (3)
C(9)—C(4)—C(5)	118.6 (3)	C(17)—C(16)—C(15)	121.4 (3)
C(4)—C(5)—O(1)	111.5 (3)	C(16)—C(17)—C(12)	119.4 (4)

Table 3. *Geometric parameters (Å, °) of the related benzofuran derivatives (1), (2), (3) and (4)*

The atoms used to calculate the mean planes are in square brackets. R_3 is one of the substituents at C(10) (see *Scheme*). *X* is O(2) in compounds (1) and (2), and N(2) in compounds (3) and (4).

	(1)	(4)	(3)	(2)
[O(1)–C(9)]^ [S(1), C(12)–C(17)]	77.4 (1)	65.6 (1)	46.1 (2)	
[O(1)–C(9)]^ [C(11), C(10), R_3]	0.7 (1)	3.5 (1)	11.1 (2)	7.9 (1)
C(3)—N(1)—S—C(12)	−55.2 (3)	−57.4 (3)	−52.8 (4)	
N(1)—S—C(12)—C(13)	−72.9 (3)	−83.7 (4)	−95.2 (4)	
N(1)—S—C(12)	106.8 (1)	108.2 (1)	106.7 (3)	
S—N(1)—C(3)—C(2)	140.8 (3)	124.8 (2)	106.5 (3)	
N(1)—H· · ·*X*	2.756 (4)	2.817 (4)	2.843 (6)	2.853 (3)
S—N(1)—C(3)	124.3 (2)	121.6 (2)	116.2 (3)	
C(2)—C(3)—N(1)	119.8 (3)	122.8 (3)	122.8 (5)	126.4 (3)
N(1)—H· · ·*X*	106	92	80	
[C(2), C(10), C(11), R_3]^ [C(3), N(1), S(1)]	41.2 (1)	56.1 (1)	79.5 (2)	

The structure was solved by direct methods (*SHELXTL-Plus*; Sheldrick, 1991) and refined by full-matrix least-squares methods. All the non-H atoms were refined anisotropically. The H atoms of the methyl groups were introduced at geometrically idealized positions. All other H atoms could be located on a difference Fourier map. All H atoms were refined riding on their parent atoms.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1246). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Two Polymorphic Forms of 3-Hydroxy-2-methyl-4*H*-pyran-4-one (Maltol)

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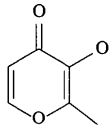
(*Received 26 April 1996; accepted 30 May 1996*)

Abstract

The crystal structures of two polymorphic forms of maltol, $C_6H_6O_3$, have been determined. The polymorphs exhibit different crystal-packing arrangements through intermolecular hydrogen bonding involving the hydroxyl H atoms. Form (1) has a near-planar chain of molecules linked by hydrogen bonds while form (2) has mutually hydrogen-bonded dimers. In both polymorphic forms there are also weaker C—H· · ·O bonds which give greater stability to the chains of form (1) and link the dimers in form (2).

Comment

In the structures of both polymorphic forms, the hydroxyl atoms H1 bonded to the O1 atoms are involved in intermolecular hydrogen bond to a carbonyl atom, O2. In the case of polymorph (1), there are two crystallographically unique molecules (*A* and *B*) arranged alternately in the chain, with successive pairs related by a cell translation along the *c* axis. Molecules *A* and *B* are approximately related by a non-crystallographic twofold screw axis parallel to **c** at $x = 0.75$, $y = 0.236$. The hydrogen bonds link the molecules to form a near planar chain. Adjacent molecules in the chain are arranged such that there are also weaker hydrogen bonds involving the carbon-bonded atom H5 and the carbonyl atom, O2 (Fig. 1).



Maltol

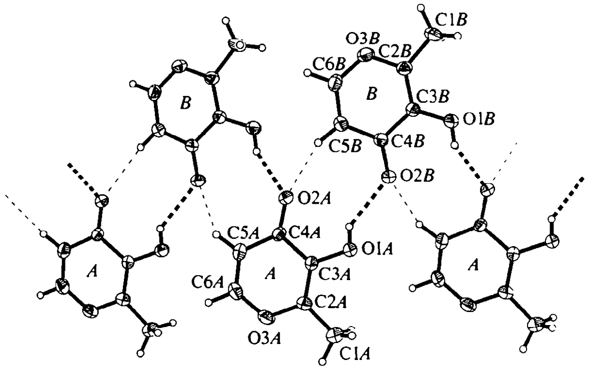


Fig. 1. Structure of polymorph (1) (*SHELXTL/PC XP*; Sheldrick, 1990*a*) showing the atom-numbering scheme of the near-planar chain of hydrogen-bonded molecules. Intermolecular O—H···O bonds are shown as dashed lines and C—H···O bonds are shown as dotted lines. Displacement ellipsoids are drawn at the 30% probability level.

In polymorph (2), three crystallographically unique molecules (*A*, *B* and *C*) are found. One molecule (*C*) forms hydrogen-bonded dimeric pairs mutually linked across a crystallographic centre of symmetry while the other molecules (*A* and *B*) are hydrogen bonded to each other in a similar dimeric arrangement. In polymorph (2), further weaker C—H···O hydrogen bonds from H5 to O2 link dimeric units into chains (Fig. 2). The two polymorphs of maltol are similar to two of the three polymorphic forms reported for ethyl maltol (Brown *et al.*, 1995).

The bond distances for the two polymorphs are essentially the same despite the data for polymorphs (1) and (2) being collected at 293 and 163 K, respectively. The intermolecular contact parameters are summarized in Table 5. In both forms, the H atom H1 was located as the highest residual electron-density peak after all other atoms were included in the refinement. The distances between the O atoms O1 and O2 of adjacent molecules of polymorph (1) are 2.738 (3) and 2.752 (3) Å, and the equivalent distances for the three unique molecules of polymorph (2) are 2.718 (1), 2.700 (1) and 2.731 (1) Å. The equivalent O···O distances for the related ethyl maltol polymorphs are 2.724 (6) and 2.711 (4) Å, respectively (Brown *et al.*, 1995). It is noteworthy that the H1 atoms all make the closest possible intramolecular approach to O2, suggesting further hydrogen-bonding interaction.

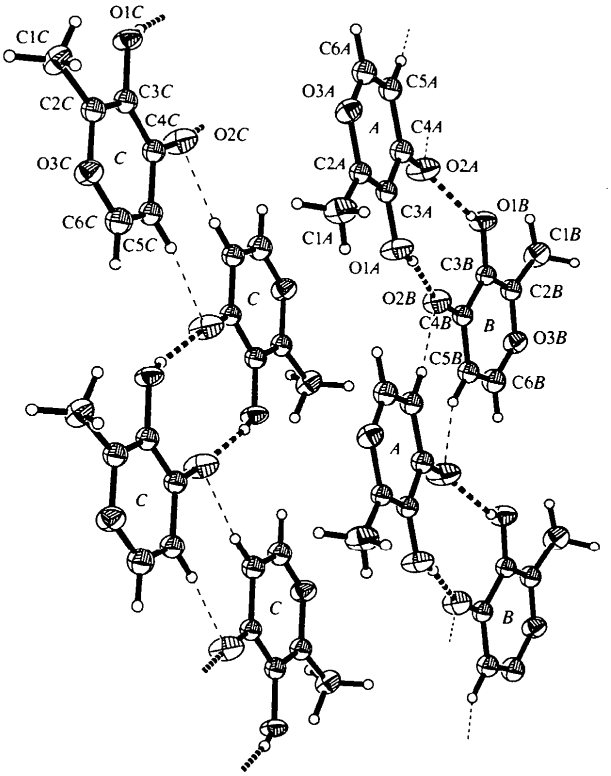


Fig. 2. Structure of polymorph (2) (*SHELXTL/PC XP*; Sheldrick, 1990*a*) showing the atom-numbering scheme of the hydrogen-bonded dimeric units linked by intermolecular O—H···O bonds with weaker C—H···O bonds linking the dimeric units into chains. Displacement ellipsoids are drawn at the 30% probability level.

The C···O distances for the weaker C5—H5···O2 intermolecular contacts are 3.193 (4) and 3.287 (4) Å for polymorph (1) and 3.309 (2), 3.341 (2) and 3.293 (2) Å for polymorph (2). The distances are within or close to the conservative upper limit for the C···O distance in this type of hydrogen bond suggested by Desiraju (1991) and Braga, Grepioni, Biradha, Pedireddi & Desiraju (1995).

Experimental

Crystals of (1) were obtained from an ethanol/water mixture. Crystals of (2) were obtained from an ethanol solution equilibrated with heptane.

Compound (1)

Crystal data

$C_6H_6O_3$
$M_r = 126.11$
Orthorhombic
$Pca2_1$
$a = 7.134\,(1)$ Å
$b = 12.152\,(2)$ Å
$c = 13.304\,(1)$ Å
$V = 1153.4\,(3)$ Å^3
$Z = 8$
$D_x = 1.453$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 4.6$–$12.4°$
$\mu = 0.118$ mm^{-1}
$T = 293\,(2)$ K
Block
0.72 × 0.54 × 0.35 mm
Colourless

Data collection

Siemens $P4$ diffractometer
ω scans
Absorption correction: none
1616 measured reflections
1277 independent reflections
1098 observed reflections [$I > 2\sigma(I)$]
$R_{\rm int} = 0.0174$

$\theta_{\rm max} = 25.99°$
$h = -1 \rightarrow 8$
$k = -1 \rightarrow 14$
$l = -1 \rightarrow 16$
3 standard reflections monitored every 100 reflections
intensity decay: <2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0324$
$wR(F^2) = 0.0876$
$S = 1.054$
1277 reflections
211 parameters
H atoms riding, $U_{\rm iso}$ values refined
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.021$

$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.14$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983)
Polarity not reliably determined

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (1)*

$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	$U_{\rm eq}$
O1*A*	0.2134 (3)	0.5948 (2)	0.5621 (2)	0.0531 (6)
O2*A*	0.1517 (3)	0.73941 (15)	0.7191 (2)	0.0553 (6)
O3*A*	0.0906 (3)	0.41124 (15)	0.7623 (2)	0.0470 (5)
C1*A*	0.1887 (5)	0.3624 (3)	0.5975 (3)	0.0547 (8)
C2*A*	0.1470 (4)	0.4507 (2)	0.6710 (2)	0.0399 (6)
C3*A*	0.1627 (4)	0.5603 (2)	0.6546 (2)	0.0376 (6)
C4*A*	0.1291 (4)	0.6384 (2)	0.7343 (2)	0.0391 (6)
C5*A*	0.0717 (4)	0.5912 (2)	0.8281 (2)	0.0447 (6)
C6*A*	0.0530 (4)	0.4831 (2)	0.8370 (2)	0.0478 (7)
O1*B*	0.1688 (4)	0.9359 (2)	0.8214 (2)	0.0596 (7)
O2*B*	0.1717 (3)	0.78859 (15)	0.9773 (2)	0.0536 (6)
O3*B*	0.1092 (3)	1.1131 (2)	1.0343 (2)	0.0535 (6)
C1*B*	0.1383 (8)	1.1684 (3)	0.8642 (4)	0.0675 (11)
C2*B*	0.1320 (4)	1.0771 (2)	0.9381 (2)	0.0443 (7)
C3*B*	0.1482 (4)	0.9691 (2)	0.9174 (2)	0.0401 (6)
C4*B*	0.1483 (4)	0.8877 (2)	0.9972 (2)	0.0394 (6)
C5*B*	0.1200 (5)	0.9318 (3)	1.0956 (2)	0.0501 (8)
C6*B*	0.1011 (5)	1.0393 (3)	1.1093 (2)	0.0550 (8)

Table 2. *Selected geometric parameters (Å, °) for (1)*

O1*A*—C3*A*	1.350 (3)	O1*B*—C3*B*	1.347 (4)
O2*A*—C4*A*	1.254 (3)	O2*B*—C4*B*	1.244 (3)
O3*A*—C6*A*	1.351 (4)	O3*B*—C6*B*	1.343 (4)
O3*A*—C2*A*	1.366 (4)	O3*B*—C2*B*	1.362 (4)
C1*A*—C2*A*	1.482 (4)	C1*B*—C2*B*	1.483 (5)
C2*A*—C3*A*	1.354 (4)	C2*B*—C3*B*	1.346 (4)
C3*A*—C4*A*	1.444 (4)	C3*B*—C4*B*	1.452 (4)
C4*A*—C5*A*	1.433 (4)	C4*B*—C5*B*	1.429 (4)
C5*A*—C6*A*	1.325 (4)	C5*B*—C6*B*	1.326 (5)

Compound (2)

Crystal data

$C_6H_6O_3$
$M_r = 126.11$
Monoclinic
$P2_1/c$
$a = 7.166\,(2)$ Å
$b = 35.909\,(10)$ Å
$c = 6.982\,(2)$ Å
$\beta = 109.79\,(3)°$
$V = 1690.5\,(8)$ Å^3
$Z = 12$
$D_x = 1.486$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 24 reflections
$\theta = 15$–$25°$
$\mu = 1.033$ mm^{-1}
$T = 163$ (2) K
Rod
0.40 × 0.15 × 0.10 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
3467 measured reflections
3467 independent reflections
2830 observed reflections [$I > 2\sigma(I)$]

$\theta_{\rm max} = 74.98°$
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 44$
$l = 0 \rightarrow 8$
3 standard reflections monitored every 200 reflections
intensity decay: <1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0434$
$wR(F^2) = 0.1274$
$S = 1.071$
3467 reflections
244 parameters
H atoms riding, $U_{\rm iso}$ values refined
$w = 1/[\sigma^2(F_o^2) + (0.067P)^2 + 0.334P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = 0.007$
$\Delta\rho_{\rm max} = 0.28$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.31$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (2)*

$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	$U_{\rm eq}$
O1*A*	0.0755 (2)	0.60590 (3)	0.9257 (2)	0.0318 (3)
O2*A*	0.3393 (2)	0.65787 (3)	0.8788 (2)	0.0338 (3)
O3*A*	0.4999 (2)	0.54927 (3)	0.9596 (2)	0.0266 (3)
C1*A*	0.1913 (3)	0.52807 (5)	0.9750 (3)	0.0339 (4)
C2*A*	0.3149 (2)	0.55984 (4)	0.9529 (2)	0.0243 (3)
C3*A*	0.2595 (2)	0.59623 (4)	0.9292 (2)	0.0235 (3)
C4*A*	0.3925 (2)	0.62463 (4)	0.9061 (2)	0.0242 (3)
C5*A*	0.5864 (2)	0.61170 (5)	0.9193 (2)	0.0251 (3)
C6*A*	0.6287 (2)	0.57535 (5)	0.9432 (2)	0.0263 (3)

O1*B*	0.1905 (2)	0.72636 (3)	0.8964 (2)	0.0306 (3)
O2*B*	−0.1015 (2)	0.67398 (3)	0.8514 (2)	0.0318 (3)
O3*B*	−0.2381 (2)	0.78377 (3)	0.8292 (2)	0.0285 (3)
C1*B*	0.0900 (3)	0.80473 (5)	0.8833 (3)	0.0332 (4)
C2*B*	−0.0474 (2)	0.77285 (4)	0.8591 (2)	0.0243 (3)
C3*B*	0.0009 (2)	0.73626 (4)	0.8666 (2)	0.0232 (3)
C4*B*	−0.1469 (2)	0.70756 (4)	0.8452 (2)	0.0237 (3)
C5*B*	−0.3431 (2)	0.72099 (5)	0.8163 (3)	0.0265 (3)
C6*B*	−0.3784 (2)	0.75781 (5)	0.8089 (3)	0.0299 (4)
O1*C*	0.4277 (2)	0.56081 (3)	0.4663 (2)	0.0267 (3)
O2*C*	0.7144 (2)	0.50828 (3)	0.4955 (2)	0.0355 (3)
O3*C*	0.8266 (2)	0.61682 (3)	0.4193 (2)	0.0272 (3)
C1*C*	0.5152 (3)	0.63870 (4)	0.4205 (3)	0.0303 (4)
C2*C*	0.6482 (2)	0.60656 (4)	0.4325 (2)	0.0236 (3)
C3*C*	0.6063 (2)	0.57026 (4)	0.4546 (2)	0.0212 (3)
C4*C*	0.7507 (2)	0.54141 (4)	0.4688 (2)	0.0239 (3)
C5*C*	0.9342 (2)	0.55404 (5)	0.4493 (3)	0.0271 (3)
C6*C*	0.9623 (2)	0.59056 (5)	0.4271 (3)	0.0287 (4)

Table 4. *Selected geometric parameters (Å, °) for (2)*

O1*A*—C3*A*	1.356 (2)	C2*B*—C3*B*	1.355 (2)
O2*A*—C4*A*	1.248 (2)	C3*B*—C4*B*	1.449 (2)
O3*A*—C6*A*	1.347 (2)	C4*B*—C5*B*	1.435 (2)
O3*A*—C2*A*	1.365 (2)	C5*B*—C6*B*	1.344 (2)
C1*A*—C2*A*	1.484 (2)	O1*C*—C3*C*	1.352 (2)
C2*A*—C3*A*	1.359 (2)	O2*C*—C4*C*	1.245 (2)
C3*A*—C4*A*	1.441 (2)	O3*C*—C6*C*	1.343 (2)
C4*A*—C5*A*	1.438 (2)	O3*C*—C2*C*	1.363 (2)
C5*A*—C6*A*	1.338 (2)	C1*C*—C2*C*	1.481 (2)
O1*B*—C3*B*	1.351 (2)	C2*C*—C3*C*	1.358 (2)
O2*B*—C4*B*	1.246 (2)	C3*C*—C4*C*	1.444 (2)
O3*B*—C6*B*	1.343 (2)	C4*C*—C5*C*	1.440 (2)
O3*B*—C2*B*	1.368 (2)	C5*C*—C6*C*	1.344 (2)
C1*B*—C2*B*	1.482 (2)		

Table 5. *Hydrogen-bonding parameters (Å, °)*

D	*A*	*D*···*A*	*D*—H†	H···*A*†	*D*—H···*A*†
Polymorph (1)					
O1*A*	O2*B*$^{\text{i}}$	2.738 (3)	0.86	2.035	146
O1*B*	O2*A*	2.752 (3)	0.81	2.102	138
C5*A*	O2*B*	3.193 (4)	0.96	2.410	139
C5*B*	O2*A*$^{\text{ii}}$	3.287 (4)	0.85	2.616	137
Polymorph (2)					
O1*A*	O2*B*	2.718 (1)	0.82	1.949	156
O1*B*	O2*A*	2.700 (1)	0.88	1.876	156
O1*C*	O2*C*$^{\text{iii}}$	2.731 (1)	0.86	1.925	155
C5*A*	O2*B*$^{\text{iv}}$	3.309 (2)	0.92	2.397	172
C5*B*	O2*A*$^{\text{v}}$	3.341 (2)	0.94	2.434	162
C5*C*	O2*C*$^{\text{vi}}$	3.293 (2)	0.93	2.364	175

† Uncertainties when H atoms were refined freely were approximately 0.05 Å. However, no e.s.d.'s are given here as in the final cycles, a riding model was used for the H atoms.

Symmetry codes: (i) $\frac{1}{2}-x, y, \frac{1}{2}-z$; (ii) $\frac{1}{2}-x, y, \frac{1}{2}+z$; (iii) $1-x, 1-y, 1-z$; (iv) $1+x, y, z$; (v) $x-1, y, z$; (vi) $2-x, 1-y, 1-z$.

Data collection: *XSCANS* (Fait, 1991) for (1); *CAD*-4 *Software* (Enraf–Nonius, 1989) for (2). Cell refinement: *XSCANS* for (1); local program for (2). Data reduction: *XSCANS* for (1); local program for (2). Program(s) used to solve structures: *SHELXTL/PC* (Sheldrick, 1990*a*) for (1); *SHELXS*86 (Sheldrick, 1990*b*) for (2). For both compounds, program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *SHELXTL/PC XP*; software used to prepare material for publication: *SHELXTL/PC*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BM1083). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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2,2-Dimethyl-6-nitro-3,4-dihydro-2*H*-benzo[*b*]pyran-4-one *O*-Benzoyloxime

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(*Received 6 February 1996; accepted 25 June 1996*)

Abstract

The title compound, $C_{18}H_{16}N_2O_5$, has a pyran ring in a half-chair conformation fused to a benzene ring. The substituent groups at C3 and C5 are approximately coplanar with the benzopyran nucleus, with dihedral angles of 8.5 (5) and 4.2 (5)°, respectively. The benzoyloxy carbonyl group and the benzene ring of the benzopyran moiety both adopt a *cis* configuration.

Comment

There is interest at present in the structures of benzopyran compounds and their biological activity as potassium-channel activators which relax smooth muscle and lower blood pressure (Arch *et al.*, 1991; Buckle *et al.*, 1990; Buckle, Arch *et al*, 1991; Buckle, Eggleston *et al.*, 1991; Burrell, Cassidy, Evans, Lightowler & Stemp, 1990; Cassidy *et al.*, 1989). A representative compound is cromakalim [(II); Cassidy *et al.*, 1989]. Praeruptorin C, (III), isolated from the Chinese herbal drug 'Qian-Hu', is also a benzopyran compound and has been shown to cause inhibition of the calcium-