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2,7-Diacetylxanthene

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.128
Data-to-parameter ratio = 8.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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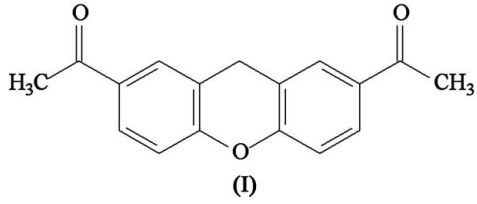
In the crystal structure of the title compound, $C_{17}H_{14}O_3$, the asymmetric unit comprises one half-molecule; a mirror plane passes through the pyran O atom and the *para*-carbon atom.

Comment

The title compound, (I), was synthesized from xanthene and acetyl chloride (Ng & Ng, 1952). Recently, we found that it exhibits anti-xanthine oxidase activity with an inhibition ratio of 71.28% at a concentration of 10^{-6} g ml^{-1}. In the light of this, we have synthesized this compound and determined its structure by X-ray analysis.



(I)

Compound (I) crystallizes in the space group $Cmc2_1$ with one half-molecule in the asymmetric unit (Fig. 1). The dihedral angle between the two benzene rings is 11.1 (1)°, and the pyran ring adopts a boat conformation, in which atoms C4, C5, C4^{i} and C5^{i} form the bottom of the boat, O2 the prow and C9 the stern [deviations from the C4/C5/C4^{i}/C5^{i} mean plane = 0.132 (2) and 0.1921 (17) Å for O2 and C9, respectively; symmetry code: (i) $-x, y, z$]. Atoms O2 and C9 are located on a mirror plane. No hydrogen-bond interactions are observed between molecules (Fig. 2)

Experimental

The title compound was prepared according to the procedure of Ng & Ng (1952). A single crystal was obtained by slow evaporation of a saturated methanol–hexane(1:1) solution at 283 K.

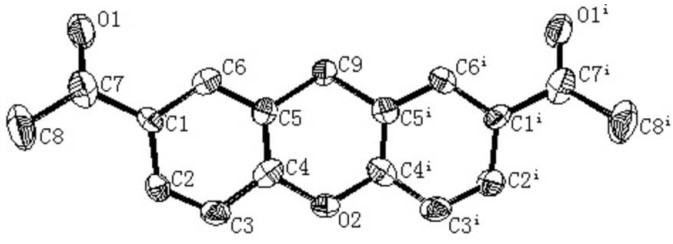


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry code: (i) $-x, y, z$.]

Crystal data

$C_{17}H_{14}O_3$	$Z = 4$
$M_r = 266.28$	$D_x = 1.354$ Mg m^{-3}
Orthorhombic, $Cmc2_1$	Mo $K\alpha$ radiation
$a = 29.875$ (6) Å	$\mu = 0.09$ mm^{-1}
$b = 6.0270$ (12) Å	$T = 296$ (1) K
$c = 7.2560$ (15) Å	Block, pale yellow
$V = 1306.5$ (5) Å^3	0.30 × 0.20 × 0.10 mm

Data collection

MAC DIP 2030K diffractometer	785 independent reflections
ω scans	782 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.023$
1899 measured reflections	$\theta_{max} = 27.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2 + 0.4024P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.048$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.128$	$\Delta\rho_{max} = 0.11$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.11$ e Å^{-3}
785 reflections	Extinction correction: *SHELXL97*
95 parameters	Extinction coefficient: 0.010 (3)
H-atom parameters constrained	

Table 1
Selected bond and torsion angles (°).

C4—O2—C4^i	118.6 (2)	C5—C9—C5^i	112.0 (2)
C4^i—O2—C4—C3	−168.35 (15)	C3—C4—C5—C9	−176.8 (3)
C4^i—O2—C4—C5	12.8 (4)	O2—C4—C5—C9	2.0 (3)
C3—C4—C5—C6	0.2 (3)	C6—C5—C9—C5^i	167.84 (16)
O2—C4—C5—C6	179.0 (2)	C4—C5—C9—C5^i	−15.3 (4)

Symmetry code: (i) $-x, y, z$.

In the absence of significant anomalous scattering, Friedel pairs were merged. Methyl H atoms were constrained to an ideal geometry, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *DENZO* (Otwinowski & Minor, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

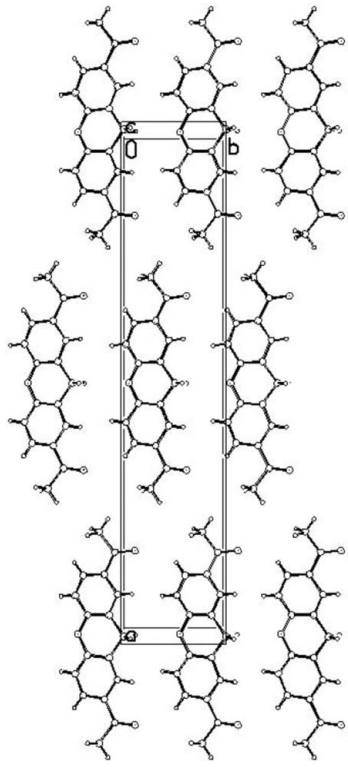


Figure 2
The molecular packing of (I), viewed along the *c* axis.

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