Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

3-Hydroxy-4-oxo-2-phenyl-4*H*-chromene-6-carboxylic acid dimethylformamide solvate

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Received 14 November 2006
Accepted 26 November 2006

Key indicators

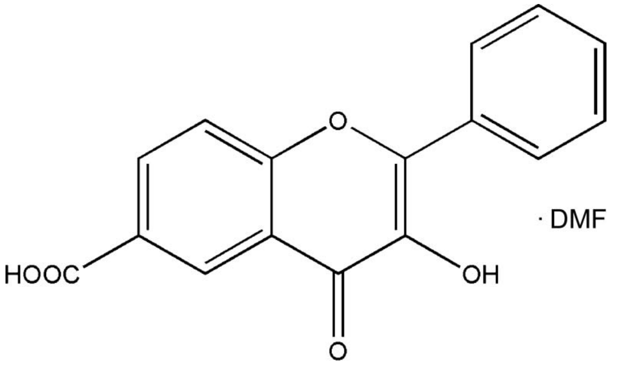
Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 13.2

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

The chromene molecule of the title compound, $C_{16}H_{10}O_5 \cdot C_3H_7NO$, is roughly planar. The H atom of the carboxylic acid group is hydrogen bonded to the dimethylformamide solvent molecule; an infinite planar chain is formed through intermolecular O(hydroxyl)—H···O(carboxyl) hydrogen bonds.

Comment

Flavonols have long been an important class of flavonoids with interesting pharmacological properties (Hammad & Abdalla, 1997). Being widely present in nature, they are usually obtained by extraction from plants. With the purpose of finding new flavonols possessing further pharmacological activities and studying their structure–activity relationships, the title compound, (I), has been synthesized and its structure is reported here.



(I)

The chromene molecule of (I) is roughly planar, the largest deviation from the mean plane being 0.241 (2) Å for O4 (Fig. 1). The dimethylformamide solvent and the 3-hydroxo-4-oxo-2-phenyl-4*H*-chromene-6-carboxylic acid are connected through an O—H···O hydrogen bond involving the H atom of the carboxylic acid group (Fig. 1, Table 1). An infinite planar chain along [010], with its plane parallel to (10$\bar{1}$), is formed through intermolecular O(hydroxyl)—H···O(carboxyl) hydrogen bonds (Table 1 and Fig. 2).

Experimental

The title compound was synthesized by the route published by Pfister *et al.* (1980), the only difference being that a phase-transfer catalyst (benzyltriethylammonium chloride) was added in the first step and the total yield rose to 57%. Single crystals of (I) suitable for X-ray diffraction analysis were obtained from a solution in *N*,*N*-dimethylformamide.

Crystal data

$C_{16}H_{10}O_5{\cdot}C_3H_7NO$
$M_r = 355.34$
Triclinic, $P\overline{1}$
$a = 7.5036$ (17) Å
$b = 9.666$ (2) Å
$c = 12.509$ (3) Å
$\alpha = 106.806$ (2)°
$\beta = 93.680$ (3)°
$\gamma = 95.967$ (3)°
$V = 859.5$ (3) Å^3
$Z = 2$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 291$ (2) K
Block, yellow
$0.35 \times 0.25 \times 0.17$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.965$, $T_{\max} = 0.983$
6465 measured reflections
3157 independent reflections
1996 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.131$
$S = 1.03$
3157 reflections
239 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.0483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4$\cdots$O6	0.82	1.80	2.6121 (19)	170
O2—H2$\cdots$O5$^{\rm i}$	0.82	2.05	2.765 (2)	146

Symmetry code: (i) $x, y + 1, z$.

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å (CH) or 0.96 Å (CH_3) and O—H = 0.82 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C,O) for CH or OH, and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(C) for methyl H.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

This work was supported by the National Natural Science Foundation of China (grant No. 20662007).

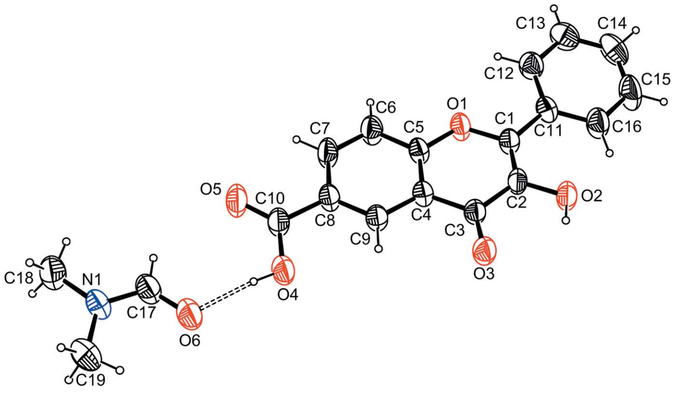


Figure 1
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radii. The hydrogen bond is shown as a dashed line.

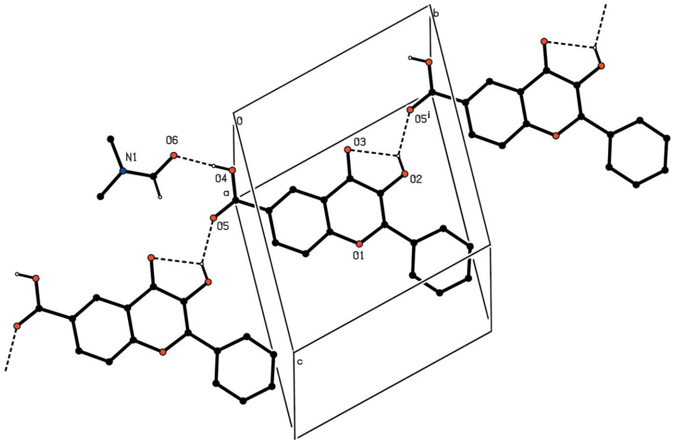


Figure 2
A partial packing view, showing the formation of the infinite planar chain. H atoms not involved in hydrogen bonding have been omitted for clarity. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) x, 1 + y, z]

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