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2-(2,3-Dimethoxyphenyl)chroman-4-one

Hui Wu,[a]* Zhou Xu,[a] Jun Zhou[a] and Yong-Min Liang[b]

[a]Department of Chemistry, Xuzhou Normal University, Xuzhou, Jiangsu, 221116, People's Republic of China, and [b]Department of Chemistry, Lanzhou University, State Key Laboratory of Applied Organic Chemistry, Lanzhou, Gansu, 730000, People's Republic of China

Correspondence e-mail: wuhui72@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.126
Data-to-parameter ratio = 12.7

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

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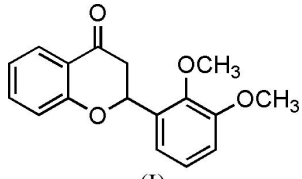
The title compound, $C_{17}H_{16}O_4$, was synthesized by the reaction of 2,3-dimethoxybenzaldehyde and 2-hydroxyacetophenone in 20% NaOH solution for 2 h, followed by crystallization from ethyl acetate. The pyrone ring adopts a chair conformation.

Comment

Flavanones are present in a wide variety of natural products exhibiting interesting biological activities (Heinisch & Holzer, 1991; Salvatore *et al.*, 1998). Thus, the synthesis of flavanones and their derivatives is of great interest in organic chemistry. It is found from biological examination that the flavanone (I) has good molluscicidal activity, and we report its crystal structure here. In (I), the pyrone ring is slightly distorted and adopts a chair conformation (Fig. 1). The bond lengths and angles in (I) show normal values (Table 1).



(I)

Experimental

The title compound, (I), was prepared from 2,3-dimethoxybenzaldehyde (2 mmol, 0.033 g) and 2-hydroxyacetophenone (2 mmol, 0.027 g) in 20% NaOH solution by stirring at room temperature for 2 h (yield 90%, m.p 365–366 K). Crystals of (I) suitable for X-ray diffraction were obtained by crystallization from ethyl acetate.

Crystal data

$C_{17}H_{16}O_4$
M_r = 284.30
Triclinic, $P\overline{1}$
a = 7.547 (3) Å
b = 9.122 (2) Å
c = 11.437 (3) Å
α = 107.905 (2)°
β = 108.506 (4)°
γ = 92.139 (3)°
V = 702.4 (4) Å^3
Z = 2
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 732 reflections
θ = 2.5–22.9°
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, colorless
0.48 × 0.34 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.983
3693 measured reflections
2443 independent reflections
1262 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 9$
$l = -13 \rightarrow 13$

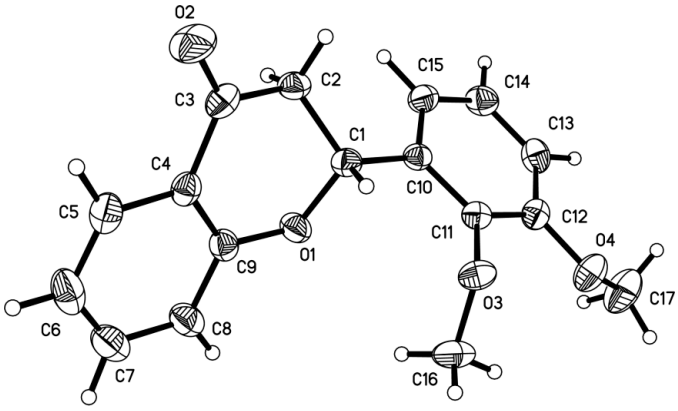


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

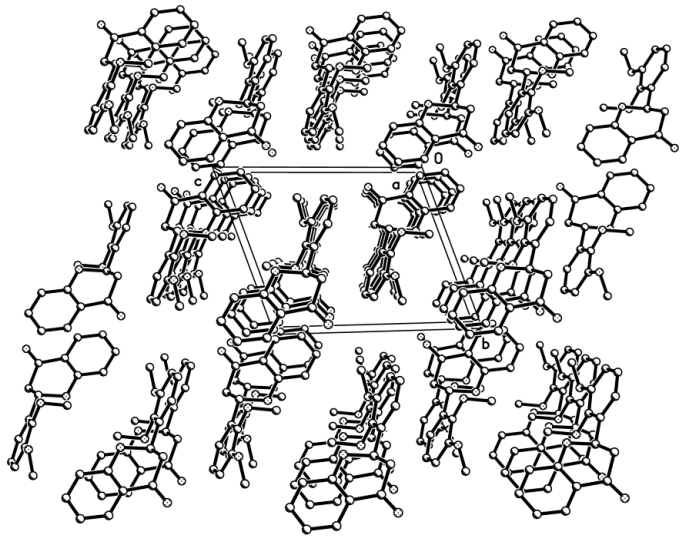


Figure 2
The molecular packing of (I). H atoms have been omitted.

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
2443 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}
192 parameters	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.458 (3)	C1—C10	1.500 (3)
O2—C3	1.207 (3)	C1—C2	1.502 (3)
C9—O1—C1	114.26 (19)	O1—C1—C2	109.0 (2)
O1—C1—C10	105.98 (18)	C10—C1—C2	117.5 (2)
C9—O1—C1—C10	178.8 (2)	C1—C2—C3—O2	143.9 (3)
O1—C1—C2—C3	63.2 (3)	O1—C1—C10—C11	−75.1 (3)
C10—C1—C2—C3	−176.3 (2)	O1—C1—C10—C15	103.3 (3)

All H atoms were placed in calculated positions and treated using a riding model, with C—H distances of 0.93–0.98 Å and U_{iso}(H) values of $1.2U_{eq}$(C) [$1.5U_{eq}$(C) for methyl groups].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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