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Methyl 2-[(1-oxo-1*H*-isochromen-3-yl)-methyl]benzoate

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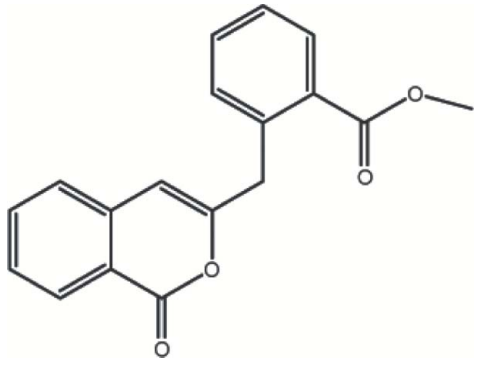
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.098; data-to-parameter ratio = 17.7.

In the nonplanar title compound, $C_{18}H_{14}O_4$, the dihedral angle between the isochromene and benzene ring systems is 83.32 (6)°. The crystal structure is stabilized by intra- and intermolecular C—H···O interactions, the latter resulting in centrosymmetric dimers.

Related literature

For related literature, see: Bogdanov *et al.* (2007); Burdzhiev & Stanoeva (2006); Dobson & Gerkin (1996); Kokila *et al.* (1996); Bogdanov & Palamareva (2004); Kandinska *et al.* (2006); Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{14}O_4$
M_r = 294.29
Triclinic, $P\overline{1}$
a = 8.1628 (7) Å
b = 8.8981 (8) Å
c = 11.0236 (9) Å
α = 105.048 (7)°
β = 108.266 (6)°
γ = 97.981 (7)°
V = 712.78 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 200 K
0.21 × 0.20 × 0.15 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.980, T_{max} = 0.986
16802 measured reflections
3545 independent reflections
2478 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
S = 1.01
3545 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O3	0.97	2.39	2.8706 (18)	110
C15—H15···O4	0.93	2.34	2.6766 (19)	101
C3—H3···O1^{i}	0.93	2.58	3.3178 (19)	136

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

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD* and *SADABS* (Sheldrick, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2399).

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supplementary materials

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Methyl 2-[(1-oxo-1*H*-isochromen-3-yl)methyl]benzoate

M. Akkurt, S. Ö. Yildirim, M. G. Bogdanov, Y. N. Mitrev and F. W. Heinemann

Comment

As a part of our systematic studies on the reactions of anhydrides with compounds containing activated double bonds (Burdzhiev & Stanoeva 2006; Kandinska *et al.*, 2006) we focused our attention on the reactions of homophthalic anhydride with carbonyl compounds (Bogdanov & Palamareva 2004; Bogdanov *et al.*, 2007). The title compound (I) was synthesized while searching for new antibiotics with an isocoumarin core. In this paper, we report our X-ray crystallographic studies of (I).

A displacement ellipsoid plot with the atomic numbering scheme of the title compound (I) is shown in Fig. 1. The bond lengths and angles observed in (I) are normal (Allen *et al.*, 1987). The isochromene system (C1—C9/O1/O2) of the molecule is planar. The dihedral angle between the benzene ring C2—C7 and the fused pyran ring in the isochromene system is 3.56 (6)°. The average deviation of these atoms from the mean plane of the coumarin system is -0.066 (1) Å for atom C1; this value is in agreement with those found in analogous coumarin derivatives (Dobson & Gerkin, 1996; Kokila *et al.*, 1996). The isochromene and benzene ring rings are nearly perpendicular to each other [dihedral angle = 83.32 (6)°].

In the crystal structure of (I), there are two acute intramolecular C—H···O interactions (Table 1). An intermolecular C—H···O bond results in inversion dimers (Fig. 2).

Experimental

Compound (I) was synthesized by the reaction between homophthalic anhydride and paraformaldehyde in boiling pyridine and subsequent treatment of the isolated carboxylic acid with ether solution of diazomethane. After working up the reaction mixture, compound crystallized as colourless prisms from ethyl acetate (yield 0.2 g, 80 %; m.p. 375–376 K). Analysis, calculated for $C_{18}H_{14}O_4$: C 73.46, H 4.79 %; found: C 73.31, H 4.46 %. The product was characterized by ^{1}H NMR, MS and IR spectra. Single crystals of (I) were obtained by slow evaporation of a solution of in a chloroform–ethyl acetate mixture (3:1 v/v) at room temperature.

IR ($CHCl_3$) 1600 cm^{-1}(ArH), 1650 cm^{-1} (C═C), 1710 cm^{-1} (C═O), 1715 cm^{-1} (C═O). The mass spectrum was recorded on Trace DSQ (Termo-Finnigan) instrument with EI (70 eV), equipped with quadruple EI mass analyzer. MS: m/z (%) 294 (4), 262 (73), 234 (100), 219 (6), 206 (20), 178 (61), 145 (3), 133 (7), 117 (17), 89 (74). The ^{1}H NMR spectrum of (I) was obtained on a Bruker Avance DRX250 spectrometer at 250.13 MHz in $CDCl_3$ at 293 K. ^{1}H NMR (250 MHz, $CDCl_3$) δ = 3.64 (s, 3H, *OCH$_3$*), 4.08 (s, 2H, -*CH$_2$*-), 5.98 (s, 1H, *H-vinyl*), 7.10-7.45 (m, 5H, *Ph—H*), 7.60 (dt, 1H, J= 1.3 and 7.5 Hz, *Ph—H*), 7.92 (dd, 1H, J= 1.5 and 7.5 Hz, *Ph—H*), 8.18 (dd, 1H, J= 1.5 and 7.8 Hz, *Ph—H*).

Refinement

The H atoms were placed in idealized positions (C—H = 0.93-0.97 Å) and treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

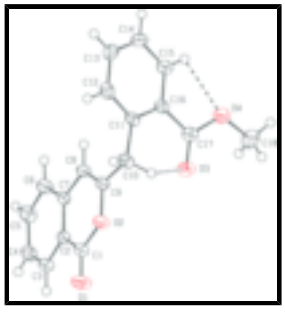


Fig. 1. View of (I) with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. The intra molecular C—H···O interactions are shown as dashed lines.

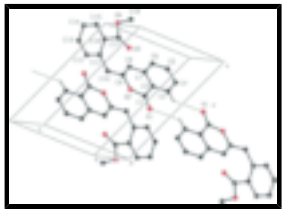


Fig. 2. View of the hydrogen bonding diagram of (I). Dashed lines show intermolecular C—H···O hydrogen bonding interactions. For clarity, H atoms not involved in this type hydrogen bonding have been omitted.

Methyl 2-[(1-oxo-1*H*-isochromen-3-yl)methyl]benzoate

Crystal data

$C_{18}H_{14}O_4$	$Z = 2$
$M_r = 294.29$	$F_{000} = 308$
Triclinic, $P\overline{1}$	$D_x = 1.371$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1628$ (7) Å	Cell parameters from 121 reflections
$b = 8.8981$ (8) Å	$\theta = 6$–20º
$c = 11.0236$ (9) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 105.048$ (7)º	$T = 200$ K
$\beta = 108.266$ (6)º	Prism, colourless
$\gamma = 97.981$ (7)º	0.21 × 0.20 × 0.15 mm
$V = 712.78$ (12) Å^3	

Data collection

Bruker–Nonius KappaCCD diffractometer	3545 independent reflections
Radiation source: fine-focus sealed tube	2478 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.046$

Detector resolution: 9 pixels mm^{-1}

T = 200 K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2002)

T_{min} = 0.980, T_{max} = 0.986

16802 measured reflections

θ_{max} = 28.5º

θ_{min} = 3.7º

h = −10→10

k = −11→11

l = −14→14

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.042

$wR(F^2)$ = 0.098

S = 1.01

3545 reflections

200 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2 + 0.1587P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.22 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.20 e $Å^{-3}$

Extinction correction: none

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.18577 (13)	0.16525 (13)	0.44383 (11)	0.0383 (3)
O2	0.46676 (11)	0.29825 (11)	0.53778 (9)	0.0263 (3)
O3	0.71541 (13)	0.62739 (13)	0.86170 (11)	0.0389 (3)
O4	0.96272 (13)	0.79415 (13)	1.02380 (11)	0.0402 (3)
C1	0.33053 (16)	0.17680 (16)	0.52388 (13)	0.0254 (4)
C2	0.37572 (16)	0.07659 (15)	0.60971 (12)	0.0222 (3)
C3	0.24074 (17)	−0.03931 (16)	0.60986 (14)	0.0286 (4)
C4	0.28196 (18)	−0.13486 (16)	0.68940 (15)	0.0312 (4)

C5	0.45829 (19)	−0.11968 (17)	0.76684 (15)	0.0329 (4)
C6	0.59279 (17)	−0.00575 (16)	0.76802 (14)	0.0294 (4)
C7	0.55308 (16)	0.09646 (14)	0.69088 (12)	0.0214 (3)
C8	0.68633 (16)	0.22290 (15)	0.69299 (13)	0.0232 (3)
C9	0.64026 (16)	0.32037 (15)	0.62138 (12)	0.0217 (3)
C10	0.75531 (17)	0.46250 (16)	0.61556 (13)	0.0262 (4)
C11	0.94433 (16)	0.50474 (15)	0.71511 (13)	0.0233 (4)
C12	1.07127 (18)	0.44492 (16)	0.66982 (15)	0.0296 (4)
C13	1.24714 (19)	0.47860 (17)	0.75392 (16)	0.0338 (4)
C14	1.30077 (18)	0.57203 (17)	0.88678 (15)	0.0311 (4)
C15	1.17855 (17)	0.63349 (16)	0.93482 (14)	0.0285 (4)
C16	1.00054 (16)	0.60148 (15)	0.85036 (13)	0.0237 (4)
C17	0.87454 (17)	0.67161 (16)	0.90832 (14)	0.0268 (4)
C18	0.8566 (2)	0.8684 (2)	1.09349 (17)	0.0446 (5)
H3	0.12320	−0.05150	0.55610	0.0340*
H4	0.19200	−0.20970	0.69150	0.0370*
H5	0.48590	−0.18690	0.81840	0.0390*
H6	0.71020	0.00320	0.82020	0.0350*
H8	0.80510	0.23650	0.74460	0.0280*
H10A	0.70400	0.55400	0.63380	0.0320*
H10B	0.75680	0.44060	0.52510	0.0320*
H12	1.03660	0.38060	0.58050	0.0360*
H13	1.32920	0.43810	0.72070	0.0410*
H14	1.41860	0.59370	0.94390	0.0370*
H15	1.21500	0.69700	1.02460	0.0340*
H18A	0.78230	0.91870	1.03860	0.0670*
H18B	0.93340	0.94750	1.17750	0.0670*
H18C	0.78370	0.78820	1.11060	0.0670*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0211 (5)	0.0427 (6)	0.0448 (6)	0.0025 (4)	0.0005 (4)	0.0207 (5)
O2	0.0201 (4)	0.0266 (5)	0.0291 (5)	0.0018 (4)	0.0039 (4)	0.0123 (4)
O3	0.0216 (5)	0.0437 (6)	0.0452 (6)	0.0064 (4)	0.0110 (5)	0.0064 (5)
O4	0.0287 (5)	0.0463 (7)	0.0345 (6)	0.0084 (5)	0.0111 (4)	−0.0040 (5)
C1	0.0190 (6)	0.0251 (6)	0.0280 (7)	0.0024 (5)	0.0064 (5)	0.0061 (5)
C2	0.0213 (6)	0.0205 (6)	0.0222 (6)	0.0027 (5)	0.0082 (5)	0.0035 (5)
C3	0.0194 (6)	0.0265 (7)	0.0350 (8)	0.0001 (5)	0.0086 (6)	0.0064 (6)
C4	0.0279 (7)	0.0251 (7)	0.0393 (8)	−0.0026 (6)	0.0151 (6)	0.0095 (6)
C5	0.0351 (8)	0.0273 (7)	0.0362 (8)	0.0015 (6)	0.0108 (6)	0.0160 (6)
C6	0.0228 (7)	0.0300 (7)	0.0318 (7)	0.0024 (5)	0.0043 (6)	0.0134 (6)
C7	0.0208 (6)	0.0194 (6)	0.0211 (6)	0.0015 (5)	0.0073 (5)	0.0040 (5)
C8	0.0166 (6)	0.0249 (6)	0.0241 (6)	0.0011 (5)	0.0033 (5)	0.0085 (5)
C9	0.0183 (6)	0.0233 (6)	0.0200 (6)	0.0018 (5)	0.0060 (5)	0.0041 (5)
C10	0.0248 (7)	0.0264 (7)	0.0242 (7)	−0.0003 (5)	0.0049 (5)	0.0111 (5)
C11	0.0229 (6)	0.0191 (6)	0.0271 (7)	−0.0015 (5)	0.0080 (5)	0.0108 (5)
C12	0.0318 (7)	0.0247 (7)	0.0320 (7)	0.0016 (6)	0.0152 (6)	0.0070 (6)

C13	0.0286 (7)	0.0296 (7)	0.0488 (9)	0.0081 (6)	0.0218 (7)	0.0117 (7)
C14	0.0195 (6)	0.0323 (7)	0.0412 (8)	0.0049 (5)	0.0081 (6)	0.0159 (6)
C15	0.0238 (7)	0.0299 (7)	0.0280 (7)	0.0031 (5)	0.0058 (5)	0.0093 (6)
C16	0.0206 (6)	0.0227 (6)	0.0284 (7)	0.0020 (5)	0.0088 (5)	0.0109 (5)
C17	0.0243 (7)	0.0287 (7)	0.0274 (7)	0.0052 (5)	0.0085 (5)	0.0110 (6)
C18	0.0415 (9)	0.0511 (10)	0.0397 (9)	0.0175 (8)	0.0191 (7)	0.0039 (8)

Geometric parameters (Å, °)

O1—C1	1.2046 (18)	C12—C13	1.383 (2)
O2—C1	1.3789 (18)	C13—C14	1.376 (2)
O2—C9	1.3799 (16)	C14—C15	1.381 (2)
O3—C17	1.2003 (19)	C15—C16	1.400 (2)
O4—C17	1.3470 (18)	C16—C17	1.496 (2)
O4—C18	1.446 (2)	C3—H3	0.9300
C1—C2	1.4619 (19)	C4—H4	0.9300
C2—C3	1.401 (2)	C5—H5	0.9300
C2—C7	1.4009 (19)	C6—H6	0.9300
C3—C4	1.374 (2)	C8—H8	0.9300
C4—C5	1.391 (2)	C10—H10A	0.9700
C5—C6	1.381 (2)	C10—H10B	0.9700
C6—C7	1.4021 (19)	C12—H12	0.9300
C7—C8	1.4423 (19)	C13—H13	0.9300
C8—C9	1.3330 (19)	C14—H14	0.9300
C9—C10	1.495 (2)	C15—H15	0.9300
C10—C11	1.5131 (19)	C18—H18A	0.9600
C11—C12	1.395 (2)	C18—H18B	0.9600
C11—C16	1.4034 (18)	C18—H18C	0.9600
O1···C3^{i}	3.3178 (19)	C3···H18B^{vii}	3.1000
O2···C10^{ii}	3.4198 (18)	C4···H18B^{vii}	3.0300
O3···C9	3.1009 (17)	C4···H10B^{vi}	3.0100
O3···C10	2.8706 (18)	C6···H15^{v}	2.9200
O1···H3^{i}	2.5800	C7···H15^{v}	3.0200
O1···H3	2.6200	C8···H15^{v}	2.8200
O1···H12^{iii}	2.7800	C11···H8	2.6400
O2···H10A^{ii}	2.7200	C12···H4^{x}	3.0200
O2···H13^{iii}	2.7200	C13···H5^{x}	3.1000
O3···H5^{iv}	2.6800	C13···H4^{x}	3.0800
O3···H10A	2.3900	C14···H5^{x}	2.8500
O3···H14^{iii}	2.8500	C17···H10A	2.7400
O3···H18A	2.6700	H3···O1	2.6200
O3···H18C	2.5800	H3···O1^{i}	2.5800
O4···H15	2.3400	H3···H3^{i}	2.4400
O4···H6^{v}	2.7400	H4···C12^{viii}	3.0200
O4···H8^{v}	2.7700	H4···C13^{viii}	3.0800

C1···C13^{iii}	3.487 (2)	H5···O3^{xi}	2.6800
C1···C6^{vi}	3.471 (2)	H5···C13^{viii}	3.1000
C1···C7^{vi}	3.3885 (19)	H5···C14^{viii}	2.8500
C2···C7^{vi}	3.5348 (18)	H6···H8	2.5400
C2···C8^{vi}	3.5272 (18)	H6···O4^{v}	2.7400
C3···C9^{vi}	3.551 (2)	H8···C11	2.6400
C3···O1^{i}	3.3178 (19)	H8···H6	2.5400
C3···C8^{vi}	3.585 (2)	H8···O4^{v}	2.7700
C4···C18^{vii}	3.482 (2)	H8···H15^{v}	2.5200
C5···C14^{viii}	3.591 (2)	H10A···O3	2.3900
C6···C1^{vi}	3.471 (2)	H10A···C17	2.7400
C7···C1^{vi}	3.3885 (19)	H10A···O2^{ii}	2.7200
C7···C2^{vi}	3.5348 (18)	H10B···H12	2.3500
C8···C12	3.589 (2)	H10B···C4^{vi}	3.0100
C8···C3^{vi}	3.585 (2)	H12···O1^{ix}	2.7800
C8···C2^{vi}	3.5272 (18)	H12···H10B	2.3500
C8···C16	3.566 (2)	H13···O2^{ix}	2.7200
C9···O3	3.1009 (17)	H13···C1^{ix}	2.7400
C9···C3^{vi}	3.551 (2)	H14···O3^{ix}	2.8500
C9···C17	3.5841 (19)	H14···H14^{xii}	2.5900
C10···O3	2.8706 (18)	H15···O4	2.3400
C10···O2^{ii}	3.4198 (18)	H15···C6^{v}	2.9200
C12···C8	3.589 (2)	H15···C7^{v}	3.0200
C13···C1^{ix}	3.487 (2)	H15···C8^{v}	2.8200
C14···C5^{x}	3.591 (2)	H15···H8^{v}	2.5200
C16···C8	3.566 (2)	H18A···O3	2.6700
C17···C9	3.5841 (19)	H18B···C3^{vii}	3.1000
C18···C4^{vii}	3.482 (2)	H18B···C4^{vii}	3.0300
C1···H13^{iii}	2.7400	H18C···O3	2.5800
C1—O2—C9	122.79 (11)	O3—C17—C16	126.23 (13)
C17—O4—C18	116.75 (12)	O4—C17—C16	111.11 (12)
O1—C1—O2	116.89 (13)	C2—C3—H3	120.00
O1—C1—C2	126.47 (14)	C4—C3—H3	120.00
O2—C1—C2	116.63 (11)	C3—C4—H4	120.00
C1—C2—C3	119.58 (12)	C5—C4—H4	120.00
C1—C2—C7	120.00 (12)	C4—C5—H5	120.00
C3—C2—C7	120.41 (12)	C6—C5—H5	120.00
C2—C3—C4	120.03 (13)	C5—C6—H6	120.00
C3—C4—C5	119.95 (14)	C7—C6—H6	120.00
C4—C5—C6	120.68 (14)	C7—C8—H8	120.00
C5—C6—C7	120.28 (13)	C9—C8—H8	120.00
C2—C7—C6	118.58 (12)	C9—C10—H10A	109.00
C2—C7—C8	118.48 (12)	C9—C10—H10B	109.00

C6—C7—C8	122.93 (12)	C11—C10—H10A	109.00
C7—C8—C9	120.42 (13)	C11—C10—H10B	109.00
O2—C9—C8	121.38 (13)	H10A—C10—H10B	108.00
O2—C9—C10	109.93 (11)	C11—C12—H12	119.00
C8—C9—C10	128.69 (13)	C13—C12—H12	119.00
C9—C10—C11	113.11 (11)	C12—C13—H13	120.00
C10—C11—C12	118.16 (12)	C14—C13—H13	120.00
C10—C11—C16	124.07 (12)	C13—C14—H14	120.00
C12—C11—C16	117.76 (13)	C15—C14—H14	120.00
C11—C12—C13	121.88 (14)	C14—C15—H15	120.00
C12—C13—C14	120.00 (15)	C16—C15—H15	120.00
C13—C14—C15	119.60 (14)	O4—C18—H18A	109.00
C14—C15—C16	120.92 (13)	O4—C18—H18B	109.00
C11—C16—C15	119.83 (13)	O4—C18—H18C	109.00
C11—C16—C17	121.77 (12)	H18A—C18—H18B	110.00
C15—C16—C17	118.40 (12)	H18A—C18—H18C	109.00
O3—C17—O4	122.66 (14)	H18B—C18—H18C	110.00
C9—O2—C1—O1	−177.05 (12)	C6—C7—C8—C9	−177.53 (13)
C9—O2—C1—C2	4.02 (18)	C7—C8—C9—C10	176.46 (13)
C1—O2—C9—C8	0.80 (19)	C7—C8—C9—O2	−3.7 (2)
C1—O2—C9—C10	−179.31 (11)	O2—C9—C10—C11	174.24 (11)
C18—O4—C17—C16	−177.43 (13)	C8—C9—C10—C11	−5.9 (2)
C18—O4—C17—O3	2.2 (2)	C9—C10—C11—C16	−85.15 (17)
O1—C1—C2—C3	−4.7 (2)	C9—C10—C11—C12	95.29 (15)
O1—C1—C2—C7	175.15 (14)	C10—C11—C16—C15	179.86 (13)
O2—C1—C2—C3	174.12 (12)	C10—C11—C16—C17	0.3 (2)
O2—C1—C2—C7	−6.03 (18)	C12—C11—C16—C15	−0.6 (2)
C3—C2—C7—C6	2.30 (19)	C12—C11—C16—C17	179.84 (13)
C1—C2—C7—C6	−177.54 (12)	C16—C11—C12—C13	0.0 (2)
C1—C2—C7—C8	3.44 (18)	C10—C11—C12—C13	179.57 (14)
C3—C2—C7—C8	−176.72 (12)	C11—C12—C13—C14	0.8 (2)
C1—C2—C3—C4	179.53 (13)	C12—C13—C14—C15	−0.9 (2)
C7—C2—C3—C4	−0.3 (2)	C13—C14—C15—C16	0.3 (2)
C2—C3—C4—C5	−1.9 (2)	C14—C15—C16—C17	−179.95 (14)
C3—C4—C5—C6	2.0 (2)	C14—C15—C16—C11	0.5 (2)
C4—C5—C6—C7	0.0 (2)	C11—C16—C17—O3	18.3 (2)
C5—C6—C7—C8	176.83 (13)	C15—C16—C17—O4	18.30 (19)
C5—C6—C7—C2	−2.2 (2)	C11—C16—C17—O4	−162.11 (13)
C2—C7—C8—C9	1.45 (19)	C15—C16—C17—O3	−161.25 (15)

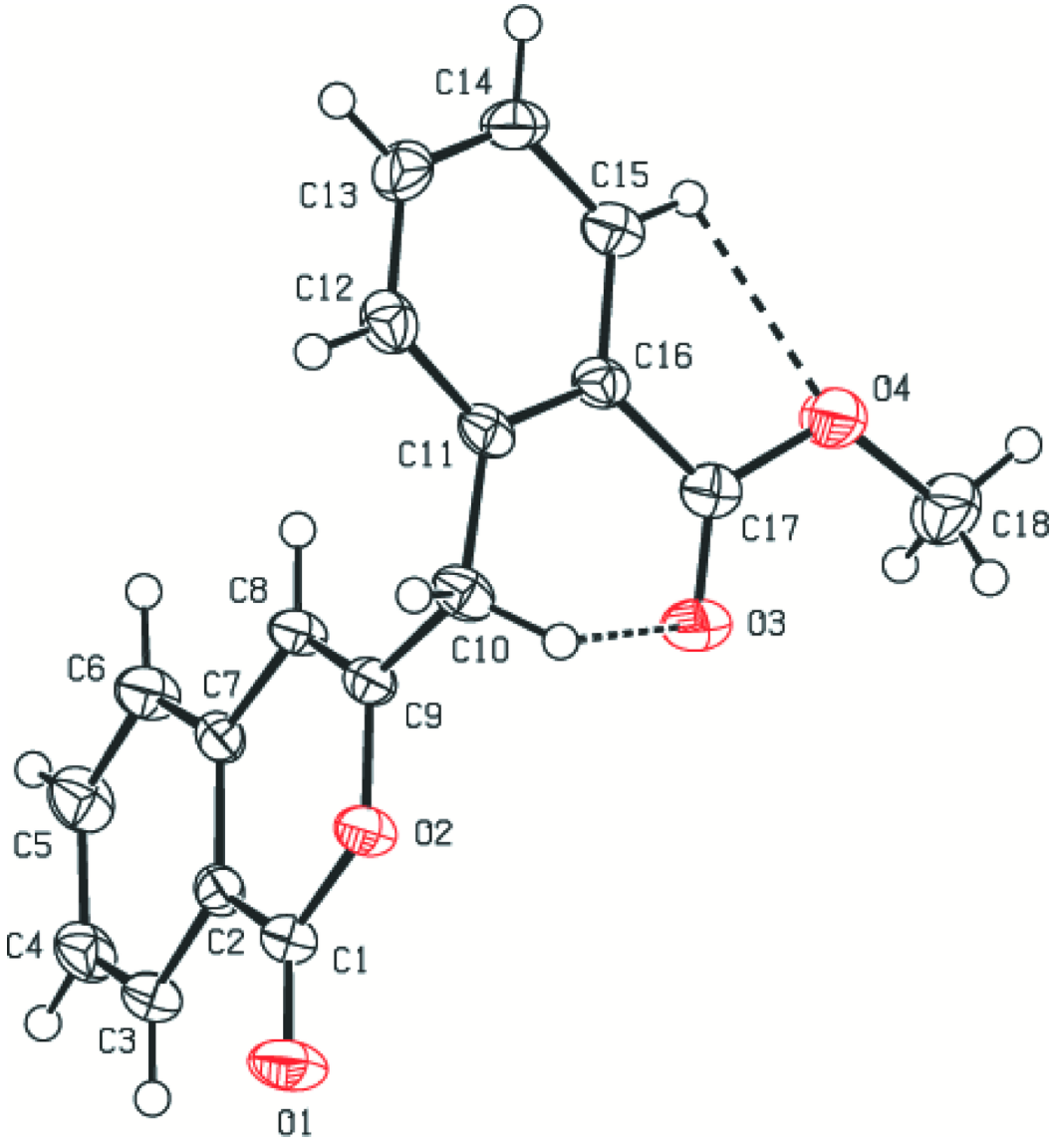
Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*; (iv) *x*, *y*+1, *z*; (v) −*x*+2, −*y*+1, −*z*+2; (vi) −*x*+1, −*y*, −*z*+1; (vii) −*x*+1, −*y*+1, −*z*+2; (viii) *x*−1, *y*−1, *z*; (ix) *x*+1, *y*, *z*; (x) *x*+1, *y*+1, *z*; (xi) *x*, *y*−1, *z*; (xii) −*x*+3, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10A···O3	0.97	2.39	2.8706 (18)	110
C15—H15···O4	0.93	2.34	2.6766 (19)	101
C3—H3···O1^{i}	0.93	2.58	3.3178 (19)	136

Symmetry codes: (i) −*x*, −*y*, −*z*+1.

Fig. 1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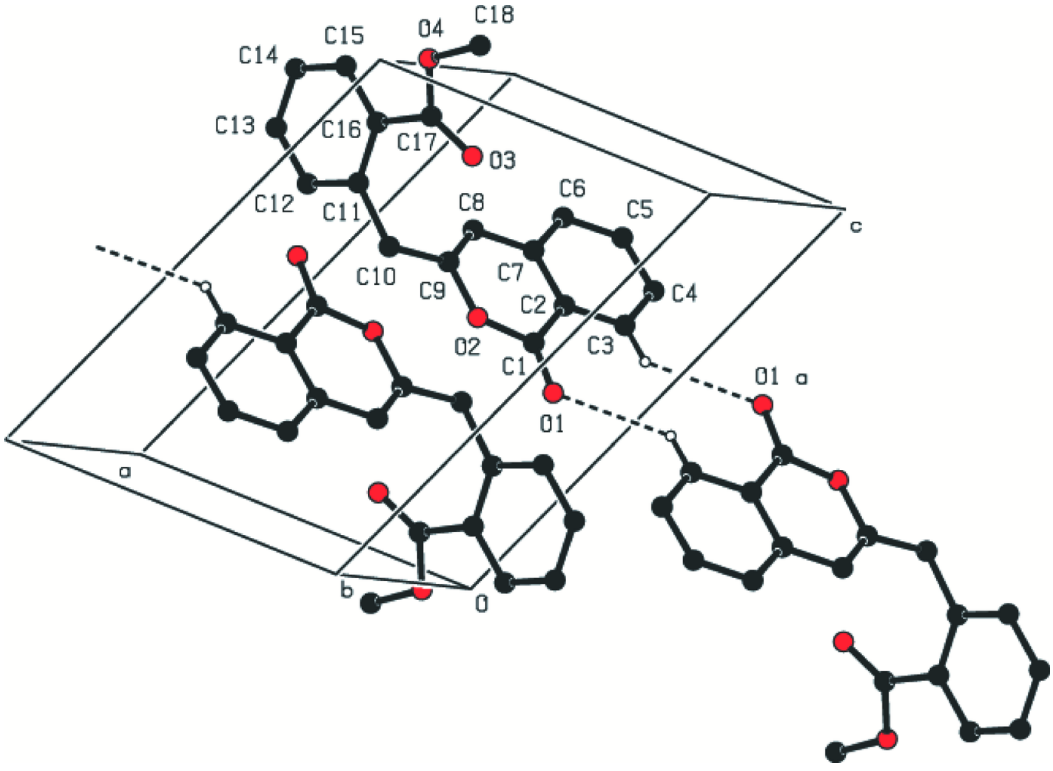
C13
C15
C12
C16
O4
C11
C17
C18
C8
O3
C10
C6
C7
C9
O2
C5
C4
C2
C1
C3
O1

Fig. 2


C18
O4
C15
C14
C13
C16
C17
O3
C12
C11
C8
C6
C5
C10
C9
C7
C4
C2
O2
C1
C3
O1 a
O1
a
b
0
c