Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

(3*E*,4*E*)-3-(1,3-Benzodioxol-5-ylmethylene)-4-(1-phenylethylidene)tetrahydrofuran-2,5-dione

Liang-Wen Zheng, Wen-Liang Dong, Jin-Hua Zhang and Bao-Xiang Zhao*

School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China
Correspondence e-mail: sduzhao@hotmail.com

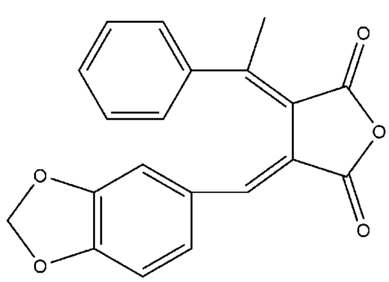
Received 29 June 2007; accepted 17 July 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 8.4.

In the title compound, $C_{20}H_{14}O_5$, the methylenedioxyphenyl ring system is essentially planar. There are short C—H···π interactions. The vinyl group is inclined with respect to the tetrahydrofuran ring by 21.43 (7)°. The dihedral angles made by the atoms defining the planar part of the tetrahydrofuran ring with the phenyl and methylenedioxyphenyl rings are 35.24 (12) and 26.39 (9)°, respectively, while that between the two aryl rings is 14.43 (10)°.

Related literature

For related literature, see: Asiri *et al.* (2003); Heller *et al.* (2000); Uchida *et al.* (1995).



Experimental

Crystal data

$C_{20}H_{14}O_5$
M_r = 334.31
Orthorhombic, $Pna2_1$
a = 7.2201 (2) Å
b = 18.0627 (5) Å
c = 12.2046 (4) Å
V = 1591.66 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 (2) K
0.38 × 0.19 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.963, T_{max} = 0.993
9796 measured reflections
1918 independent reflections
1606 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.04
1918 reflections
227 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

Table 1
X—H···π-ring interactions calculated by *PLATON* (Spek, 2003).

*Cg*1 is the centroid of the benzene ring C1–C6 and *Cg*2 is the centroid of the benzene ring C14-C19.

X—H···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C19—H19···*Cg*1^{i}	0.93	2.83	3.671 (2)	151
C3—H3···*Cg*2^{ii}	0.93	2.94	3.837 (2)	163

Symmetry code: (i) $x, -1+y, z$; (ii) $\frac{1}{2}-x, -\frac{1}{2}+y-\frac{1}{2}+z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This study was supported by the Natural Science Foundation of Shandong Province (grant No. Y2005B12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2028).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Asiri, A. M. (2003). *J. Photochem. Photobiol. A Chem.* **159**, 1–5.
Bruker (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Heller, H. G., Hughes, D. S., Hursthouse, M. B. & Rowles, N. G. (2000). *Chem. Commun.* pp. 1397–1398.
Sheldrick, G. M. (1997). *SHELX97*. Release 97-2. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Uchida, S., Yamada, S., Yokoyama, Y. & Kurita, Y. (1995). *Bull. Chem. Soc. Jpn*, **68**, 1677–1682.

supplementary materials

Acta Cryst. (2007). E**63**, o3567   [**doi:10.1107/S160053680703485X**]

(3*E*,4*E*)-3-(1,3-Benzodioxol-5-ylmethylene)-4-(1-phenylethylidene)tetrahydrofuran-2,5-dione

L.-W. Zheng, W.-L. Dong, J.-H. Zhang and B.-X. Zhao

Comment

Organic photochromic compounds, such as fulgides, are potential candidates for application in erasable optical information media. Attempts have been made to improve their photochromic properties (Asiri, 2003; Uchida *et al.*, 1995). In order to achieve certain desirable properties such as absorption at longer wavelengths and thus higher fatigue resistance to coloration-bleaching cycles, improvements have been made by modifying the fulgide frame (Heller *et al.*, 2000). We report here the crystal structure of the title compound, (I).

Experimental

The (2*E*,3*E*)-2-(1,3-benzodioxol-5-ylmethylene)-3-(1-phenylethylidene)succinic acid (0.01 mmol) was dissolved in dichloromethane (10 ml), and to this mixture was added acetyl chloride (5 ml) dropwise with stirring at 0 degree C, and the mixture was stirred at room temperature for 5 h. After removal of the excess acetyl chloride and dichloromethane, the residue was purified using flash column chromatography on silica gel (petroleum ether/ethyl acetate = 2/1; *v*/*v*) and recrystallized with ethyl acetate to give a solid (yield 76%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in ethyl acetate at room temperature for 15 d.

Refinement

H atoms were positioned geometrically (C - H = 0.93 − 0.97 A °) and refined as riding, with U_{iso}(H) = 1.2Ueq(C). Because of the meaningless of the absolute structure parameter, Friedel-pairs (4) were merged before final refinement.

Figures

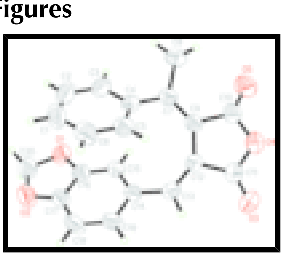


Fig. 1. The molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

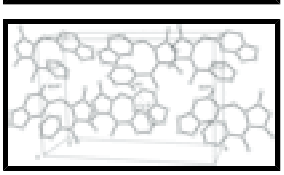


Fig. 2. The view of the structure along *a* axis. All H atoms were omited for clarity except for those which were involve with *X*—H···*Cg*(Pi-Ring) interactions. Symmetry codes: (i) *x*,-1 + *y*,*z*; (ii) 0.5 − *x*,-1/2 + *y*,-1/2 + *z*; (iii) 1 − *x*,1 − *y*,-1/2 + *z*; (iv) 1 − *x*,2 − *y*,-1/2 + *z*; (v) 1/2 + *x*,1.5 − *y*,*z*.

(3*E*,4*E*)-3-(1,3-Benzodioxol-5-ylmethylene)-4-\ (1-phenylethylidene)tetrahydrofuran-2,5-dione

Crystal data

$C_{20}H_{14}O_5$	F_{000} = 696
M_r = 334.31	D_x = 1.395 Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 3450 reflections
a = 7.2201 (2) Å	θ = 3.0–26.3°
b = 18.0627 (5) Å	μ = 0.10 mm^{-1}
c = 12.2046 (4) Å	T = 296 (2) K
V = 1591.66 (8) Å^3	Plate, orange–yellow
Z = 4	0.38 × 0.19 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	1918 independent reflections
Radiation source: fine-focus sealed tube	1606 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 296(2) K	θ_{max} = 27.5°
φ and ω scans	θ_{min} = 2.0°
Absorption correction: multi-scan APEX2 (Bruker, 2005)	$h = -9\rightarrow9$
T_{min} = 0.963, T_{max} = 0.993	$k = -23\rightarrow23$
9796 measured reflections	$l = -15\rightarrow5$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.0276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.086	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.11 e Å^{-3}
1918 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
227 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: ?
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *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}
C1	0.4507 (4)	1.08850 (14)	0.6981 (3)	0.0766 (8)
H1	0.4852	1.1381	0.6987	0.092*
C2	0.3315 (4)	1.06286 (14)	0.6196 (3)	0.0746 (8)
H2	0.2857	1.0950	0.5666	0.090*
C3	0.2793 (3)	0.98960 (13)	0.6188 (2)	0.0590 (6)
H3	0.2008	0.9723	0.5641	0.071*
C4	0.3435 (3)	0.94086 (11)	0.69979 (17)	0.0459 (4)
C5	0.4666 (3)	0.96742 (11)	0.77765 (19)	0.0501 (5)
H5	0.5136	0.9357	0.8309	0.060*
C6	0.5196 (4)	1.04076 (13)	0.7763 (3)	0.0678 (7)
H6	0.6025	1.0582	0.8287	0.081*
C7	0.2848 (3)	0.86249 (11)	0.69894 (19)	0.0451 (4)
C8	0.2857 (4)	0.82596 (15)	0.5875 (2)	0.0653 (6)
H8A	0.3729	0.7858	0.5874	0.098*
H8B	0.3207	0.8616	0.5329	0.098*
H8C	0.1642	0.8073	0.5714	0.098*
C9	0.2416 (3)	0.82442 (11)	0.79118 (19)	0.0448 (4)
C10	0.2277 (3)	0.74232 (13)	0.7893 (2)	0.0579 (6)
C11	0.2485 (3)	0.77359 (13)	0.9690 (2)	0.0578 (6)
C12	0.2296 (3)	0.84388 (11)	0.90818 (18)	0.0444 (4)
C13	0.1956 (3)	0.90390 (11)	0.97086 (17)	0.0473 (5)
H13	0.2022	0.8946	1.0457	0.057*
C14	0.1507 (3)	0.98016 (11)	0.94437 (16)	0.0438 (4)
C15	0.0488 (2)	1.00096 (11)	0.85107 (17)	0.0429 (4)
H15	−0.0007	0.9658	0.8037	0.052*
C16	0.0257 (2)	1.07498 (12)	0.83316 (17)	0.0445 (4)
C17	0.1013 (3)	1.12780 (11)	0.9026 (2)	0.0522 (5)
C18	0.1941 (3)	1.10943 (12)	0.9952 (2)	0.0618 (6)
H18	0.2411	1.1453	1.0423	0.074*
C19	0.2157 (3)	1.03414 (12)	1.01647 (19)	0.0544 (5)
H19	0.2751	1.0195	1.0805	0.065*
C20	−0.0455 (4)	1.18660 (13)	0.7682 (2)	0.0692 (7)
H20A	0.0160	1.2098	0.7063	0.083*

H20B	−0.1664	1.2092	0.7767	0.083*
O1	−0.0653 (2)	1.10928 (8)	0.74889 (14)	0.0585 (4)
O2	0.0608 (3)	1.19719 (8)	0.86474 (16)	0.0709 (5)
O3	0.2660 (3)	0.76142 (11)	1.06471 (17)	0.0809 (6)
O4	0.2406 (3)	0.71527 (9)	0.89574 (18)	0.0691 (5)
O5	0.2125 (3)	0.69889 (10)	0.71649 (18)	0.0878 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0858 (17)	0.0437 (12)	0.100 (2)	−0.0096 (11)	0.0383 (18)	−0.0003 (16)
C2	0.0857 (17)	0.0588 (14)	0.0794 (19)	0.0115 (13)	0.0310 (16)	0.0223 (15)
C3	0.0655 (12)	0.0621 (13)	0.0495 (12)	0.0050 (10)	0.0081 (11)	0.0086 (12)
C4	0.0498 (10)	0.0477 (10)	0.0401 (10)	0.0006 (8)	0.0098 (9)	−0.0006 (9)
C5	0.0456 (10)	0.0530 (11)	0.0518 (12)	−0.0043 (8)	0.0075 (10)	−0.0038 (10)
C6	0.0630 (14)	0.0603 (14)	0.0801 (19)	−0.0166 (11)	0.0202 (14)	−0.0152 (14)
C7	0.0472 (9)	0.0465 (10)	0.0416 (10)	−0.0012 (8)	0.0001 (9)	−0.0047 (10)
C8	0.0885 (16)	0.0634 (14)	0.0439 (12)	−0.0034 (12)	0.0010 (12)	−0.0127 (12)
C9	0.0478 (10)	0.0408 (10)	0.0458 (11)	−0.0037 (7)	0.0021 (9)	−0.0055 (10)
C10	0.0686 (13)	0.0465 (12)	0.0585 (14)	−0.0100 (10)	0.0083 (12)	−0.0055 (13)
C11	0.0696 (13)	0.0483 (13)	0.0556 (15)	0.0053 (10)	0.0036 (11)	0.0049 (12)
C12	0.0491 (9)	0.0416 (10)	0.0427 (11)	−0.0008 (8)	0.0009 (9)	0.0026 (10)
C13	0.0548 (10)	0.0505 (11)	0.0365 (10)	0.0022 (9)	0.0004 (9)	0.0017 (9)
C14	0.0483 (10)	0.0455 (10)	0.0375 (10)	0.0044 (8)	0.0027 (9)	−0.0041 (9)
C15	0.0426 (9)	0.0468 (10)	0.0394 (10)	−0.0012 (8)	0.0018 (8)	−0.0067 (9)
C16	0.0420 (8)	0.0501 (11)	0.0414 (10)	0.0040 (8)	0.0024 (9)	−0.0010 (9)
C17	0.0579 (11)	0.0434 (11)	0.0555 (13)	0.0052 (9)	0.0014 (10)	−0.0075 (11)
C18	0.0766 (13)	0.0503 (12)	0.0586 (15)	0.0054 (10)	−0.0152 (12)	−0.0211 (12)
C19	0.0667 (12)	0.0574 (13)	0.0391 (11)	0.0113 (10)	−0.0107 (10)	−0.0108 (11)
C20	0.0816 (16)	0.0540 (13)	0.0719 (17)	0.0067 (11)	−0.0073 (14)	0.0106 (13)
O1	0.0640 (9)	0.0567 (8)	0.0549 (9)	0.0022 (7)	−0.0134 (7)	0.0073 (7)
O2	0.0881 (11)	0.0445 (8)	0.0802 (13)	0.0049 (8)	−0.0127 (10)	−0.0021 (9)
O3	0.1243 (16)	0.0638 (10)	0.0544 (11)	0.0120 (10)	−0.0018 (11)	0.0152 (10)
O4	0.1004 (12)	0.0409 (8)	0.0660 (12)	−0.0016 (8)	0.0077 (10)	0.0034 (8)
O5	0.1352 (17)	0.0545 (10)	0.0737 (14)	−0.0265 (10)	0.0139 (12)	−0.0191 (11)

Geometric parameters (Å, °)

C1—C2	1.369 (4)	C11—O4	1.383 (3)
C1—C6	1.379 (4)	C11—C12	1.477 (3)
C1—H1	0.9300	C12—C13	1.349 (3)
C2—C3	1.376 (4)	C13—C14	1.451 (3)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.403 (3)	C14—C19	1.395 (3)
C3—H3	0.9300	C14—C15	1.407 (3)
C4—C5	1.387 (3)	C15—C16	1.365 (3)
C4—C7	1.478 (3)	C15—H15	0.9300
C5—C6	1.379 (3)	C16—O1	1.369 (3)
C5—H5	0.9300	C16—C17	1.388 (3)

C6—H6	0.9300	C19—H19	0.9300
C7—C9	1.356 (3)	C17—C18	1.355 (3)
C7—C8	1.512 (3)	C17—O2	1.368 (3)
C8—H8A	0.9600	C18—C19	1.393 (3)
C8—H8B	0.9600	C18—H18	0.9300
C8—H8C	0.9600	C19—H19	0.9300
C9—C12	1.473 (3)	C20—O2	1.419 (3)
C9—C10	1.487 (3)	C20—O1	1.424 (3)
C10—O5	1.191 (3)	C20—H20A	0.9700
C10—O4	1.391 (3)	C20—H20B	0.9700
C11—O3	1.195 (3)		

C2—C1—C6	120.0 (2)	O4—C11—C12	109.0 (2)
C2—C1—H1	120.0	C13—C12—C9	138.8 (2)
C6—C1—H1	120.0	C13—C12—C11	115.0 (2)
C1—C2—C3	120.2 (3)	C9—C12—C11	106.07 (19)
C1—C2—H2	119.9	C12—C13—C14	132.6 (2)
C3—C2—H2	119.9	C12—C13—H13	113.7
C2—C3—C4	120.5 (3)	C14—C13—H13	113.7
C2—C3—H3	119.7	C19—C14—C15	120.00 (18)
C4—C3—H3	119.7	C19—C14—C13	116.60 (19)
C5—C4—C3	118.5 (2)	C15—C14—C13	123.40 (18)
C5—C4—C7	121.34 (19)	C16—C15—C14	117.07 (18)
C3—C4—C7	120.1 (2)	C16—C15—H15	121.5
C6—C5—C4	120.1 (2)	C14—C15—H15	121.5
C6—C5—H5	119.9	C15—C16—O1	128.48 (19)
C4—C5—H5	119.9	C15—C16—C17	121.83 (19)
C5—C6—C1	120.6 (3)	O1—C16—C17	109.68 (18)
C5—C6—H6	119.7	C18—C17—O2	127.7 (2)
C1—C6—H6	119.7	C18—C17—C16	122.4 (2)
C9—C7—C4	123.10 (19)	O2—C17—C16	109.8 (2)
C9—C7—C8	121.79 (18)	C17—C18—C19	116.7 (2)
C4—C7—C8	115.0 (2)	C17—C18—H18	121.6
C7—C8—H8A	109.5	C19—C18—H18	121.6
C7—C8—H8B	109.5	C18—C19—C14	121.8 (2)
H8A—C8—H8B	109.5	C18—C19—H19	119.1
C7—C8—H8C	109.5	C14—C19—H19	119.1
H8A—C8—H8C	109.5	O2—C20—O1	108.90 (19)
H8B—C8—H8C	109.5	O2—C20—H20A	109.9
C7—C9—C12	134.23 (18)	O1—C20—H20A	109.9
C7—C9—C10	120.60 (19)	O2—C20—H20B	109.9
C12—C9—C10	104.40 (18)	O1—C20—H20B	109.9
O5—C10—O4	118.2 (2)	H20A—C20—H20B	108.3
O5—C10—C9	132.4 (2)	C16—O1—C20	105.74 (18)
O4—C10—C9	109.39 (19)	C17—O2—C20	105.82 (17)
O3—C11—O4	119.7 (2)	C11—O4—C10	109.81 (17)
O3—C11—C12	131.2 (3)		

C6—C1—C2—C3	0.4 (4)	C9—C12—C13—C14	1.0 (4)
C1—C2—C3—C4	1.7 (4)	C11—C12—C13—C14	−173.1 (2)

C2—C3—C4—C5	−2.7 (3)	C12—C13—C14—C19	−147.5 (2)
C2—C3—C4—C7	179.3 (2)	C12—C13—C14—C15	31.9 (3)
C3—C4—C5—C6	1.8 (3)	C19—C14—C15—C16	3.0 (3)
C7—C4—C5—C6	179.78 (19)	C13—C14—C15—C16	−176.44 (18)
C4—C5—C6—C1	0.2 (3)	C14—C15—C16—O1	179.41 (18)
C2—C1—C6—C5	−1.3 (4)	C14—C15—C16—C17	0.9 (3)
C5—C4—C7—C9	42.2 (3)	C15—C16—C17—C18	−3.5 (3)
C3—C4—C7—C9	−139.8 (2)	O1—C16—C17—C18	177.8 (2)
C5—C4—C7—C8	−134.7 (2)	C15—C16—C17—O2	178.71 (18)
C3—C4—C7—C8	43.2 (3)	O1—C16—C17—O2	0.0 (2)
C4—C7—C9—C12	3.0 (4)	O2—C17—C18—C19	179.3 (2)
C8—C7—C9—C12	179.7 (2)	C16—C17—C18—C19	1.9 (3)
C4—C7—C9—C10	−165.19 (19)	C17—C18—C19—C14	2.1 (4)
C8—C7—C9—C10	11.5 (3)	C15—C14—C19—C18	−4.6 (3)
C7—C9—C10—O5	−16.8 (4)	C13—C14—C19—C18	174.8 (2)
C12—C9—C10—O5	171.9 (3)	C15—C16—O1—C20	−179.0 (2)
C7—C9—C10—O4	161.4 (2)	C17—C16—O1—C20	−0.4 (2)
C12—C9—C10—O4	−9.9 (2)	O2—C20—O1—C16	0.7 (3)
C7—C9—C12—C13	27.4 (4)	C18—C17—O2—C20	−177.2 (2)
C10—C9—C12—C13	−163.0 (3)	C16—C17—O2—C20	0.4 (2)
C7—C9—C12—C11	−158.1 (2)	O1—C20—O2—C17	−0.7 (3)
C10—C9—C12—C11	11.4 (2)	O3—C11—O4—C10	−177.6 (3)
O3—C11—C12—C13	−12.5 (4)	C12—C11—O4—C10	3.2 (3)
O4—C11—C12—C13	166.54 (19)	O5—C10—O4—C11	−177.2 (2)
O3—C11—C12—C9	171.5 (3)	C9—C10—O4—C11	4.3 (2)
O4—C11—C12—C9	−9.4 (2)		

X—H···π-ring interactions calculated by PLATON (Spek, 2003). Cg1 is the centroid of the benzene ring C1–C6 and Cg2 is the centroid of the benzene ring C14-C19.

X—H···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C19—H19···*Cg*1[i]	0.93	2.83	3.671 (2)	151
C3—H3···*Cg*2[ii]	0.93	2.94	3.837 (2)	163

Symmetry code: (i) *x*,-1 + *y*,*z*, (ii) 1/2 − *x*,-1/2 + *y*,-1/2 + *z*.

Fig. 1

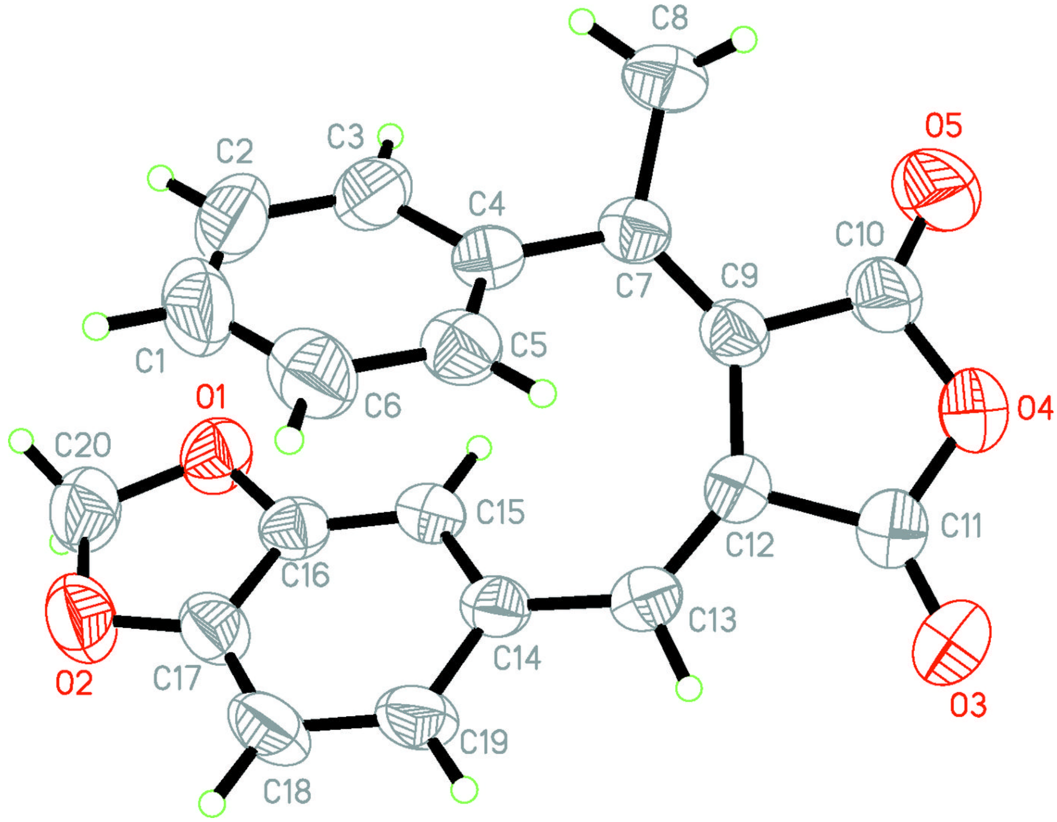

C8
O5
C2
C3
C4
C10
C7
C9
C1
C5
O1
C6
O4
C20
C15
C11
C12
C16
C13
C14
O2
C17
O3
C19
C18

Fig. 2