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(3*Z*,4*Z*)-3,4-Bis(1,3-benzodioxol-5-ylmethylene)-tetrahydrofuran-2,5-dione

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.170
Data-to-parameter ratio = 8.8

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

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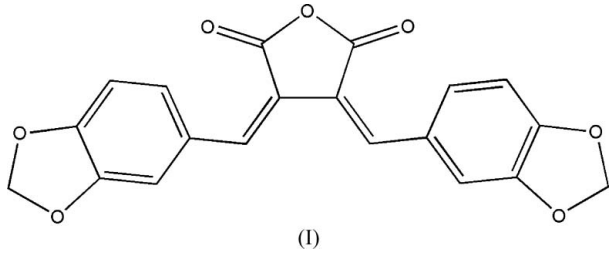
In the title compound, $C_{20}H_{12}O_7$, all bond lengths and angles show normal values. The dihedral angles between the tetrahydrofuran ring and the two aryl rings are 9.62 (3) and 34.53 (3)°, while that between the two aryl rings is 43.68 (17)°.

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). Photochromic fulgides are derivatives of dimethylene succinic anhydrides, containing a hexatriene frame (Liang *et al.*, 2001). The crystal structure of the title compound, (I), is reported here.



(I)

Experimental

2,3-Bis(benzo[*d*][1,3]dioxol-5-ylmethylene)succinic acid (33 mmol) was dissolved in dichloromethane (100 ml); to this mixture was added acetyl chloride (50 ml) dropwise with stirring at 273 K. The mixture was then stirred at room temperature for 5 h. After removal of 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 from ethyl acetate to give a solid (yield 62%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a dichloromethane solution at room temperature over a period of 15 d.

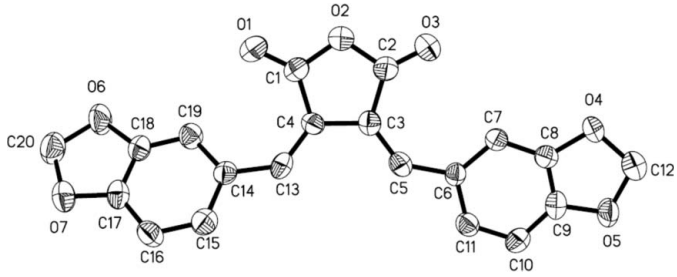


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms have been omitted.

Crystal data

$C_{20}H_{12}O_7$	V = 1581.20 (12) Å^3
M_r = 364.30	Z = 4
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
a = 4.6461 (2) Å	μ = 0.12 mm^{-1}
b = 14.2262 (6) Å	T = 296 (2) K
c = 23.9227 (11) Å	0.36 × 0.12 × 0.05 mm

Data collection

Bruker APEX2 CCD area-detector diffractometer	6462 measured reflections 2138 independent reflections
Absorption correction: multi-scan (*APEX2*; Bruker, 2005) T_{min} = 0.693, T_{max} = 1.000	1127 reflections with $I > 2\sigma(I)$ R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058	244 parameters
$wR(F^2)$ = 0.170	H-atom parameters constrained
S = 0.99	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
2138 reflections	$\Delta\rho_{min}$ = −0.22 e Å^{-3}

H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

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).

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