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3,3′-Diphenylbi-1*H*-indene-1,1′-dione

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.099
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.

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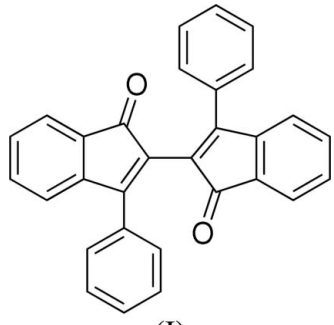
The title compound, $C_{30}H_{18}O_2$, was synthesized by the reaction of phenylmagnesium bromide with 2,2′-biindanylidene-1,1′,3,3′-tetraone under a nitrogen atmosphere. The dihedral angle between the two indenone ring systems is 50.66 (3)°.

Comment

In recent years, organic photochromic compounds have received considerable attention in view of their general applicability as optical information storage materials or switching devices (Irie, 2000). Among many types of photochromic compounds, the biindenylidene derivatives are unusual in that they simultaneously undergo photochromism in the crystalline state as well as the generation of radicals (Li *et al.*, 2005; Xu, Huang *et al.*, 2002; Xu, Sugiyama *et al.*, 2002; Tanak *et al.*, 2004). We report here the crystal structure of the title compound, (I) (Fig.1).



(I)

The O1/C1–C9 and O2/C16–C24 indenone ring systems are essentially planar with r.m.s deviations of 0.014 and 0.036 Å, respectively. The dihedral angle between the O1/C1–C9 and O2/C16–C24 planes is 50.66 (3)°. The C10–C15 and C25–C30 phenyl rings are twisted away from the attached indenone rings by 46.13 (6) and 50.79 (5)°, respectively.

The crystal structure is stabilized by C6—H6···O1^{i} [H6···O1^{i} = 2.51 Å, C6···O1^{i} = 3.368 (2) Å and C6—H6···O1^{i} 154°; symmetry code: (i) $\frac{1}{2}+x, y, \frac{1}{2}-z$] intermolecular hydrogen bonds.

Experimental

The title compound was synthesized by the reaction of phenylmagnesium bromide (3.14 g, 20 mmol) with 2,2′-biindanylidene-1,1′,3,3′-tetraone (1.54 g, 5 mmol) under a nitrogen atmosphere. Crystals suitable for X-ray analysis were grown by slow evaporation of a dichloromethane solution at room temperature.

Crystal data

$C_{30}H_{18}O_2$
M_r = 410.44
Orthorhombic, *Pbca*
a = 14.5873 (15) Å
b = 16.8272 (17) Å
c = 17.5740 (18) Å
V = 4313.8 (8) Å^3
Z = 8
D_x = 1.264 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, red
0.28 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.987
22167 measured reflections
3809 independent reflections
2757 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.02
3809 reflections
289 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 1.0083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

H atoms were positioned geometrically (C—H = 0.93 Å) and refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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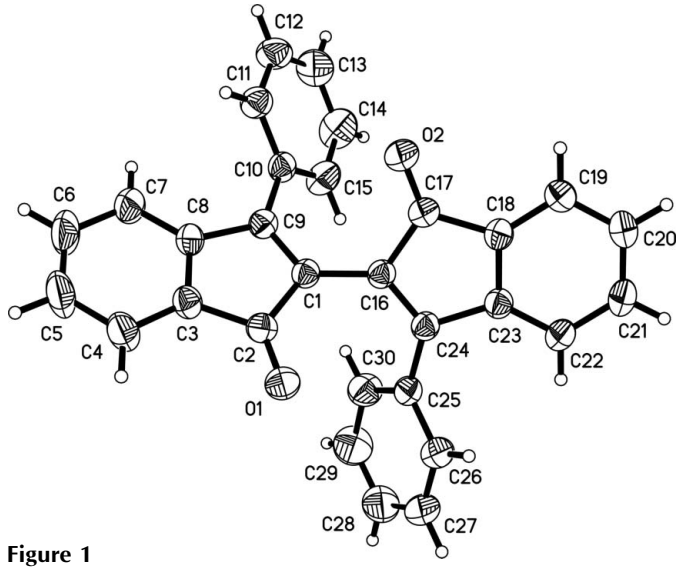

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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