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3,3′-Dibenzyl-3,3′-dihydroxy-[2,2′-bi-1*H*-indene]-1,1′-dione

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 14.7

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

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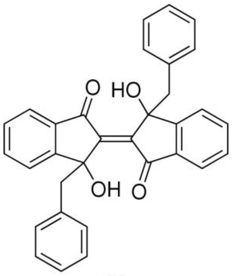
The title compound, $C_{32}H_{24}O_4$, was synthesized by the reaction of benzylmagnesium bromide with 2,2′-biindanylidene-1,1′,3,3′-tetraone. The molecule lies across a crystallographic inversion centre. The cyclopentenone ring adopts a flattened envelope conformation.

Comment

Photochromism is defined as light-induced reversible transformation of chemical species between two isomers having different absorption spectra. 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.*, 2007; Nakatsuji, 2004; Tanak *et al.*, 2004). We report here the crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) contains one-half molecule with the other half generated by a centre of inversion (Fig. 1); the centre of inversion lies at the mid-point of the C2═C2^i bond [symmetry code: (i) $1 - x$, $1 - y$, $1 - z$]. The bond distance C2═C2^i of 1.357 (3) Å confirms its double-bond character. The cyclopentenone ring adopts a flattened envelope conformation, with atom C2 at the flap. The dihedral angle between the O1/C1/C3–C9 and C11–C16 planes is 53.11 (5)°.

Intramolecular O—H⋯O hydrogen bonds generate *S*(7) ring motifs. The crystal structure is stabilized by C—H⋯π intermolecular interactions (Table 1) involving the phenyl ring (centroid *Cg*1).

Experimental

The title compound was synthesized by the reaction of benzylmagnesium bromide (3.42 g, 20 mmol) with 2,2′-biindanylidene-

1,1′,3,3′-tetraone (1.54 g, 5 mmol) under a nitrogen atmosphere, followed by exposure to the air for another 3 h. Crystals suitable for X-ray analysis were grown by slow evaporation of a dichloromethane solution at room temperature.

Crystal data

$C_{32}H_{24}O_4$	$Z = 4$
$M_r = 472.51$	$D_x = 1.299$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 15.576$ (6) Å	$\mu = 0.09$ mm^{-1}
$b = 9.611$ (4) Å	$T = 294$ (2) K
$c = 16.139$ (6) Å	Block, yellow
$V = 2416.1$ (17) Å^3	0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	12722 measured reflections
φ and ω scans	2462 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1482 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.979$, $T_{\max} = 0.989$	$R_{\rm int} = 0.046$
	$\theta_{\max} = 26.4°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0521P)^2 + 0.4227P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.121$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.02$	$\Delta\rho_{\max} = 0.19$ e Å^{-3}
2462 reflections	$\Delta\rho_{\min} = -0.14$ e Å^{-3}
167 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1$^{\rm i}$	0.94 (3)	1.76 (3)	2.685 (2)	164 (3)
C5—H5···*Cg*1$^{\rm ii}$	0.93	2.79	3.640 (3)	153

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$. Cg1 is the centroid of the phenyl ring C11–C16.

The hydroxyl H atom was located in a difference map and refined isotropically. All other H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

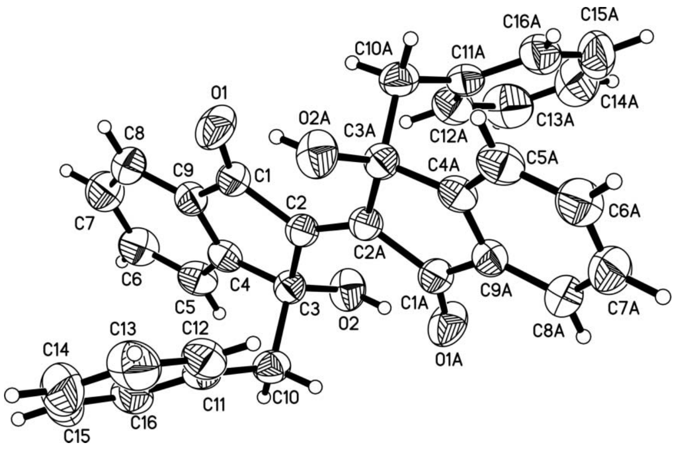


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Atoms labelled with the suffix A are generated by the symmetry operation ($1-x, 1-y, 1-z$).

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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