Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

3,3′-Diethyl-3,3′-dihydroxy-5,5′-dimethyl-2,2′-bi-1*H*-indanylidene-1,1′-dione

Xu Li,* Xing-Yi Zhao, Min Zhao, Jing-Jun Liu and Yong-Ming Wang

Chinese People's Armed Police Forces Academy, Langfang 065000, People's Republic of China

Correspondence e-mail:
lixu.wjxy@yahoo.com.cn

Received 26 March 2007
Accepted 26 March 2007

Key indicators

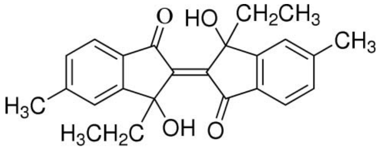
Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.119
Data-to-parameter ratio = 15.4

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

The title compound, $C_{24}H_{24}O_4$, was synthesized by the reaction of ethylmagnesium bromide with 5,5′-bimethyl-2,2′-biindanylidene-1,1′,3,3′-tetraone under an argon atmosphere. 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) $1 - x, 2 - y, 2 - z$]. The C2═C2^{i} bond distance of 1.352 (3) Å confirms its double-bond character.

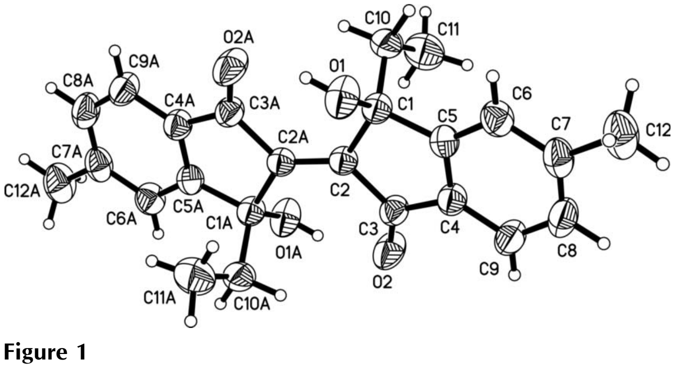


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Atoms labelled with the suffix A are generated by the symmetry operation $(1 - x, 2 - y, 2 - z)$.

The cyclopentenone ring adopts a flattened envelope conformation, with atom C2 at the flap.

Intramolecular O—H···O hydrogen bonds generate *S*(7) ring motifs. The crystal structure is stabilized by C—H···O intermolecular interactions (Table 1).

Experimental

The title compound was synthesized by the reaction of ethylmagnesium bromide (2.16 g, 20 mmol) with 5,5′-bimethyl-2,2′-biindanylidene-1,1′,3,3′-tetraone (1.59 g, 5 mmol) under an argon atmosphere. Crystals suitable for X-ray analysis were grown by slow evaporation of a dichloromethane solution at room temperature.

Crystal data

$C_{24}H_{24}O_4$
$M_r = 376.43$
Monoclinic, $P2_1/n$
$a = 8.584$ (2) Å
$b = 7.4860$ (15) Å
$c = 15.554$ (4) Å
$\beta = 100.564$ (8)°
$V = 982.6$ (4) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.947$, $T_{\max} = 0.983$
5475 measured reflections
2030 independent reflections
1403 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.119$
$S = 1.03$
2030 reflections
132 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2$^{\rm i}$	0.833 (9)	1.935 (14)	2.7019 (18)	153 (2)
C10—H10*A*···O2$^{\rm i}$	0.97	2.58	3.247 (3)	126
C10—H10*B*···O1$^{\rm ii}$	0.97	2.58	3.476 (2)	153

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

The hydroxyl H atom was located in a difference map and refined with an O—H distance restraint of 0.84 (1) Å. All other H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined in the riding-model approximation, with $U_{\rm iso}({\rm H}) = 1.2$–$1.5U_{\rm eq}({\rm C})$.

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*.

This work was financially supported by the Department of Education of Hebei Province (grant No. Z2006119).

References

Bruker (1998). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Irie, M. (2000). *Chem. Rev.* **100**, 1683–1890.
Li, X., Liu, J.-J., Zhao, M., Wang, Y.-M. & Xia, C.-F. (2007). *Acta Cryst.* E**63**, o436–o437.
Nakatsuji, S. (2004). *Chem. Soc. Rev.* **33**, 348–353.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tanak, K., Yamamoto, Y. & Caira, M. R. (2004). *CrystEngComm*, **6**, 1–4.

Acta Cryst. (2007). E**63**, o2182–o2183 Li *et al.* • $C_{24}H_{24}O_4$ **o2183**