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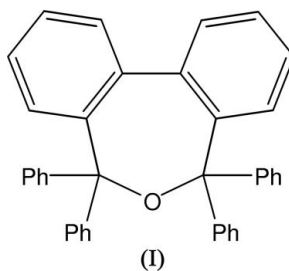
Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.078
 wR factor = 0.199
Data-to-parameter ratio = 17.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2,2',7,7'-Tetraphenyl-2,7-dihydrodibenz-
[c,e]oxepine

The structure of the title compound, $\text{C}_{38}\text{H}_{28}\text{O}$, has previously been reported by Hirano, Toyota & Toda [*Heterocycles* (2004), **62**, 749–756]. Since these authors did not publish any coordinates, we present here a redetermination of this structure using new intensity data. The molecule has chemical but not crystallographic C_2 symmetry. The central seven-membered ring adopts a twist-boat conformation.

Comment

2,2',7,7'-Tetraphenyl-2,7-dihydrodibenz[*c,e*]oxepine, (I), was obtained as an unexpected product during our investigation of the $\text{Bi}(\text{OTf})_3$ -catalysed (OTf is trifluoromethanesulfonate) intramolecular benzylation of arenes (Rueping *et al.*, 2006). Surprisingly, the etherification yielding the oxepine derivative occurred more rapidly than the Friedel–Crafts-type *C*-alkylation of the arene ring. The product could be isolated in good yield, suggesting that this methodology may be applied in the synthesis of further oxepine derivatives.

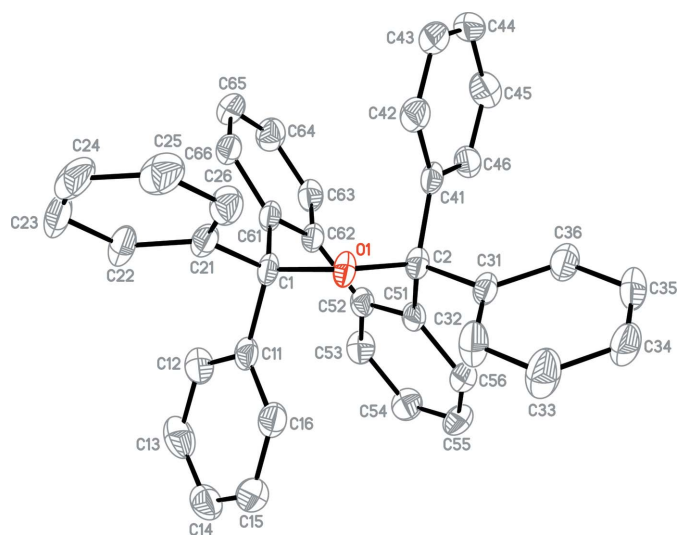


A perspective view of (I) is shown in Fig. 1. It shows molecular but not crystallographic C_2 symmetry. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27 plus one update; *MOGUL* Version 1.1; Allen, 2002). The central seven-membered ring adopts a twist-boat conformation (Table 1). The dihedral angle between the two benzene rings of the biphenyl system is $47.43(12)^\circ$. Since no coordinates from the previous structure determination (Hirano *et al.*, 2004) are available, no comparison between the two structure determinations can be made. However, Carey *et al.* (2002) published the structure of the toluene solvate of the title compound. A least-squares fit of (I) with this solvate (r.m.s. deviation for all non-H atoms = 0.201 Å) shows that the molecular conformation is not significantly influenced by the solvent (Fig. 2).

Experimental

2,2'-Bis(diphenylhydroxymethyl)biphenyl (0.2593 g, 0.50 mmol) and $\text{Bi}(\text{OTf})_3 \cdot 4\text{H}_2\text{O}$ (0.0036 g, 0.005 mmol) in CH_2Cl_2 (4 ml) were added

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**Figure 1**

Perspective view of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

to a 10 ml round-bottomed flask and the reaction mixture was refluxed for 2 h. The reaction mixture was allowed to cool to room temperature and CH_2Cl_2 was removed *in vacuo*. The crude product was purified by column chromatography (SiO_2), using hexane and ethyl acetate (50:1) as eluent, affording (I) (yield 0.2009 g, 80%). Slow evaporation of a CH_2Cl_2 solution of (I) gave colourless crystals of (I) (m.p. >503 K).

Crystal data

$\text{C}_{38}\text{H}_{28}\text{O}$
 $M_r = 500.60$
 Monoclinic, $P2_1/c$
 $a = 13.6436$ (17) Å
 $b = 11.5482$ (9) Å
 $c = 17.1442$ (19) Å
 $\beta = 90.306$ (10)°
 $V = 2701.2$ (5) Å³
 $Z = 4$

$D_x = 1.231$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 10503 reflections
 $\theta = 3.6$ – 27.6°
 $\mu = 0.07$ mm⁻¹
 $T = 173$ (2) K
 Block, colourless
 $0.24 \times 0.23 \times 0.21$ mm

Data collection

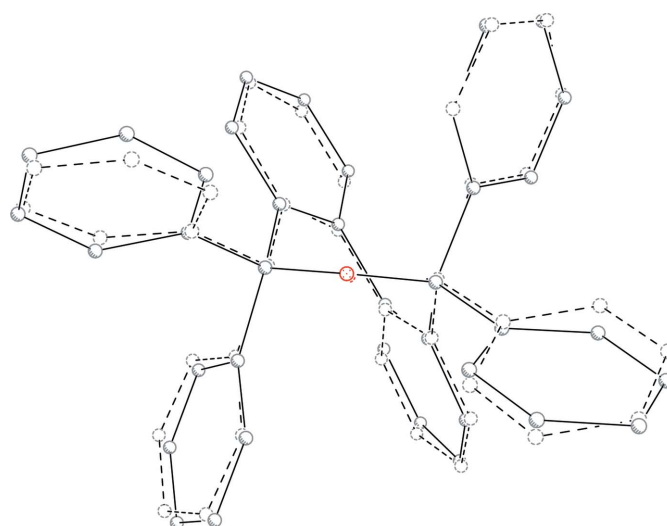
Stoe IPDS-II two-circle diffractometer
 ω scans
 Absorption correction: none
 31915 measured reflections
 6240 independent reflections

3318 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.097$
 $\theta_{\text{max}} = 27.7^\circ$
 $h = -17 \rightarrow 17$
 $k = -14 \rightarrow 15$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.078$
 $wR(F^2) = 0.199$
 $S = 0.96$
 6240 reflections
 353 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.089P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0083 (19)

**Figure 2**

Least-squares fit of (I) (solid lines) with the toluene solvate (dashed lines).

Table 1

Selected geometric parameters (Å, °).

C1—O1	1.463 (3)	C52—C62	1.496 (4)
O1—C2	1.463 (3)		
C2—O1—C1	121.4 (2)		
C61—C1—O1—C2	−36.7 (3)	O1—C1—C61—C62	70.8 (3)
C1—O1—C2—C51	−45.5 (3)	C1—C61—C62—C52	−7.1 (4)
O1—C2—C51—C52	66.2 (3)	C51—C52—C62—C61	−46.2 (4)
C2—C51—C52—C62	3.3 (4)		

H atoms were located in a difference map, but were repositioned with idealized geometry and refined with fixed individual displacement parameters [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$] using a riding model ($\text{C—H} = 0.95$ Å).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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