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9,9′-Bi-10*H*-anthracene-9,9′-diol

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The title compound, $C_{28}H_{22}O_2$, is a intermediate in the synthesis of 10,10′-dibromo-9,9′-bianthracenyl. The molecule forms both intra- and intermolecular O—H⋯O hydrogen bonds.

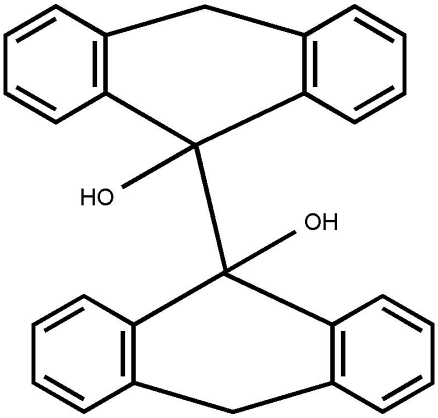
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.062
wR factor = 0.121
Data-to-parameter ratio = 13.1

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

Comment

Organic electroluminescence materials have many advantages, such as high brightness, high efficiency, wide visual view, fast response, rich colour and low cost. In addition, they can be driven by low-voltage direct current, processed into various shapes owing to their excellent mechanical properties, or made into large full-colour displays (Tsutsui & Fujita, 2002). In this promising field, therefore, much research effort is being devoted to the investigation of synthesis techniques and photophysical behaviour of new and promising electroluminescent materials. The title compound, (I), is an intermediate of many organic electroluminescence materials. Due to its versatility and utility in organic synthesis, we have now investigated the crystal structure of (I).



(I)

The molecule of (I) has two ring systems, which are connected by the C14—C15 bond (Fig. 1). The C14—C15 bond of 1.594 (3) Å is longer than the standard C—C bond of 1.53 Å (Allen *et al.*, 1987). The difference is considered to be the result of steric hindrance.

The title compound forms intra- and intermolecular O—H⋯O hydrogen bonds (Table 2). The intermolecular hydrogen-bond chains run along the c axis (Fig. 2). There are two benzene rings in each ring system, connected by two sp^3-hybridized C atoms (C7/C14 and C15/C22). The dihedral

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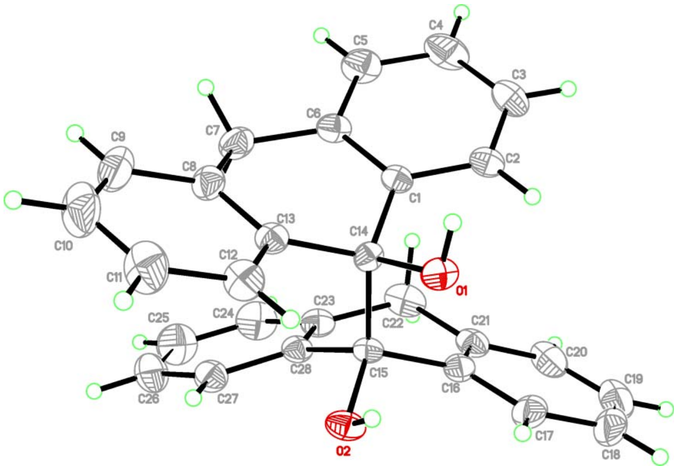

Figure 1
The molecular structure of (I), showing the atom-labelling scheme and 40% probability displacement ellipsoids.

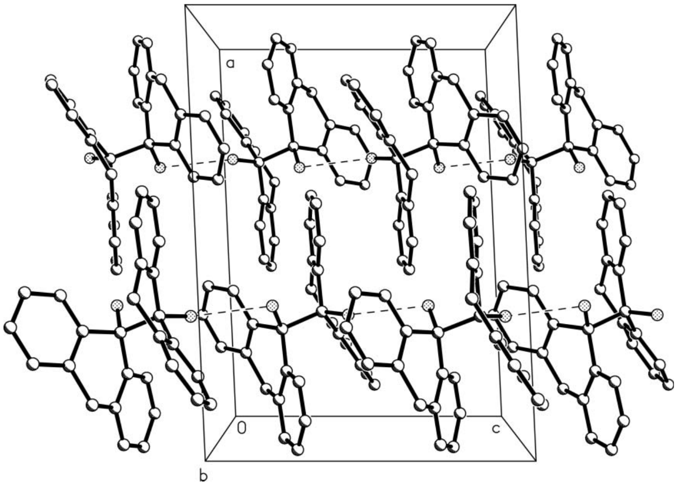

Figure 2
A packing diagram for (I), viewed along the *b* axis. Broken lines indicate hydrogen bonds. H atoms have been omitted, except for those involved in the hydrogen bonding.

angles between the pairs of benzene rings, C1–C6 and C8–C13, and C16–C21 and C23–C28, are 152.16 (11) and 148.29 (9)°, respectively.

Experimental

A mixture of anthrone (20 g), Zn (100 g), $ZnCl_2$ (20 g), tetrahydrofuran (THF; 100 ml) and water (100 ml) was stirred at room temperature for 4 h (Tanaka *et al.*, 1990). The reaction mixture was then combined wth 3 *N* HCl (50 ml) for 20 min, after which THF (100 ml) and toluene (100 ml) were added. The mixture was stirred for 10 min and then filtered to remove Zn powder. The filtrate was worked up as above three times. The oil layer was separated to remove $ZnCl_2$ and then evaporated to give the crude target compound. The product, (I), was recrystallized from THF and toluene (1:1), giving a yield of 95%.

Crystal data

$C_{28}H_{22}O_2$
$M_r = 390.46$
Monoclinic, $P2_1/c$
$a = 14.789$ (6) Å
$b = 12.853$ (5) Å
$c = 10.688$ (4) Å
$\beta = 92.549$ (6)°
$V = 2029.6$ (13) Å^3
$Z = 4$

$D_x = 1.278$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1379 reflections
$\theta = 2.5$–20.7°
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.40 × 0.30 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.750$, $T_{\max} = 0.992$
8162 measured reflections

3566 independent reflections
2239 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\max} = 25.0°$
$h = -17 \rightarrow 15$
$k = -13 \rightarrow 15$
$l = -8 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.121$
$S = 1.03$
3566 reflections
273 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.19$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C14	1.520 (3)	C15—C28	1.513 (3)
C13—C14	1.520 (3)	C15—C16	1.525 (3)
C14—C15	1.594 (3)		
O1—C14—C15—O2	58.0 (2)	C1—C14—C15—C16	57.7 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O2—H2⋯O1	0.82	2.22	2.675 (2)	115
O1—H1⋯O2$^{\rm i}$	0.82	2.01	2.801 (2)	163

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

H atoms were placed in idealized positions and allowed to ride on their respective parent atoms, with O—H = 0.82 Å and C—H 0.93–0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

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