# 3-(Anthracen-9-yl)-3*H*-isobenzofuran-1-one

K. Palani,[a] P. Amaladass,[b] A. K. Mohanakrishnan[b] and M. N. Ponnuswamy[a]*

[a]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India

Correspondence e-mail:
mnpsy2004@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.125
Data-to-parameter ratio = 11.3

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

In the title compound, $C_{22}H_{14}O_2$, the dihedral angle between the planes of the anthracene and the benzofuranone ring systems is 70.74 (4)°. The crystal packing is stabilized by C—H···π interactions.

Comment

The design of fluorescent chemosensors is an aspect of the field of supramolecular chemistry (de Silva *et al.*, 1997). Many fluorescent sensors containing the anthracene ring system have been designed and investigated (Wang *et al.*, 2002). The fluorescence intensity of compounds with anthracene chromophores can be effectively modulated by introducing different substituents (Luigi & Antonio, 1995). In view of this, the crystal structure of the title compound (I) was determined to establish the conformation of the molecule.

(I)
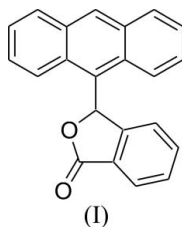
A *ORTEP-3* (Farrugia, 1997) plot of the molecule is shown in Fig.1. The bond lengths and bond angles in the anthracene ring system are comparable to those reported for 9-oxo-10-diphenylphosphinoylanthracene (Liu & Song, 2005). The anthracene ring system is approximately planar, with a maximum deviation of 0.138 (2) Å for C3. The dihedral angle between the planes of the anthracene and the isobenzofuranone ring systems is 70.74 (4)°.

An intramolecular C2—H2···O1 hydrogen bond leads to the formation of an *S*(5) ring motif (Bernstein, *et al.*, 1995). The crystal structure is stabilized by C—H···π interactions (Table 2) involving the C1–C6 benzene ring (Fig. 2).

Experimental

A dry 50 ml round-bottom flask was charged with ethyl-2-iodo-benzoate (7.24 mmol) in dry THF (10 ml) and cooled to 253 K; isopropyl magnesium bromide (7.24 mmol) was slowly added. After 1 h, when the exchange was completed, 9-anthracene carbaldehyde (7.24 mmol) was added as a solution in THF (5 ml). The reaction mixture was allowed to warm to room temperature over a period of 30 min. The reaction mixture was poured into 30% aqueous NH₄Cl solution (20 ml) and extracted with ethyl acetate (50 ml). The crude
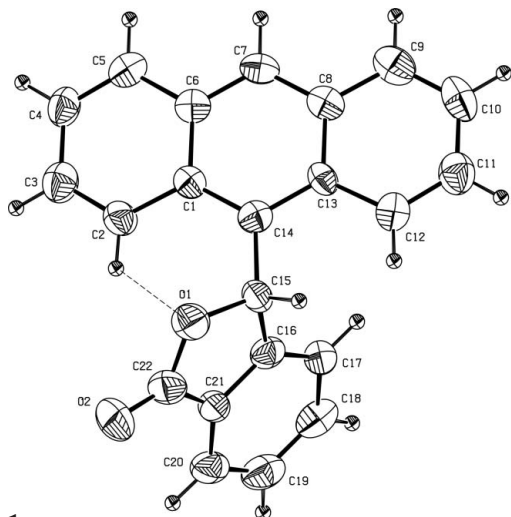
Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.
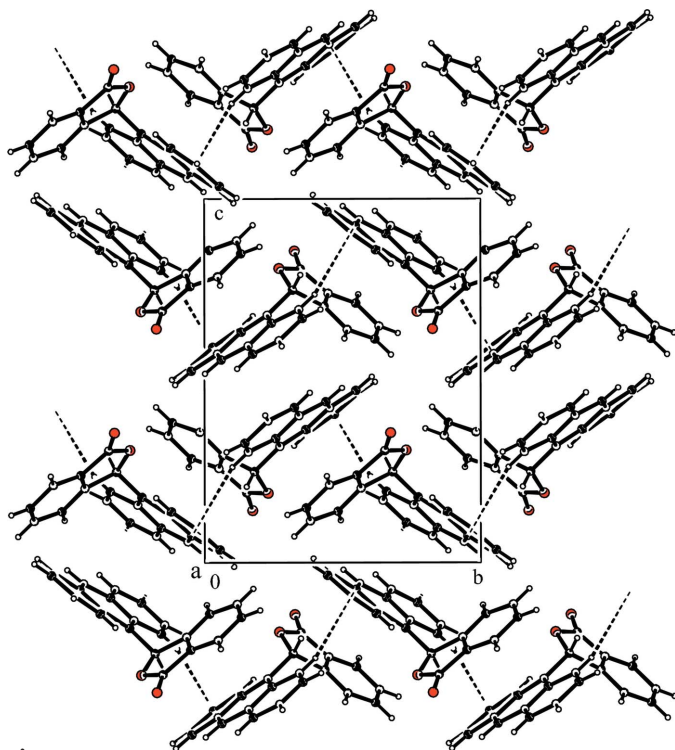

Figure 2
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate C—H···π interactions.

residue was recrystallized from boiling hexane to afford good quality crystals.

Crystal data

$C_{22}H_{14}O_2$	Mo $K\alpha$ radiation
$M_r = 310.33$	Cell parameters from 25
Orthorhombic, $P2_12_12_1$	reflections
$a = 9.961$ (4) Å	$\theta = 10-15°$
$b = 10.677$ (5) Å	$\mu = 0.09$ mm^{-1}
$c = 14.073$ (5) Å	$T = 293$ (2) K
$V = 1496.7$ (11) Å^3	Prism, yellow
$Z = 4$	$0.34 \times 0.20 \times 0.18$ mm
$D_x = 1.377$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4	$\theta_{max} = 30.1°$
diffractometer	$h = 0 \rightarrow 13$
ω scans	$k = 0 \rightarrow 15$
Absorption correction: none	$l = 0 \rightarrow 19$
2462 measured reflections	3 standard reflections
2462 independent reflections	frequency: 60 min
1469 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$+ 0.0612P]$
$wR(F^2) = 0.125$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
2462 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

C1—C14	1.412 (3)	C15—C14	1.504 (3)
C1—C2	1.438 (3)	C16—C21	1.380 (3)
O1—C22	1.368 (3)	C21—C22	1.459 (4)
O1—C15	1.454 (3)	C22—O2	1.203 (3)
C15—C16	1.501 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.93	2.33	2.914 (4)	120
C12—H12···$Cg2^i$	0.93	2.94	3.746 (4)	147

Symmetry code: (i) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$. $Cg1$ is the centroid of the C1–C6 benzene ring.

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 or 0.98 Å and $U_{iso}(H)$ = $1.2U_{eq}(C)$. Owing to the absence of any significant anomalous scatterers in the molecule, the Friedel data were not measured and the absolute configuration was assigned arbitrarily.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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