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9-Oxo-10-diphenylphosphinoylanthracene

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In the title anthraquinone derivative, $C_{26}H_{19}O_2P$, the dihedral angle of the two benzene rings is 30.2 (1)°. The diphenylphosphinoyl unit lies out of the plane of the tricyclic core.

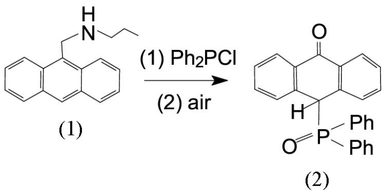
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.083
Data-to-parameter ratio = 11.1

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

Comment

The design of fluorescent chemosensors is an aspect of supramolecular chemistry (de Silva *et al.*, 1997). Many of these fluorescent sensors containing an 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 substituents (Luigi & Antonio, 1995). We report here the synthesis and crystal structure of 9-oxo-10-diphenylphosphinoylanthracene, (2).



(9–Anthracenemethyl)propylamine, (1), was reacted with diphenylphosphorus chloride to afford a yellow powder of (2). Compound (2) has a structure analogous to anthraquinone

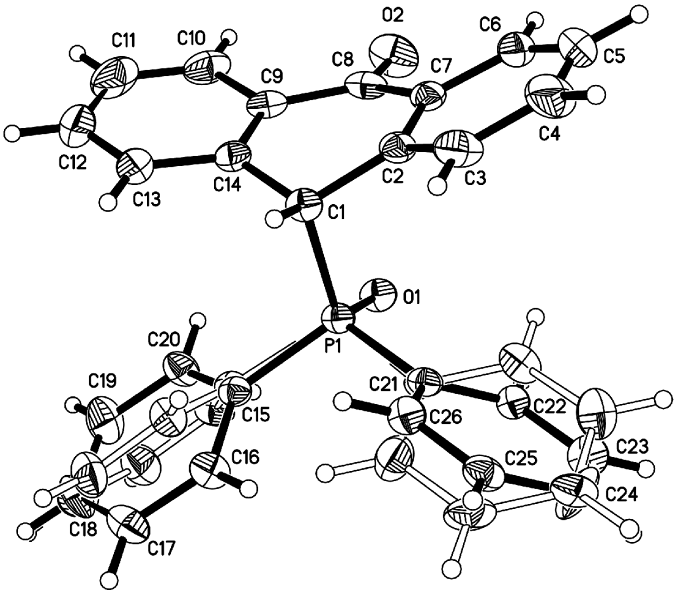


Figure 1
A view of (2), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Both disorder components are shown.

(Fig. 1). The dihedral angle of the two benzene rings is 30.2 (1)°. The diphenylphosphinoyl unit lies out of the plane of the tricyclic core. The distances P1—O1, P1—C1 and O2—C8 are 1.480 (18), 1.858 (3) and 1.220 (4) Å, respectively. The bond angles C9—C8—C7 and C2—C1—C14 are 115.9 (3) and 112.9 (3)°, respectively.

Experimental

Diphenylphosphorus chloride (0.904 g, 4.10 mmol) was added dropwise to a benzene solution of (9-anthracenemethyl)propylamine (1.00 g, 4.02 mmol) under nitrogen in an ice–water bath. After stirring for 5 h, the solution was warmed to room temperature and stirring was continued for 2 h in air. The solvent was removed *in vacuo* to afford a yellow powder of (2) (0.839 g, 53%; m.p. 467–469 K). ^{1}H NMR (300 MHz, CDCl$_3$): δ 5.31 (*d*, $J_{\rm H-P}$ = 30 Hz, H, CH), 7.01 (*d*, J = 7.6 Hz, 2H, PhH), 7.24 (*t*, J = 7.6 Hz, 2H, PhH), 7.39–7.53 (*m*, 8H, PhH and ArH), 7.68 (*t*, J = 7.6 Hz, 4H, ArH), 8.00 (*d*, J = 7.6 Hz, 2H, ArH). ^{31}P NMR (300 MHz, CDCl$_3$): δ 36.5. Analysis calculated for $C_{26}H_{19}O_2P$: C 79.18, H 19.15%; found: C 78.76, H 19.32%. IR (KBr, cm^{-1}): 1665 (C═O), 1599, 1439, 1309, 1179, 1117, 931, 788, 755, 723, 694, 564.

Crystal data

$C_{26}H_{19}O_2P$
M_r = 394.38
Orthorhombic, $Pca2_1$
a = 19.386 (6) Å
b = 5.5840 (15) Å
c = 17.928 (5) Å
V = 1940.7 (10) Å^3
Z = 4
D_x = 1.350 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 543 reflections
θ = 2.1–25.0°
μ = 0.16 mm^{-1}
T = 293 (2) K
Prism, yellow
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.953, $T_{\rm max}$ = 0.968
7475 measured reflections

3286 independent reflections
2286 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.056
$\theta_{\rm max}$ = 25.0°
$h = -23 \rightarrow 14$
$k = -6 \rightarrow 6$
$l = -21 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.083
S = 0.95
3286 reflections
296 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.21 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0013 (5)
Absolute structure: Flack (1983); 1510 Friedel pairs
Flack parameter = −0.16 (11)

Table 1
Selected geometric parameters (Å, °).

P1—O1	1.4803 (18)	O2—C8	1.220 (4)
P1—C1	1.858 (3)		
C2—C1—C14	112.9 (3)	C7—C8—C9	115.9 (3)

All H atoms were initially located in a difference Fourier map and then placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The phenyl rings are disordered over two positions each and were refined as ideal hexagons, with C—C = 1.39 Å and equal occupancy.

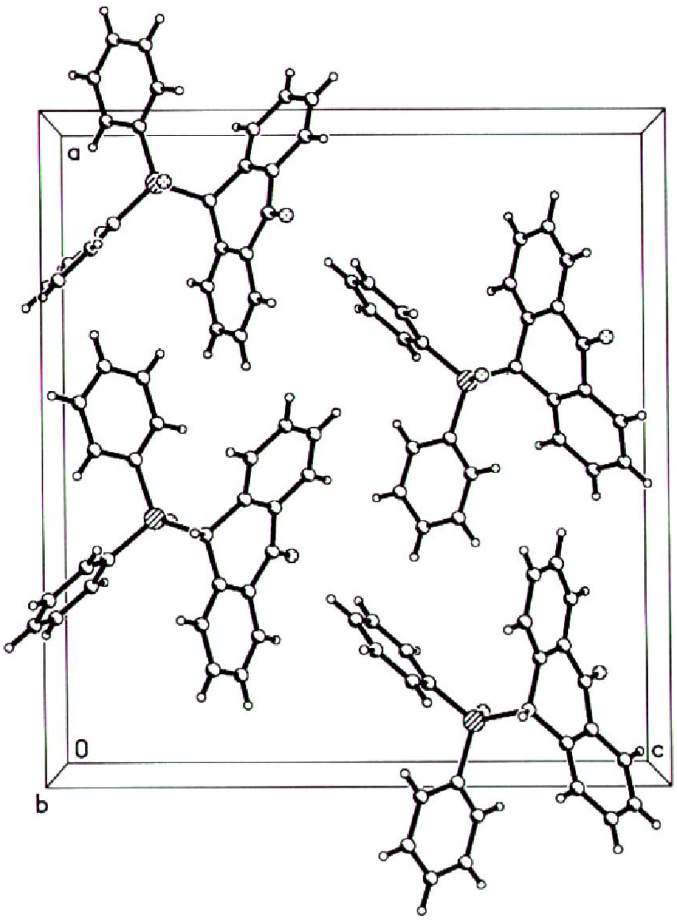


Figure 2
A view, down the *b* axis, of the packing arrangement in the crystal structure.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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