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1,3-Diphenyl-2*H*-cyclopenta[*l*]phenanthren-2-one

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Key indicators

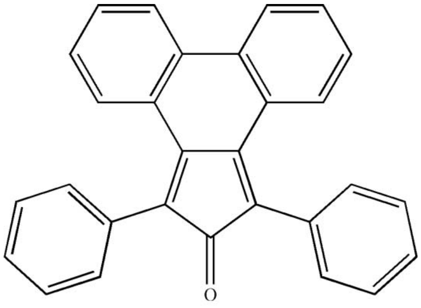
Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 12.9

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

The title compound, $C_{29}H_{18}O$, crystallizes as dark-red plates. The molecule shows a twisted and partial paddle-wheel conformation.

Comment

Tetraaryl-substituted cyclopentadienones (tetracyclones) are an interesting class of compounds due to their potential in organic synthesis (Eisch *et al.*, 1998). Despite this, only the crystal structure of the parent compound, tetracyclone (Barnes *et al.*, 1991; Alvarez-Toledano *et al.*, 1997), has been reported. The geometry of the tetracyclone molecule is mainly the result of steric hindrance, whereas the crystal packing is determined by weak C—H···O and C—H···π interactions. A similar situation is found in the crystal structure of the title compound, phencyclone (I), although (I) differs from tetracyclone in the conformation of the central six-membered ring fused to the cyclopentadienone ring. This particular six-membered ring, defined by atoms C9/C10/C15/C16/C21/C22, shows loss of planarity and thus also of aromatic character, similarly to 9,10-dihydrophenanthrene (Cosmo *et al.*, 1987). The endocyclic torsion angles for this ring and the five-membered ring are given in Table 1.



(I)

In summary, (I) should be considered a substituted cyclopentadienone rather than a condensed phenanthrene. The phenyl substituents of (I) are arranged in a paddle-wheel fashion (Fig. 2), which is also a typical feature of tetraphenylcyclone and the related compound, 2,5-diphenyl-3,4-bis(2-pyridyl)cyclopenta-2,4-dien-1-one (Siemeling *et al.*, 2004). Intermolecular C—H···π contacts, where π is an aromatic-ring centroid, ranging from 2.53 to 2.93Å give rise to the formation of molecular chains extended along the *a* axis.

Experimental

The title compound, (I), was synthesized according to the procedure described by Dilthey *et al.* (1935) from phenanthrene quinone, dibenzyl ketone and finely powdered potassium hydroxide in ethanol. Recrystallization from toluene gave dark-red crystals in 67% yield.

Crystal data

$C_{29}H_{18}O$
$M_r = 382.43$
Triclinic, $P\overline{1}$
$a = 10.4562$ (3) Å
$b = 10.5242$ (3) Å
$c = 10.5842$ (3) Å
$\alpha = 60.9600$ (10)°
$\beta = 70.1500$ (10)°
$\gamma = 89.446$ (2)°

$V = 940.59$ (5) Å^3
$Z = 2$
$D_x = 1.350$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 93$ (2) K
Plate, dark red
0.32 × 0.26 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
28645 measured reflections

3495 independent reflections
3224 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\rm max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.090$
$S = 1.04$
3495 reflections
271 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.331P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.008$
$\Delta\rho_{\rm max} = 0.24$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C23	1.5043 (15)	C10—C15	1.4142 (15)
C1—C2	1.5117 (14)	C15—C16	1.4868 (15)
C2—C9	1.3568 (15)	C16—C21	1.4156 (15)
C9—C10	1.4681 (15)	C21—C22	1.4637 (15)
C9—C22	1.5062 (14)	C22—C23	1.3528 (15)
C23—C1—C2—C9	−3.62 (11)	C16—C21—C22—C9	12.06 (14)
C1—C2—C9—C22	7.03 (11)	C2—C9—C22—C23	−8.53 (12)
C22—C9—C10—C15	13.00 (14)	C10—C9—C22—C21	−21.88 (14)
C9—C10—C15—C16	5.18 (14)	C9—C22—C23—C1	5.74 (11)
C10—C15—C16—C21	−15.52 (15)	C2—C1—C23—C22	−1.56 (11)
C15—C16—C21—C22	6.31 (15)		

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95Å and $U_{\rm iso}$ = 1.2 or 1.5 times $U_{\rm eq}$(parent atom).

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL97* and *PLATON* (Spek, 2003).

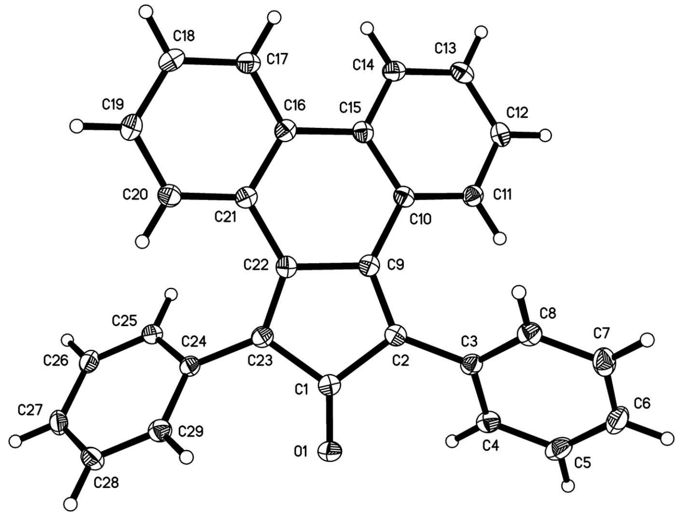


Figure 1
Perspective view of (I), showing 50% probability displacement ellipsoids.

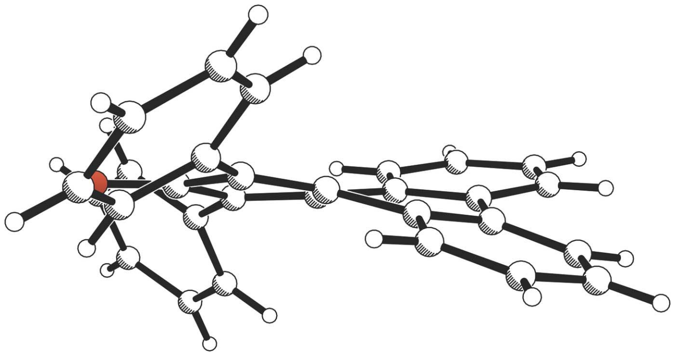


Figure 2
The non-planar conformation of (I).

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