Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

1-Phenylaceanthrylene-2,6-dione

Zhe Li,[a] Hoong-Kun Fun,[b]* Suchada Chantrapromma[c]‡ and Jian-Hua Xu[a]

[a]Department of Chemistry, Nanjing University, Nanjing 210093, People's Republic of China, [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c]Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand

‡ Additional correspondence author, email: suchada.c@psu.ac.th.

Correspondence e-mail: hkfun@usm.my

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.008 Å
R factor = 0.069
wR factor = 0.168
Data-to-parameter ratio = 6.8

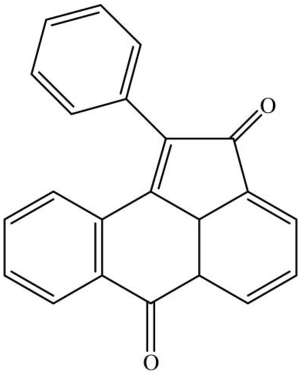
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 13 March 2007
Accepted 5 April 2007

In the title compound, $C_{22}H_{12}O_2$, the aceanthrylene-2,6-dione unit is essentially planar. The dihedral angle between the aceanthrylene system and the phenyl ring is 67.3 (2)°. C—H$\cdots\pi$ interactions involving the phenyl ring are observed in the crystal structure. The molecules are arranged into sheets parallel to the bc plane and stacked in an antiparallel manner along the a axis.

Comment

The photochemistry of quinone compounds is of continuing research interest (Patai & Rappoport, 1988; Thomson, 1997). In continuation of our recent work on photoinduced reactions of quinones with alkynes (Zhang *et al.*, 2000), the title compound, (I), was obtained by the reaction of photoexcited anthraquinone with trimethylsilylphenylethyne. A crystallographic analysis of (I) was carried out to elucidate its structure.


(I)

In the asymmetric unit of (I) (Fig. 1), the aceanthrylene-2,6-dione unit (C1–C16/O1–O2) is essentially planar. The dihedral angle between the aceanthrylene unit and the C17–C22 phenyl ring is 67.3 (2)°. All bond lengths and angles in (I) show normal values (Allen *et al.*, 1987).

The crystal packing (Fig. 2) shows that the molecules are arranged into two-dimensional sheets parallel to the bc plane. These sheets are stacked in an antiparallel manner along the a axis The crystal is stabilized by C—H$\cdots\pi$ interactions involving the phenyl ring (Table 1).

Experimental

Compound (I) was synthesized by a photoinduced reaction between anthraquinone (0.025 M) and an excess amount of 1-trimethylsilyl-2-phenylacetylene in a chloroform solution. The title compound was isolated using silica-gel column chromatography with petroleum ether-ethyl acetate as eluents for gradient elution.. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvents from a petroleum ether–chloroform solution (1:5 *v*/*v*), m.p. 527–528 K.

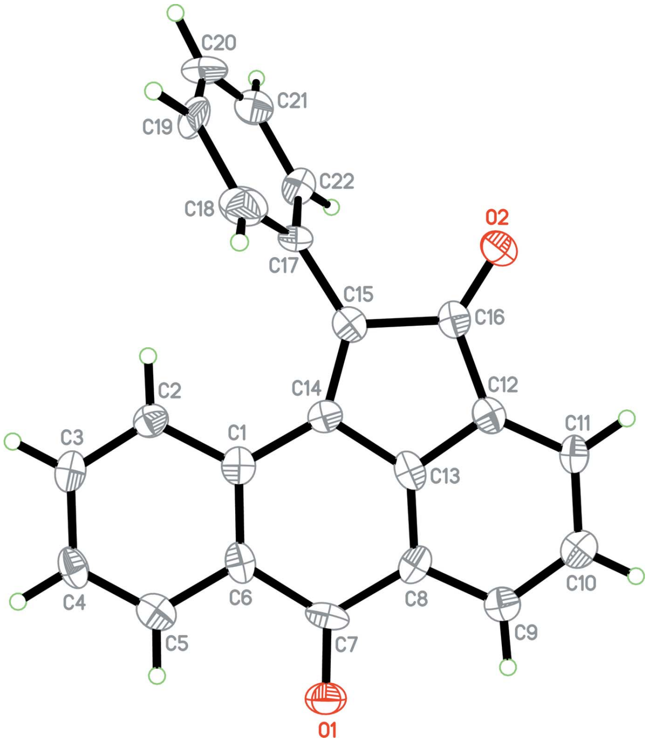


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

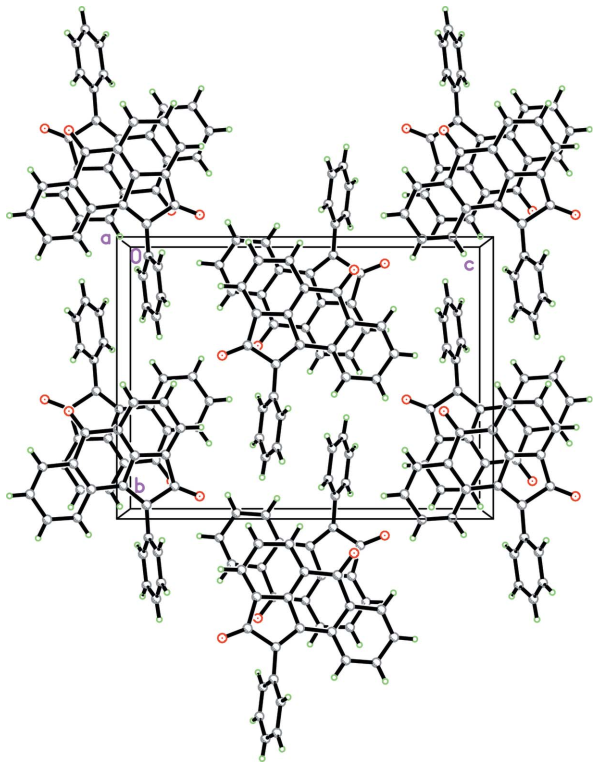


Figure 2
The crystal packing of (I), viewed down the *a* axis.

Crystal data

$C_{22}H_{12}O_2$
$M_r = 308.32$
Orthorhombic, $P2_12_12_1$
$a = 6.7144$ (4) Å
$b = 12.6734$ (7) Å
$c = 16.9009$ (10) Å
$V = 1438.17$ (14) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 100.0$ (1) K
0.26 × 0.13 × 0.08 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\rm min} = 0.977$, $T_{\rm max} = 0.993$
9082 measured reflections
1475 independent reflections
1190 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.168$
$S = 1.09$
1475 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.50$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.21$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C17–22 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19*A*···*Cg*1$^{\rm i}$	0.93	3.11	3.814 (8)	134

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

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). A total of 1044 Friedel pairs were merged before the final refinement as there is no significant anomalous dispersion.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

This work was supported by the National Natural Science Foundation of China and the Natural Science Foundation of Jiangsu Province. The authors also thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Patai, S. & Rappoport, Z. (1988). *The Chemistry of Functional Groups: The Chemstry of the Quinoid Coumpounds.* New York: Wiley.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Thomson, R. H. (1997). *Natural Occurring Quinones*, 4th ed. London/New York: Chapman & Hall.
Zhang, Y., Quian, S.-P., Fun, H.-K. & Xu, J.-H. (2000). *Tetrahedron Lett.* **41**, 8141–8145.

o2500 Li *et al.* • $C_{22}H_{12}O_2$ *Acta Cryst.* (2007). E**63**, o2499–o2500