Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,5-Diacetylanthracene

Ming-Qi Li* and Lin-Hai Jing

Department of Chemistry, China West Normal University, Nanchong 637002, People's Republic of China

Correspondence e-mail: jlhhxg@yahoo.com.cn

Received 30 July 2006
Accepted 9 August 2006

The title molecule, $C_{18}H_{14}O_2$, possesses a crystallographically imposed inversion centre. The carbonyl groups are twisted away from the anthracene mean plane by 21.03 (1)°. The crystal packing is stabilized by C—H···π interactions and C—H···O hydrogen bonds.

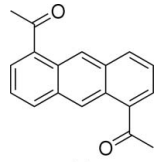
Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.001 Å
R factor = 0.034
wR factor = 0.108
Data-to-parameter ratio = 15.5

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

Comment

1,5-Disubstituted anthracenes constitute a class of intermediates important for applications as monomers in the preparation of triptycene (Wolpaw *et al.*, 2003). We report here the crystal structure of the title compound, (I).



(I)

The molecule of (I) possesses a crystallographically imposed inversion centre (Fig. 1) and shows normal values of bond lengths and angles (Allen et al., 1987). The anthracene ring system is essentially planar, with a maximum deviation from the mean plane of 0.041 (2) Å (atom C2). The carbonyl groups are twisted away from the anthracene mean plane by

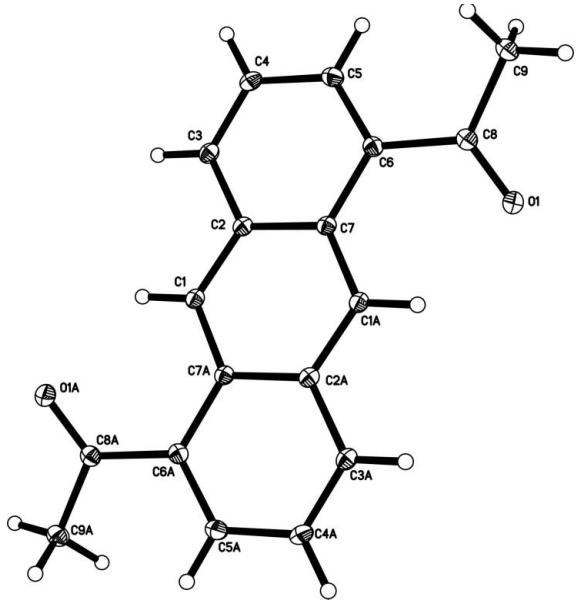


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering [symmetry code: (A) $1-x, 1-y, 1-z$].

21.03 (1)°. The crystal packing is stabilized by the C—H···π interactions and weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the procedure of Wolpaw *et al.* (2003). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from acetone.

Crystal data

$C_{18}H_{14}O_2$
M_r = 262.29
Monoclinic, $P2_1/c$
a = 9.8245 (3) Å
b = 6.2085 (2) Å
c = 10.8823 (3) Å
β = 107.4720 (3)°
V = 633.15 (3) Å^3
Z = 2
D_x = 1.376 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
Block, yellow
0.40 × 0.35 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
5967 measured reflections
1445 independent reflections
1327 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.108
S = 1.02
1445 reflections
93 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.033 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···$Cg1^{i}$	0.95	2.64	3.415 (1)	140
C9—H9C···O1^{ii}	0.98	2.60	3.478 (1)	150

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$. $Cg1$ is the centroid of the C2–C7 ring

All H atoms were placed in calculated positions, with C—H = 0.95 or 0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The methyl groups were allowed to rotate but not to tip.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank the Centre for Testing and Analysis, Cheng Du Branch, Chinese Academy of Sciences, for analytical support.

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 (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Rigaku. (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wolpaw, A. J., Aizer, A. A. & Zimmt, M. B. (2003). *Tetrahedron Lett.* **44**, 7613–7615.