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2,2′-(9,10-Dioxo-9,10-dihydroanthracene-1,8-diyldioxy)bis(*N*,*N*-diethylacetamide)

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Key indicators

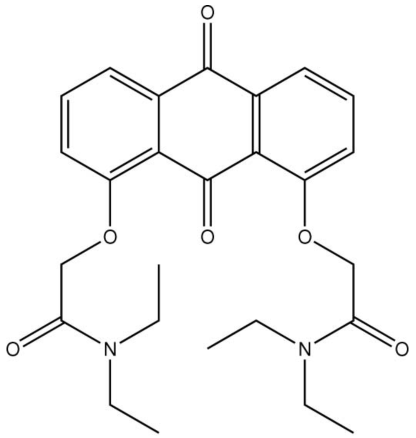
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.048
wR factor = 0.150
Data-to-parameter ratio = 13.6

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

In the title compound, $C_{26}H_{30}N_2O_6$, the anthraquinone ring system is not planar, the dihedral angle between the two benzene rings being 11.18 (13)°. The crystal structure is stabilized by C—H···O hydrogen bonds.

Comment

Anthraquinone derivatives have attracted much attention because of their optical and photosemiconducting properties (Mahajan *et al.*, 2001*a*,*b*). We report here the crystal structure of the title compound, (I) (Fig. 1).



(I)

The dihedral angle between the acetamide C15/C16/N1/O1 plane and the benzene C1–C4/C11/C12 ring is 83.60 (10)° and that between the C21/C22/N2/O2 and C5–C8/C13/C14 planes is 78.19 (12)°. The two benzene rings are not coplanar, the dihedral angle between them being 11.18 (13)°; this is comparable with the value of 10° in 1-(2-tosyloxyethoxy)-8-tosyloxy-9,10-anthraquinone (Bott *et al.*, 1996). The carbonyl atoms O3 and O4 deviate from the anthraquinone mean plane; the dihedral angle between the planes of the C12/C9/C13/O3 and C11/C10/C14/O4 fragments is 17.59 (14)°. Similar deviations from planarity have been reported for several other anthraquinone derivatives (Weber *et al.*, 2004). The crystal packing is stabilized by C—H···O hydrogen bonds (Table 1).

Experimental

To a solution of 1,8-dihydroxyanthraquinone (0.50 g, 2.08 mmol) in dry DMF (10 ml) was added anhydrous Cs_2CO_3 (3.00 g, 9.32 mmol) and the mixture was stirred at room temperature for 15 min. To this mixture was added 2-chloro-*N*,*N*-diethylacetamide (2.326 g, 15.5 mmol) and the reaction mixture was stirred at 353 K for 3 h. Most of the solvent was evaporated under reduced pressure at 353 K and the remaining solution was then cooled to ambient temperature to give (I) as a yellow solid. The crude product (m.p. 405–407 K) was purified by column chromatography with silica gel using methanol–dichloromethane (50:1 *v*/*v*) as eluent. Single crystals suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

Crystal data

$C_{26}H_{30}N_2O_6$
$M_r = 466.52$
Triclinic, $P\overline{1}$
$a = 10.313$ (4) Å
$b = 11.462$ (4) Å
$c = 11.668$ (4) Å
$\alpha = 82.418$ (7)°
$\beta = 74.330$ (7)°
$\gamma = 64.749$ (7)°
$V = 1200.9$ (8) Å^3
$Z = 2$
$D_x = 1.290$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.977$, $T_{\max} = 0.982$
6149 measured reflections
4215 independent reflections
2143 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.150$
$S = 1.00$
4215 reflections
311 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 0.0022P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.14$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O6$^{\rm i}$	0.93	2.46	3.349 (3)	161
C15—H15B···O3$^{\rm ii}$	0.97	2.45	3.380 (3)	162
C21—H21B···O1$^{\rm ii}$	0.97	2.46	3.311 (4)	147

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$.

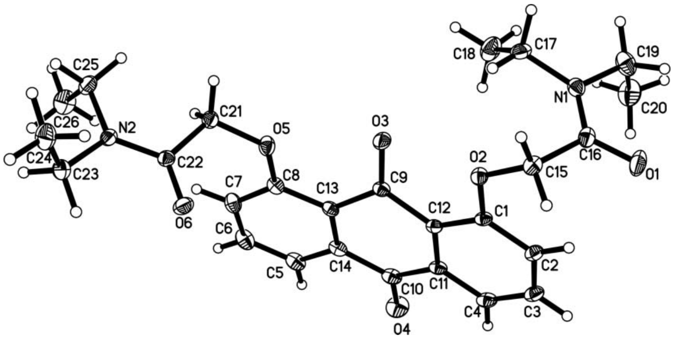


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

H atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C).

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

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o564 Gu *et al.* • $C_{26}H_{30}N_2O_6$ *Acta Cryst.* (2007). E**63**, o563–o564