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10-[2-(9-Anthryloxy)ethyl]-9-acridone

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.125
Data-to-parameter ratio = 13.7

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

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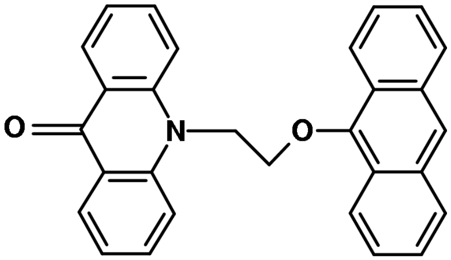
The title compound, $C_{29}H_{21}NO_2$, is an acridone derivative which crystallizes with two almost identical molecules in the asymmetric unit. The angles between the two aromatic planes in the two molecules in the asymmetric unit are 54.22 (3) and 54.04 (3)°.

Comment

Acridone derivatives are well known for their biological properties (Blanchard *et al.*, 1978). They have been reported to be anticancer active and to be applicable as antimicrobial and antiparasitic agents (Nishi *et al.*, 1981). This kind of compound is prepared by condensation of 9(10*H*)-acridinone and alkylhalogen derivatives using phase transfer catalysis. The X-ray structure analysis has been carried out to determine unambiguously the nature of the reaction product.

The title compound, (I), crystallizes with two molecules in the asymmetric unit, which are almost identical. A least-squares fit of all non-H atoms gives an r.m.s. deviation of 0.180 Å. Bond lengths and angles do not show unusual values. The angle between the acridone and the anthracene planes are 54.22 (3) and 54.04 (3)° for the two molecules in the asymmetric unit.



(I)

Experimental

The title compound was prepared in a three-necked flask containing sodium hydroxide (8 g, 200 mmol), triethylbenzylammonium chloride (0.25 g, 1 mmol) and water (25 ml). A solution of 9(10*H*)-acridone (5 mmol) in dichloromethane (125 ml) was added to 2-(9-anthryloxy)ethyl bromide (3 g, 10 mmol). At the end of the addition, the mixture was stirred and cooled in an ice water bath over 5 d. The solution was filtered and neutralized with aqueous hydrochloric acid (50 ml, 10%), sodium bicarbonate (50 ml, 5%) and water. The dichloromethane was removed on a rotary evaporator. The residue, recrystallized from ethyl ether and hexane (2/3), led to yellow crystals.

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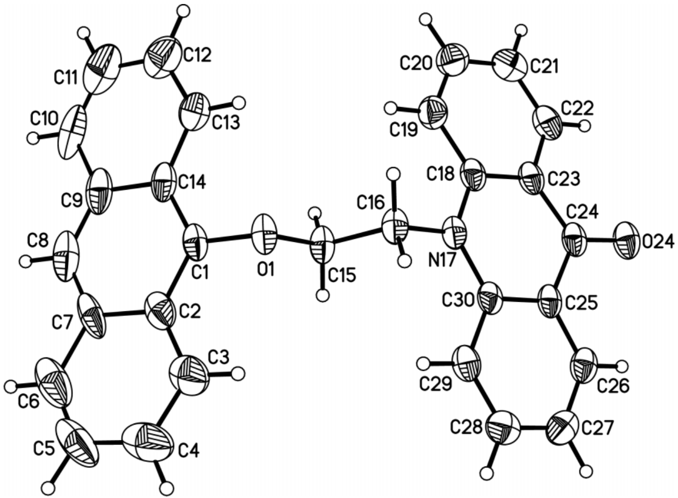

Figure 1
The molecular structure of one of the two molecules of the title compound.

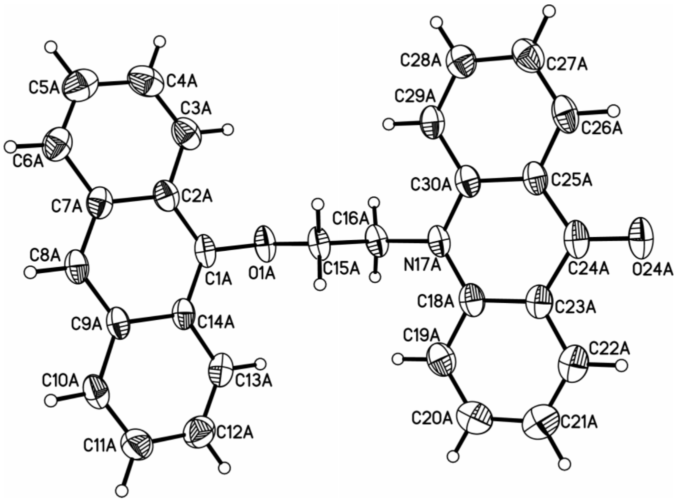

Figure 2
The molecular structure of the second of the two molecules of the title compound.

Crystal data

$C_{29}H_{21}NO_2$
$M_r = 415.47$
Triclinic, $P\overline{1}$
$a = 7.9833$ (6) Å
$b = 14.6168$ (8) Å
$c = 18.744$ (2) Å
$\alpha = 107.180$ (5)°
$\beta = 96.514$ (5)°
$\gamma = 99.570$ (5)°
$V = 2029.7$ (3) Å^3

$Z = 4$
$D_x = 1.360$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 512 reflections
$\theta = 1$–20°
$\mu = 0.09$ mm^{-1}
$T = 173$ (2) K
Plate, yellow
0.51 × 0.38 × 0.14 mm

Data collection

Siemens CCD three-circle diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.958$, $T_{\max} = 0.988$
22 246 measured reflections
7927 independent reflections
4798 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.041$
$\theta_{\max} = 27.1°$
$h = -10 \rightarrow 9$
$k = -18 \rightarrow 17$
$l = -23 \rightarrow 23$
123 standard reflections
frequency: 1440 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.125$
$S = 1.02$
7927 reflections
577 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.2959P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.393 (2)	O1*A*—C1*A*	1.390 (2)
O1—C15	1.435 (2)	O1*A*—C15*A*	1.437 (2)
C16—N17	1.468 (2)	C16*A*—N17*A*	1.466 (2)
N17—C18	1.390 (3)	N17*A*—C18*A*	1.391 (3)
N17—C30	1.396 (2)	N17*A*—C30*A*	1.397 (2)
C24—O24	1.238 (2)	C24*A*—O24*A*	1.244 (2)
C25—C24—C23	115.52 (18)	C25*A*—C24*A*—C23*A*	115.54 (18)

All H atoms were located by difference Fourier synthesis and refined with fixed individual displacement parameters [$U(\rm H) = 1.2U_{\rm eq}(\rm C)$] using a riding model with aromatic C—H = 0.95 Å or methylene C—H = 0.99 Å.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

References

Blanchard, C., Fabre, J.-M., Montginoul, C., Chaffia, B. A., Torreilles, E. & Giral, G. (1978). *J. Heterocycl. Chem.* **15**, 149–153.
Nishi, H., Kohno, H. & Kano, T. (1981). *Bull. Chem. Soc. Jpn*, **54**, 1897–1898.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1991). *SHELXTL-Plus.* Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Siemens (1995). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.