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10-(4-Fluorobenzylidene)anthrone

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.103
Data-to-parameter ratio = 12.8

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

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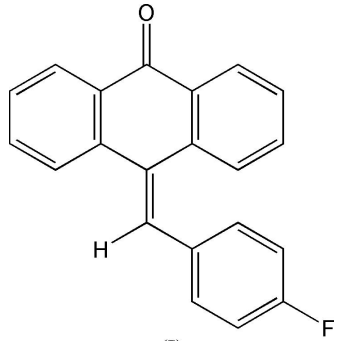
The title compound, $C_{21}H_{13}FO$, was prepared from anthrone and 4-fluorobenzaldehyde. The central six-membered ring has an asymmetric boat conformation, in which the carbonyl C and the opposite C atom deviate from the plane of the other four atoms by 0.173 (2) and 0.319 (2) Å, respectively.

Comment

It has been reported recently that derivatives of 10-substituted anthrone have a high potential for anticancer activity (Paull *et al.*, 1992). In a continuation of our work on the structure–activity relationships (SAR) of derivatives of 10-substituted anthrone (Hu & Zhou, 2004), we obtained crystals of the title compound, (I), which were prepared by reacting anthrone with 4-fluorobenzaldhyde. The structure of the product was determined by X-ray diffraction.



(I)

The molecular structure of (I) is illustrated in Fig. 1. Selected bond lengths and angles are listed in Table 1. Atoms C11–C14 are coplanar within 0.0055 (7) Å, while atoms C5 and C10 deviate from this plane by 0.173 (2) and 0.319 (2) Å, respectively.

Experimental

To a mixture of anthrone (4.0 g, 20 mmol) and 4-fluorobenzaldhyde (3.0 g, 24 mmol) were added pyridine (30 ml) and piperidine (0.5 g, 6 mmol). The reaction mixture was refluxed for 6 h. The completion of the reaction of the anthrone was confirmed by thin-layer chromatography. The mixture was cooled to room temperature, poured into methanol (75 ml) and put in a refrigerator overnight. The precipitate was collected and recrystallized twice from acetic acid to afford yellow crystals (1.4 g, yield 23.3%, m.p. 378–381 K).

Crystal data

$C_{21}H_{13}FO$
$M_r = 300.31$
Monoclinic, $P2_1/c$
$a = 10.044\ (6)$ Å
$b = 11.398\ (3)$ Å
$c = 13.820\ (3)$ Å
$\beta = 109.79\ (4)^\circ$
$V = 1488.7\ (10)$ Å^3
$Z = 4$
$D_x = 1.340$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.1$–12.7°
$\mu = 0.09$ mm^{-1}
$T = 296\ (2)$ K
Prism, colorless
$0.50 \times 0.40 \times 0.40$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3137 measured reflections
2673 independent reflections
2026 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 25.2^\circ$
$h = 0 \rightarrow 12$
$k = -1 \rightarrow 13$
$l = -16 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.103$
$S = 1.04$
2673 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.247P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0058 (11)

Table 1
Selected geometric parameters (Å, °).

F1—C19	1.3598 (19)	C5—C15	1.338 (2)
O1—C10	1.2209 (17)	C15—C16	1.470 (2)
C15—C5—C13	125.88 (13)	O1—C10—C12	121.76 (14)
C15—C5—C14	118.82 (12)	C17—C16—C15	118.41 (13)
O1—C10—C11	121.44 (14)	C21—C16—C15	123.65 (13)
C13—C5—C15—C16	4.4 (2)	C5—C15—C16—C17	−146.85 (16)
C14—C5—C15—C16	−171.30 (14)	C5—C15—C16—C21	37.3 (2)

The H atoms were placed in calculated positions (C—H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}$(parent atom).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); 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: *SHELXL97*.

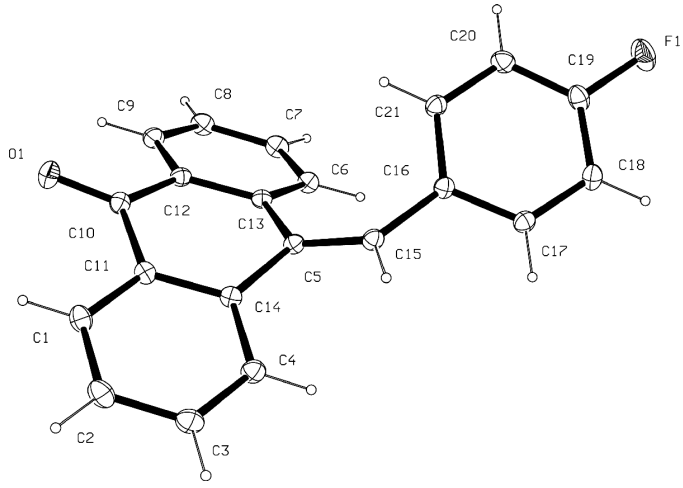


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids.

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