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10-Fluoro-6,7-dihydro-5*H*-benzo[6,7]cyclohepta[1,2-*b*]quinoline

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In the title compound, $C_{18}H_{14}FN$, the quinoline and benzene rings are essentially planar, and the two aromatic ring planes make a dihedral angle of 46.3 (1)°. The cycloheptane ring adopts a half-chair conformation.

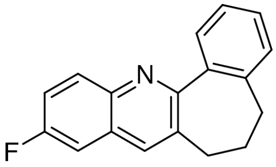
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.148
Data-to-parameter ratio = 18.2

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

Comment

Polycyclic aromatic hydrocarbons (PAHs) are well known environmental pollutants (Dong *et al.*, 1977; Harvey, 1991) and have been intensively investigated in carcinogenic studies (Harvey, 1991). Interestingly, the introduction of one F atom at a particular position has a significant effect on the carcinogenic activity of the PAHs (Harvey & Cortez, 1997; Zajc, 1999). Pan *et al.* (2001) focus on the synthesis, characterization and bioactivity of fluoro-polycyclic azaarenes (PAAs) in order to extend the carcinogenic studies, and have isolated the title compound, (I). An X-ray structure determination of (I) was undertaken to establish the conformation of the structure.



(I)

In compound (I), the bond lengths and angles show normal values and agree with those observed in a chloro-derivative of the same structure (Ray *et al.*, 1998). The cycloheptane ring adopts a half-chair conformation with an approximate twofold axis through the C10 atom and bisecting the C17—C18 bond. This is confirmed by its puckering parameters (Cremer & Pople, 1975) Q_2 = 1.032 (2) Å, φ_2 = 65.4 (1)°, Q_3 = 0.122 (2) Å, φ_3 = 324.4 (9)° and Q_T = 1.039 (2) Å. In the quinoline ring, the C2—C3, C4—C5 and C7—C8 bond distances are slightly shorter due to their localized double-bond character, while the N1—C5 bond shows partial double-bond character (Allen *et al.*, 1987). The quinoline and benzene rings are essentially planar to within ±0.007 (2) Å and to within ±0.005 (2) Å, respectively, while atom F1 deviates slightly from the quinoline plane by −0.018 (1) Å. The quinoline and benzene ring planes make a dihedral angle of 46.3 (1)°.

Experimental

The treatment of Vilsmeir–Haack reagent (phosphoryl chloride/dimethylformamide) with benzosuberone produced the β-chlorovinylaldehyde as an oil. This product was treated with p-fluoroaniline (freshly distilled) to afford the corresponding anil derivative as a red solid. After heating the anil derivative at 503–513 K for 5 min, the title compound, (I), was obtained. Single crystals suitable for X-ray structure determination were obtained by slow evaporation from a chloroform–petroleum ether solution.

Crystal data

$C_{18}H_{14}FN$
$M_r = 263.30$
Monoclinic, $P2_1/c$
$a = 8.4871$ (2) Å
$b = 10.0561$ (2) Å
$c = 16.0181$ (1) Å
$\beta = 96.536$ (1)°
$V = 1358.21$ (4) Å^3
$Z = 4$

$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4222 reflections
$\theta = 2.4$–28.3°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.48 × 0.44 × 0.28 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
9310 measured reflections
3305 independent reflections
1784 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.071$
$\theta_{\rm max} = 28.3°$
$h = -6 \rightarrow 11$
$k = -13 \rightarrow 10$
$l = -19 \rightarrow 20$
Intensity decay: negligible

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.148$
$S = 0.90$
3305 reflections
182 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.28$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.046 (4)

Table 1
Selected geometric parameters (Å, °).

N1—C18	1.323 (2)	C5—C6	1.412 (2)
N1—C1	1.370 (2)	C6—C7	1.409 (2)
F1—C4	1.366 (2)	C7—C8	1.363 (2)
C1—C2	1.411 (2)	C8—C18	1.431 (2)
C1—C6	1.416 (2)	C8—C9	1.507 (2)
C2—C3	1.358 (3)	C12—C17	1.400 (2)
C3—C4	1.385 (3)	C17—C18	1.487 (2)
C4—C5	1.344 (3)		
C18—N1—C1	118.55 (13)	C9—C10—C11	112.99 (15)
C2—C1—C6	119.06 (15)	C16—C17—C12	119.66 (15)
C5—C4—F1	118.93 (16)	C12—C17—C18	121.01 (14)
C8—C7—C6	120.92 (14)	C8—C18—C17	119.40 (15)
C18—C8—C9	120.16 (15)		
C11—C12—C13—C14	177.52 (16)	C16—C17—C18—N1	44.5 (2)
C9—C8—C18—N1	−176.58 (15)	C12—C17—C18—N1	−134.56 (16)

After checking their presence in a difference map, all H atoms were geometrically fixed and allowed to ride on their attached atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

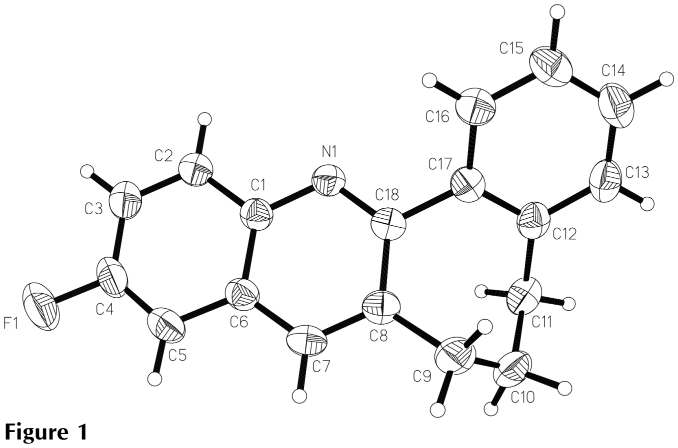


Figure 1
The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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