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9-(2-Pyridylmethyl)carbazole

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.131
Data-to-parameter ratio = 13.4

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

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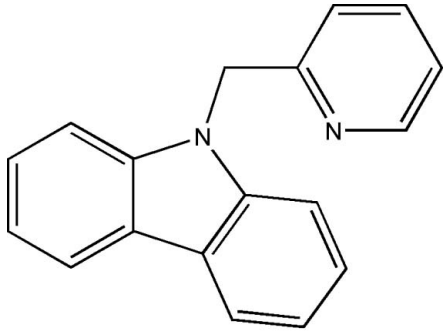
In the title compound, $C_{18}H_{14}N_2$, the carbazole and pyridine ring systems are each essentially planar. The asymmetric unit contains three independent molecules. The molecular structure is stabilized by an intermolecular C—H···N hydrogen bond.

Comment

Carbazole derivatives containing alkylpyridines possess valuable therapeutic properties. In some cases they are able to potentiate the analgesic effect without substantially influencing blood pressure and the vegetative nervous system (Chemische Fabrik Promonta GmbH, 1959). *N*-Alkylation is one of the important processes for the construction of carbazole derivatives. In this paper, the structure of the title compound, (I), is reported. The structure of the related compound 9-(3-pyridylmethyl)carbazole was reported by Duan *et al.* (2004).



(I)

The asymmetric unit of (I) consists of three molecules (Fig. 1). The carbazole ring systems containing N1, N3 and N5 are each essentially planar, with mean deviations of 0.009 (4), 0.019 (5) and 0.022 (4) Å, respectively. The dihedral angles between these carbazole ring systems and the corresponding pyridine rings are 95.9 (3), 91.2 (4) and 81.8 (3)°, respectively. The bond lengths and angles are in agreement with reported literature values (Allen *et al.*, 1987). The crystal structure is stabilized by an intermolecular C—H···N hydrogen bond (Table 1 and Fig. 2).

Experimental

A solution of potassium hydroxide (7.0 g) in dimethylformamide (DMF, 50 ml) was stirred at room temperature for 20 min. Carbazole (3.3 g, 20 mmol) was added and stirring continued for a further 40 min. A solution of 2-chloromethylpyridine hydrochloride (5.0 g,

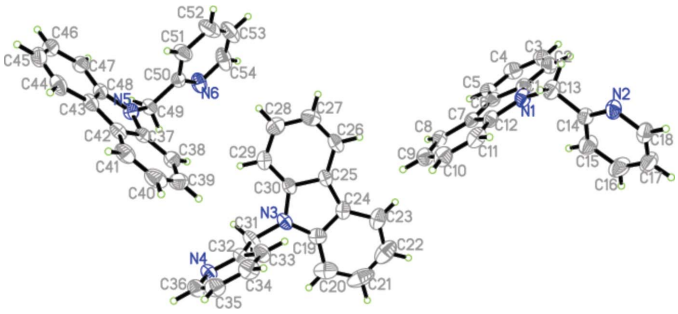


Figure 1
A view of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level.

30 mmol) in DMF (50 ml) was added dropwise with stirring. The resulting mixture was then stirred at room temperature for 12 h, poured into water (500 ml), and a white precipitate was obtained. The solid product was filtered off, washed with cool water and recrystallized from EtOH, giving crystals of (I) (yield: 4.32 g, 90.4%; m.p. 392.0–393.3 K). (I) (20 mg) was dissolved in chloroform (6 ml) and the solution was kept at room temperature for 10 d. Natural evaporation gave colorless single crystals suitable for X-ray diffraction.

Crystal data

$C_{18}H_{14}N_2$
$M_r = 258.31$
Triclinic, $P\overline{1}$
$a = 9.8420\ (16)$ Å
$b = 12.501\ (2)$ Å
$c = 17.696\ (3)$ Å
$\alpha = 80.269\ (3)^\circ$
$\beta = 81.207\ (3)^\circ$
$\gamma = 76.412\ (3)^\circ$
$V = 2071.2\ (6)$ Å^3
$Z = 6$
$D_x = 1.243$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3015 reflections
$\theta = 2.4$–22.3°
$\mu = 0.07$ mm^{-1}
$T = 294\ (2)$ K
Block, colourless
0.30 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.960$, $T_{max} = 0.988$
10635 measured reflections
7266 independent reflections
4202 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0^\circ$
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 14$
$l = -18 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.131$
$S = 1.05$
7266 reflections
541 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.1491P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

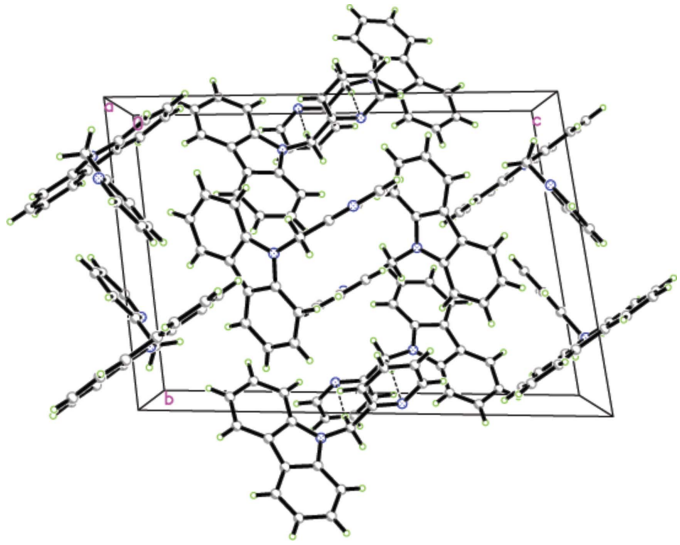


Figure 2
A packing diagram of (I), viewed down the *a* axis. Dashed lines indicate C—H···N hydrogen bonds.

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

D—H···A	D—H	H···A	D···A	D—H···A
C49—H49A···N6^{i}	0.97	2.48	3.445 (3)	172

Symmetry code: (i) $-x, -y, -z+1$.

H atoms were positioned geometrically (C—H = 0.93 or 0.97 Å) and refined in a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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