Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9-(3-Pyridylmethyl)carbazole

Xue-Min Duan, Li-Gong Chen,* Yan-Jie Xu, Yang Li, Juan Han and Le-Ping Li

College of Pharmaceuticals and Biotechnology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: dxmlhp@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.096
Data-to-parameter ratio = 9.4

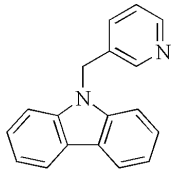
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 21 September 2004
Accepted 29 September 2004
Online 9 October 2004

The title compound, $C_{18}H_{14}N_2$, was synthesized by *N*-alkylation of 3-chloromethylpyridine hydrochloride with carbazole. The carbazole ring system is essentially planar and makes a dihedral angle of 87.9 (3)° with the plane of the pyridine ring.

Comment

Carbazole derivatives substituted by alkylpyridines possess valuable therapeutic properties. In some cases, they are able to potentiate the analgesic effect of, for example, morphine without substantially influencing the blood pressure and the vegetative nervous system (Chemische Fabrik Promonta GmbH, 1959). *N*-Alkylation is one of the important routes in the synthesis of carbazole derivatives.



(I)

In this paper, the structure of 9-(3-pyridylmethyl)carbazole, (I), is reported. It was synthesized by *N*-alkylation of 3-chloromethylpyridine hydrochloride with carbazole.

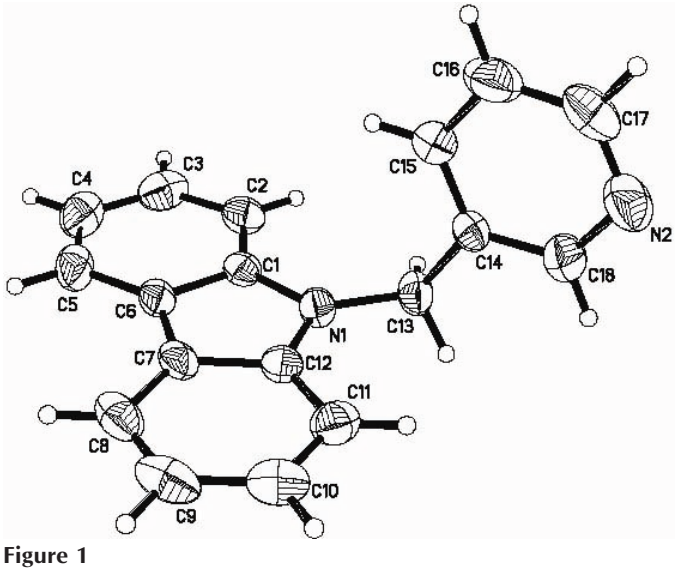


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

The molecular structure of (I) is illustrated in Fig. 1. The carbazole ring system is essentially planar, with a mean deviation of 0.003 Å. The dihedral angle between the pyridine plane and the plane of the carbazole ring system is 87.9 (3)°. The bond lengths and angles are in agreement with reported literature values (Allen *et al.*, 1987).

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 the mixture stirred for a further 40 min. A solution of 3-chloromethylpyridine hydrochloride (5.0 g, 30 mmol) in DMF (50 ml) was added dropwise with stirring. The resulting mixture was then stirred at room temperature for 12 h and poured into water (500 ml), yielding a white precipitate. The solid product was filtered off, washed with cold water and recrystallized from EtOH, giving crystals of (I) (yield 4.48 g, 93.7%; m.p. 389–390 K). ^{1}H NMR (p.p.m.): 5.52 (*s*, 2H), 7.10–7.47 (*m*, 8H), 8.14 (*d, J* = 4.1 Hz, 2H), 8.49 (*dd, J*$_1$ = 4.8, *J*$_2$ = 1.5 Hz, 1H), 8.61 (*d, J* = 0.9 Hz, 1H). 20 mg of (I) was dissolved in chloroform (6 ml) and the solution kept at room temperature for 10 d. Natural evaporation gave colorless single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{18}H_{14}N_2$
M_r = 258.31
Orthorhombic, $P2_12_12_1$
a = 5.0299 (12) Å
b = 9.777 (2) Å
c = 28.007 (8) Å
V = 1377.4 (6) Å^3
Z = 4
D_x = 1.246 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 773 reflections
θ = 2.9–23.8°
μ = 0.07 mm^{-1}
T = 293 (2) K
Rod, colorless
0.40 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
7998 measured reflections
1698 independent reflections
1288 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 26.5°
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 8$
$l = -34 \rightarrow 35$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.096
S = 1.07
1698 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.1963P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

In the absence of significant anomalous dispersion effects, Friedel pairs were averaged. H atoms were positioned geometrically, with Csp^2—H = 0.93 Å and Csp^3—H = 0.97 Å, and refined with a riding model, with U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–19.
Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chemische Fabrik Promonta GmbH (1959). GB Patent: 822 592.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.