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9-(4-Methylbenzyl)-9*H*-carbazole

Jian-Lan Cui,[a]* Peng-Mian Huang[b] and Wen-Long Guo[a]

[a]Department of Chemical Engineering, North University of China, Taiyuan 030051, People's Republic of China, and [b]School of Chemical Engineering and Techology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: cuijianlan2005@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.091
Data-to-parameter ratio = 9.3

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

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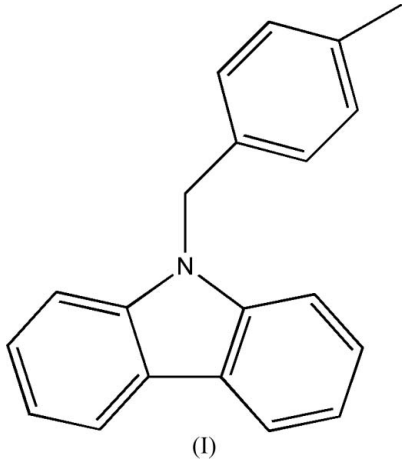
The title compound, $C_{20}H_{17}N$, was synthesized by *N*-alkylation of 1-chloromethyl-4-methylbenzene with carbazole. The carbazole ring system is essentially planar, with a mean deviation of 0.029 Å, and makes a dihedral angle of 109 (5)° with the plane of the benzene ring.

Comment

Carbazole derivatives substituted by *N*-alkylation exhibit useful pharmaceutical properties (Buu-Hoï & Royer, 1950; Harfenist & Joyner, 1983; Caulfield *et al.*, 2002; Harper *et al.*, 2002). In this paper, the structure of 9-(4-methyl-benzyl)-9*H*-carbazole (I) is reported, which was synthesized by *N*-alkylation of 1-chloromethyl-4-methylbenzene with carbazole.



(I)

The carbazole ring system is essentially planar, with a mean deviation of 0.029 Å. The dihedral angle formed between the carbazole ring system and the methylbenzyl ring is 109 (5)°.

Experimental

The title compound was prepared according to the procedure of Duan *et al.* (2005). A solution of potassium hydroxide (7.0 g) in dimethylformamide (50 ml) was stirred at room temperature for 20 min. Carbazole (3.34 g, 20 mmol) was added and the mixture stirred for a further 40 min. A solution of 1-chloromethyl-4-methylbenzene (4.23 g, 30 mmol) in dimethylformamide (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: 4.89 g (90.2%); m.p. 390 K. Compound (I) (40 mg) was dissolved in a mixture of chloroform (5 ml) and ethanol (5 ml) and the solution was kept at room temperature for 18 d. Natural evaporation of the solution gave colourless crystals suitable for X-ray analysis.

Crystal data

$C_{20}H_{17}N$
M_r = 271.35
Orthorhombic, $P2_12_12_1$
a = 5.6128 (10) Å
b = 13.627 (3) Å
c = 19.442 (4) Å
V = 1487.0 (5) Å^3
Z = 4
D_x = 1.212 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2354 reflections
θ = 2.6–24.7°
μ = 0.07 mm^{-1}
T = 294 (2) K
Rod, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.978, T_{max} = 0.993
8438 measured reflections
1783 independent reflections
1305 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.5°
$h = -7 \rightarrow 6$
$k = -17 \rightarrow 13$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
S = 1.05
1783 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.0342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

All H atoms were included in the riding model approximation with C—H distances = 0.93 (aromatic), 0.96 (methyl) and 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

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*.

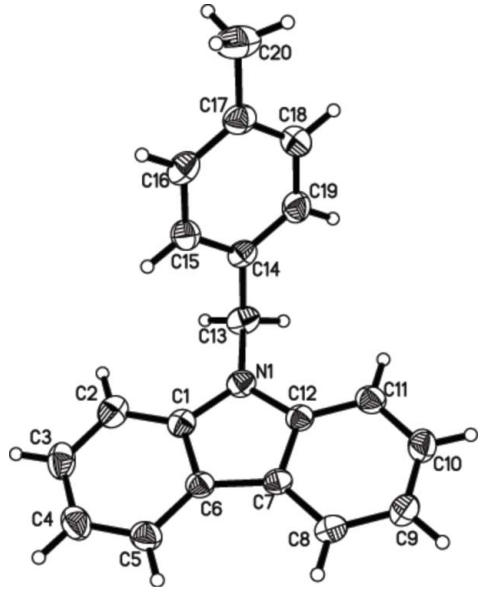


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

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