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3,6-Dibromo-9-hexyl-9*H*-carbazole

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.009 Å
R factor = 0.047
wR factor = 0.117
Data-to-parameter ratio = 17.5

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

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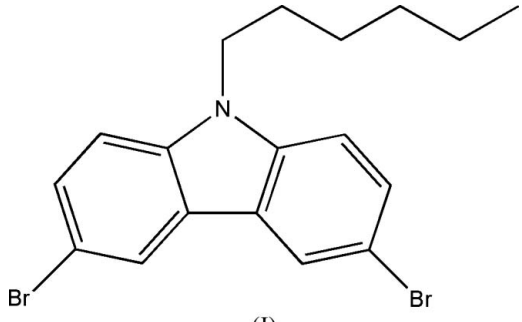
The title compound, $C_{18}H_{19}Br_2N$, was synthesized by *N*-alkylation of 1-bromohexane with 3,6-dibromo-9*H*-carbazole. The carbazole ring system is essentially planar and the *n*-hexyl chain is in the fully extended conformation.

Comment

Carbazole derivatives substituted by *N*-alkylation possess valuable pharmaceutical properties (Buu-Hoï & Royer, 1950; Harfenist & Joyner, 1983; Caulfield *et al.*, 2002; Harper *et al.*, 2002). In this paper, the structure of 3,6-dibromo-9-hexyl-9*H*-carbazole, (I), is reported, which was synthesized by *N*-alkylation of 1-bromohexane with 3,6-dibromo-9*H*-carbazole.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The carbazole ring system is essentially plannar, with an r.m.s. deviation of 0.0106 Å. The C—Br distances, in the range 1.911 (6)–1.923 (7) Å, are not statistically different from the literature value of 1.883 Å (Allen *et al.*, 1987).

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. 3,6-Dibromocarbazole (6.5 g, 20 mmol), prepared according to the method of Smith *et al.* (1992), was added and the mixture stirred for a further 40 min. A solution of 1-bromohexane (4.95 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 6.91 g, 84.5%; m.p. 373–375 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 16 d. Natural evaporation of the solution gave colourless crystals suitable for X-ray analysis.

Crystal data

$C_{18}H_{19}Br_2N$
M_r = 409.16
Orthorhombic, $Pca2_1$
a = 20.337 (3) Å
b = 4.5710 (6) Å
c = 18.456 (3) Å
V = 1715.6 (4) Å^3
Z = 4
D_x = 1.584 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2405 reflections
θ = 2.2–21.8°
μ = 4.72 mm^{-1}
T = 294 (2) K
Rod, colourless
0.24 × 0.22 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan *SADABS* (Bruker, 1997)
T_{min} = 0.320, T_{max} = 0.517
8839 measured reflections
3345 independent reflections
2056 reflections with $I > 2\sigma(I)$
R_{int} = 0.080
θ_{max} = 26.4°
$h = -25 \rightarrow 19$
$k = -5 \rightarrow 5$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.117
S = 1.01
3345 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}
Absolute structure: Flack (1983), with 1529 Friedel Pairs
Flack parameter: −0.006 (17)

All H atoms were included in the riding-model approximation, with C—H distances of 0.93 (aromatic) and 0.97 (methylene) Å, and 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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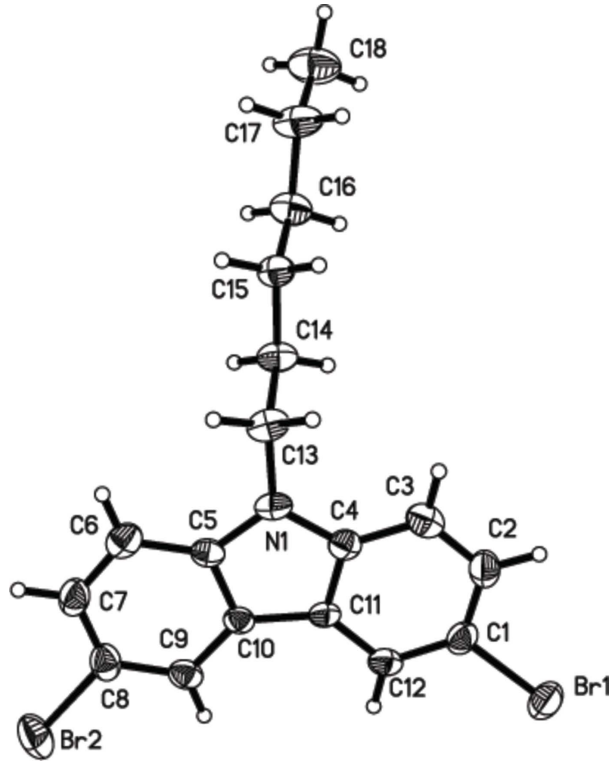

Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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