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9-Allyl-3,6-dibromo-9*H*-carbazole

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.088
Data-to-parameter ratio = 17.3

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

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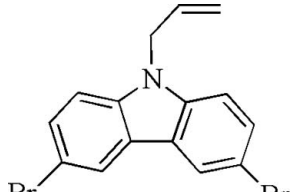
The title compound, $C_{15}H_{11}Br_2N$, was synthesized by *N*-alkylation of 3-bromopropene with 3,6-dibromo-9*H*-carbazole. The carbazole ring system is essentially planar and perpendicular to the pendant allyl substituent.

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 9-allyl-3,6-dibromo-9*H*-carbazole, (I), is reported. It was synthesized by *N*-alkylation of 3-bromopropene with 3,6-dibromo-9*H*-carbazole. The carbazole ring system is essentially planar, with a mean deviation of 0.0082 Å from the plane, consistent with recent determinations of similar structures (Huang *et al.*, 2005; Duan, Huang *et al.*, 2005). The angle between the carbazole ring system and the plane of the allyl group is 89.8 (3)°. The C—Br distances are 1.908 (4) and 1.910 (4) Å, consistent with the literature (Allen *et al.*, 1987).



(I)

Experimental

The title compound, (I), was prepared as described by Duan, Han *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 as in Smith *et al.* (1992), was added and the mixture stirred for a further 40 min. A solution of 3-bromopropene (3.63 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 6.53 g, 89.5%; m.p. 376–378 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

$C_{15}H_{11}Br_2N$	D_x = 1.778 Mg m^{-3}
M_r = 365.07	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2800 reflections
a = 8.6763 (12) Å	θ = 3.0–25.2°
b = 10.6439 (15) Å	μ = 5.93 mm^{-1}
c = 15.7934 (18) Å	T = 294 (2) K
β = 110.803 (6)°	Block, colourless
V = 1363.4 (3) Å^3	0.26 × 0.24 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2837 independent reflections
	2088 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.027
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	θ_{max} = 26.6°
	$h = -10 \rightarrow 8$
T_{min} = 0.228, T_{max} = 0.306	$k = -11 \rightarrow 13$
7598 measured reflections	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.9467P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.035	
$wR(F^2)$ = 0.088	
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
2837 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXTL*
	Extinction coefficient: 0.0155 (9)

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

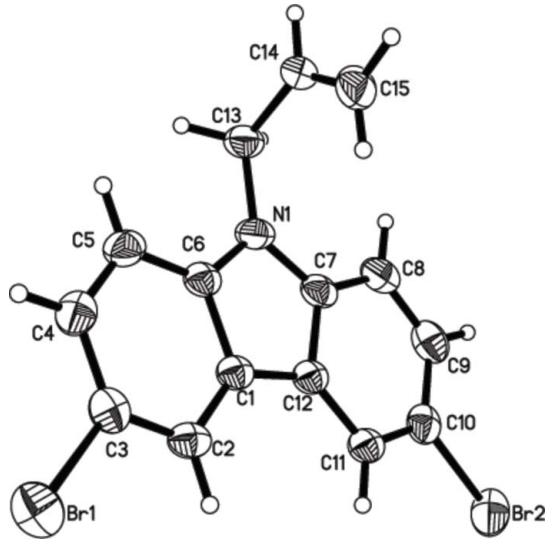


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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