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

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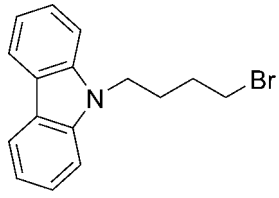
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; R factor = 0.050; wR factor = 0.145; data-to-parameter ratio = 15.1.

In the title compound, $C_{16}H_{16}BrN$, the bromobutyl group lies on one side of the carbazole ring plane and has a zigzag shape. The dihedral angle between the two benzene rings is 0.55°. In the crystal, molecules are connected by van der Waals interactions.

Related literature

For charge-transport properties and π-conjugated systems in carbazoles, see: Zhang *et al.* (2010*a*). For the bioactivity of carbazole derivatives, see: Yan *et al.* (2011). For the synthesis of the title compound, see: Zhang *et al.* (2010*b*).



Experimental

Crystal data

$C_{16}H_{16}BrN$ M_r = 302.20
Orthorhombic, *Pbca*
a = 7.696 (3) Å
b = 22.658 (8) Å
c = 16.030 (6) Å
V = 2795.3 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 296 K
0.35 × 0.33 × 0.32 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.428, T_{max} = 0.455
13981 measured reflections
2460 independent reflections
1252 reflections with $I > 2\sigma(I)$
R_{int} = 0.094

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.145
S = 0.97
2460 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2343).

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Yan, J.-P., Zhou, C.-H., Ji, Q.-G. & Geng, R.-X. (2011). *Int. J. Pharm. Res.* **38**, 118–122.
Zhang, F.-F., Gan, L.-L. & Zhou, C.-H. (2010*b*). *Bioorg. Med. Chem. Lett.* **20**, 1881–1884.
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supplementary materials

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Comment

Carbazole and its derivatives as an important type of aromatic compounds are being actively investigated for their special structural characteristics with desirable electronic charge-transport properties and π-conjugated system (Zhang *et al.*, 2010*a*). Large amount of bioactive carbazole derivatives have been reported to exert diverse biological activities such as antitumor, antimicrobial, antihistaminic, antioxidative, anti-inflammatory ones and so on (Yan *et al.*, 2011). Our interest is to develop novel carbazole compounds as medicinal agents. Herein, the molecular structure of the title compound, **I**, is reported.

The X-ray analysis of **I** shows that the carbon C4 and carbazole moiety (N1/C5–C16) belong to the same plane. The bromobutyl moiety lies in the same side of the carbon plane.

Experimental

The title compound was synthesized according to the procedure of Zhang *et al.* (2010*b*). Single crystals were grown by slow evaporation of a solution of **I** in $CHCl_3$ at room temperature.

Refinement

H atoms were placed at calculated positions with C—H = 0.93Å (aromatic) and 0.97Å (methylene). The U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

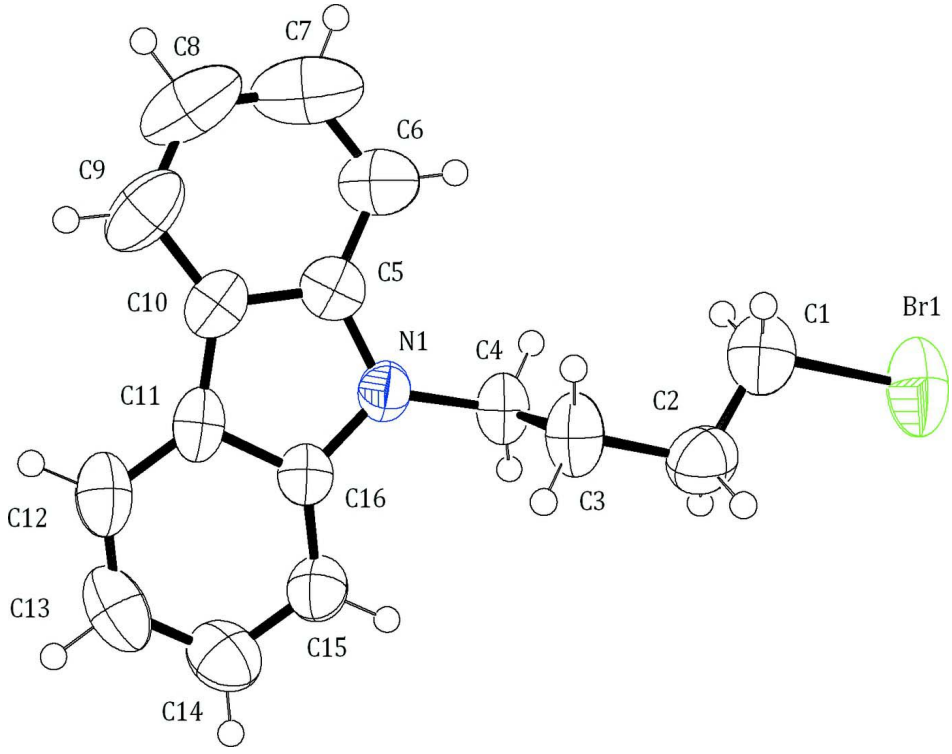

Figure 1

The molecular structure of **I**, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

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

Crystal data

$C_{16}H_{16}BrN$
$M_r = 302.20$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 7.696$ (3) Å
$b = 22.658$ (8) Å
$c = 16.030$ (6) Å
$V = 2795.3$ (18) Å^3
$Z = 8$
$F(000) = 1232$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1683 reflections
$\theta = 2.2$–$20.5°$
$\mu = 2.92$ mm^{-1}
$T = 296$ K
Block, colourless
0.35 × 0.33 × 0.32 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.428$, $T_{max} = 0.455$
13981 measured reflections
2460 independent reflections
1252 reflections with $I > 2\sigma(I)$
$R_{int} = 0.094$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -9 \rightarrow 9$
$k = -26 \rightarrow 23$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.145$
$S = 0.97$
2460 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	1.17750 (8)	0.51102 (3)	0.14901 (4)	0.0961 (4)
N1	0.4563 (4)	0.63416 (15)	0.0682 (2)	0.0503 (9)
C1	0.9838 (6)	0.5506 (2)	0.0916 (3)	0.0804 (16)
H1A	1.0214	0.5640	0.0371	0.097*
H1B	0.8887	0.5230	0.0840	0.097*
C2	0.9256 (7)	0.6005 (2)	0.1406 (3)	0.0728 (15)
H2A	1.0216	0.6275	0.1495	0.087*
H2B	0.8853	0.5869	0.1946	0.087*
C3	0.7738 (6)	0.6334 (2)	0.0939 (3)	0.0710 (16)
H3A	0.7660	0.6736	0.1143	0.085*
H3B	0.7995	0.6349	0.0347	0.085*
C4	0.6020 (6)	0.60279 (19)	0.1069 (3)	0.0589 (12)
H4A	0.6086	0.5633	0.0837	0.071*
H4B	0.5804	0.5991	0.1662	0.071*
C5	0.3858 (6)	0.6217 (2)	−0.0087 (3)	0.0534 (12)
C6	0.4334 (8)	0.5788 (2)	−0.0656 (3)	0.0744 (15)
H6	0.5249	0.5531	−0.0549	0.089*
C7	0.3397 (11)	0.5757 (3)	−0.1393 (4)	0.107 (2)
H7	0.3692	0.5475	−0.1791	0.128*
C8	0.2017 (10)	0.6140 (4)	−0.1546 (4)	0.106 (3)
H8	0.1403	0.6107	−0.2044	0.127*
C9	0.1550 (7)	0.6562 (3)	−0.0986 (4)	0.0820 (17)
H9	0.0626	0.6815	−0.1095	0.098*
C10	0.2482 (6)	0.6607 (2)	−0.0248 (3)	0.0546 (12)
C11	0.2370 (5)	0.6987 (2)	0.0468 (3)	0.0517 (12)
C12	0.1309 (6)	0.7458 (2)	0.0690 (4)	0.0684 (15)

H12	0.0438	0.7587	0.0331	0.082*
C13	0.1557 (7)	0.7729 (3)	0.1436 (4)	0.0810 (17)
H13	0.0852	0.8046	0.1584	0.097*
C14	0.2847 (7)	0.7542 (2)	0.1985 (4)	0.0744 (16)
H14	0.2990	0.7734	0.2493	0.089*
C15	0.3906 (6)	0.7079 (2)	0.1782 (3)	0.0576 (12)
H15	0.4762	0.6952	0.2150	0.069*
C16	0.3682 (5)	0.68078 (19)	0.1028 (3)	0.0462 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0657 (4)	0.1089 (6)	0.1138 (6)	0.0220 (3)	0.0026 (3)	0.0376 (4)
N1	0.046 (2)	0.051 (2)	0.054 (3)	0.0042 (18)	−0.0053 (18)	0.0027 (19)
C1	0.068 (4)	0.086 (4)	0.087 (4)	0.003 (3)	0.000 (3)	0.013 (3)
C2	0.062 (3)	0.089 (4)	0.068 (4)	−0.010 (3)	0.001 (3)	−0.007 (3)
C3	0.049 (3)	0.070 (3)	0.094 (5)	0.004 (2)	0.000 (3)	0.017 (3)
C4	0.046 (3)	0.059 (3)	0.072 (3)	0.006 (2)	−0.002 (3)	0.011 (3)
C5	0.055 (3)	0.047 (3)	0.058 (3)	−0.011 (2)	0.008 (3)	0.006 (3)
C6	0.101 (4)	0.060 (3)	0.062 (4)	−0.010 (3)	0.003 (3)	0.004 (3)
C7	0.171 (8)	0.082 (5)	0.067 (5)	−0.049 (5)	0.010 (5)	−0.003 (4)
C8	0.151 (7)	0.095 (5)	0.072 (5)	−0.050 (5)	−0.043 (5)	0.022 (4)
C9	0.090 (4)	0.085 (4)	0.071 (4)	−0.030 (3)	−0.028 (4)	0.031 (4)
C10	0.050 (3)	0.060 (3)	0.054 (4)	−0.014 (2)	−0.003 (2)	0.015 (3)
C11	0.036 (2)	0.056 (3)	0.063 (4)	−0.002 (2)	0.003 (2)	0.024 (3)
C12	0.053 (3)	0.074 (4)	0.079 (4)	0.011 (3)	0.007 (3)	0.028 (3)
C13	0.075 (4)	0.071 (4)	0.097 (5)	0.020 (3)	0.030 (4)	0.013 (4)
C14	0.087 (4)	0.077 (4)	0.060 (4)	0.007 (3)	0.018 (3)	0.004 (3)
C15	0.056 (3)	0.067 (3)	0.050 (3)	0.003 (3)	0.003 (2)	0.009 (3)
C16	0.043 (3)	0.049 (3)	0.046 (3)	−0.002 (2)	0.006 (2)	0.010 (2)

Geometric parameters (Å, º)

Br1—C1	1.968 (5)	C6—H6	0.9300
N1—C16	1.372 (5)	C7—C8	1.394 (10)
N1—C5	1.377 (5)	C7—H7	0.9300
N1—C4	1.465 (5)	C8—C9	1.361 (9)
C1—C2	1.447 (7)	C8—H8	0.9300
C1—H1A	0.9700	C9—C10	1.386 (7)
C1—H1B	0.9700	C9—H9	0.9300
C2—C3	1.575 (6)	C10—C11	1.437 (7)
C2—H2A	0.9700	C11—C12	1.391 (7)
C2—H2B	0.9700	C11—C16	1.411 (6)
C3—C4	1.507 (6)	C12—C13	1.358 (7)
C3—H3A	0.9700	C12—H12	0.9300
C3—H3B	0.9700	C13—C14	1.392 (8)
C4—H4A	0.9700	C13—H13	0.9300
C4—H4B	0.9700	C14—C15	1.367 (6)
C5—C6	1.382 (6)	C14—H14	0.9300
C5—C10	1.403 (6)	C15—C16	1.368 (6)

C6—C7	1.386 (8)	C15—H15	0.9300
C16—N1—C5	108.9 (4)	C7—C6—H6	121.3
C16—N1—C4	125.6 (4)	C6—C7—C8	121.0 (7)
C5—N1—C4	125.5 (4)	C6—C7—H7	119.5
C2—C1—Br1	109.7 (4)	C8—C7—H7	119.5
C2—C1—H1A	109.7	C9—C8—C7	121.5 (6)
Br1—C1—H1A	109.7	C9—C8—H8	119.2
C2—C1—H1B	109.7	C7—C8—H8	119.2
Br1—C1—H1B	109.7	C8—C9—C10	118.5 (6)
H1A—C1—H1B	108.2	C8—C9—H9	120.7
C1—C2—C3	110.0 (4)	C10—C9—H9	120.7
C1—C2—H2A	109.7	C9—C10—C5	120.1 (5)
C3—C2—H2A	109.7	C9—C10—C11	133.9 (5)
C1—C2—H2B	109.7	C5—C10—C11	106.0 (4)
C3—C2—H2B	109.7	C12—C11—C16	118.5 (5)
H2A—C2—H2B	108.2	C12—C11—C10	134.4 (5)
C4—C3—C2	111.6 (4)	C16—C11—C10	107.1 (4)
C4—C3—H3A	109.3	C13—C12—C11	119.4 (5)
C2—C3—H3A	109.3	C13—C12—H12	120.3
C4—C3—H3B	109.3	C11—C12—H12	120.3
C2—C3—H3B	109.3	C12—C13—C14	121.3 (5)
H3A—C3—H3B	108.0	C12—C13—H13	119.4
N1—C4—C3	113.0 (4)	C14—C13—H13	119.4
N1—C4—H4A	109.0	C15—C14—C13	120.6 (5)
C3—C4—H4A	109.0	C15—C14—H14	119.7
N1—C4—H4B	109.0	C13—C14—H14	119.7
C3—C4—H4B	109.0	C14—C15—C16	118.6 (4)
H4A—C4—H4B	107.8	C14—C15—H15	120.7
N1—C5—C6	129.1 (5)	C16—C15—H15	120.7
N1—C5—C10	109.5 (4)	C15—C16—N1	129.8 (4)
C6—C5—C10	121.4 (5)	C15—C16—C11	121.6 (4)
C5—C6—C7	117.4 (6)	N1—C16—C11	108.5 (4)
C5—C6—H6	121.3		
Br1—C1—C2—C3	178.5 (3)	C9—C10—C11—C12	−1.1 (9)
C1—C2—C3—C4	80.9 (5)	C5—C10—C11—C12	179.6 (5)
C16—N1—C4—C3	−83.0 (5)	C9—C10—C11—C16	179.2 (5)
C5—N1—C4—C3	96.9 (5)	C5—C10—C11—C16	−0.1 (5)
C2—C3—C4—N1	176.7 (4)	C16—C11—C12—C13	−0.3 (7)
C16—N1—C5—C6	179.6 (4)	C10—C11—C12—C13	180.0 (5)
C4—N1—C5—C6	−0.3 (7)	C11—C12—C13—C14	−0.3 (8)
C16—N1—C5—C10	−0.2 (5)	C12—C13—C14—C15	0.2 (8)
C4—N1—C5—C10	179.8 (4)	C13—C14—C15—C16	0.6 (7)
N1—C5—C6—C7	−180.0 (5)	C14—C15—C16—N1	179.9 (4)
C10—C5—C6—C7	−0.2 (7)	C14—C15—C16—C11	−1.2 (6)
C5—C6—C7—C8	−0.6 (8)	C5—N1—C16—C15	179.2 (4)
C6—C7—C8—C9	0.6 (10)	C4—N1—C16—C15	−0.9 (7)
C7—C8—C9—C10	0.1 (9)	C5—N1—C16—C11	0.2 (4)

C8—C9—C10—C5	−0.9 (7)	C4—N1—C16—C11	−179.9 (3)
C8—C9—C10—C11	179.9 (5)	C12—C11—C16—C15	1.1 (6)
N1—C5—C10—C9	−179.2 (4)	C10—C11—C16—C15	−179.1 (4)
C6—C5—C10—C9	0.9 (7)	C12—C11—C16—N1	−179.8 (3)
N1—C5—C10—C11	0.2 (5)	C10—C11—C16—N1	0.0 (5)
C6—C5—C10—C11	−179.6 (4)		