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9-Benzyl-3-bromo-9*H*-carbazole

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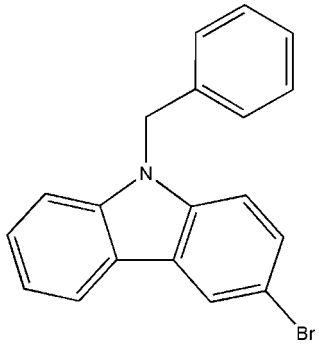
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.036; wR factor = 0.069; data-to-parameter ratio = 18.0.

The title compound, $C_{19}H_{14}BrN$, was synthesized by the *N*-alkylation of (chloromethyl)benzene with 3-bromo-9*H*-carbazole. The carbazole ring system is essentially planar (r.m.s. deviation = 0.013 Å) and forms a dihedral angle of 87.1 (2)° with the phenyl ring.

Related literature

For the synthesis, see: Duan *et al.* (2005). For the pharmaceutical properties of *N*-alkyl carbazoles, see: Buu-Hoï & Royer (1950).



Experimental

Crystal data

$C_{19}H_{14}BrN$
M_r = 336.22
Orthorhombic, $Pna2_1$
a = 17.629 (3) Å
b = 14.666 (2) Å
c = 5.6420 (8) Å
V = 1458.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.81 mm^{-1}
T = 113 K
0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.682, T_{max} = 0.755
14426 measured reflections
3441 independent reflections
2801 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.069
S = 0.98
3441 reflections
191 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 1521 Friedel pairs
Flack parameter: −0.005 (10)

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: HB5016).

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supporting information

Acta Cryst. (2009). E**65**, o1763 [doi:10.1107/S1600536809024969]

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S1. Comment

N-Alkyl carbazoles possess valuable pharmaceutical properties (Buu-Hoï & Royer, 1950). In this paper, the synthesis and the crystal structure of the title compound, (I), is reported.

The carbazole ring is essentially planar, with a r.m.s. deviation from the mean plane of 0.013 Å for the non-hydrogen atoms. The dihedral angle formed between the carbazole unit and the benzene ring is 92.9 (2) Å.

S2. Experimental

The title compound was prepared according to the procedure of Duan *et al.* (2005). The title compound (40 mg) was dissolved in a mixture of chloroform (5 ml) and ethanol (7 ml) and the solution was kept at room temperature for 11 days. Evaporation of the solution gave colourless blocks of (I).

S3. Refinement

All H atoms were included in idealized positions (C—H = 0.95–0.99Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

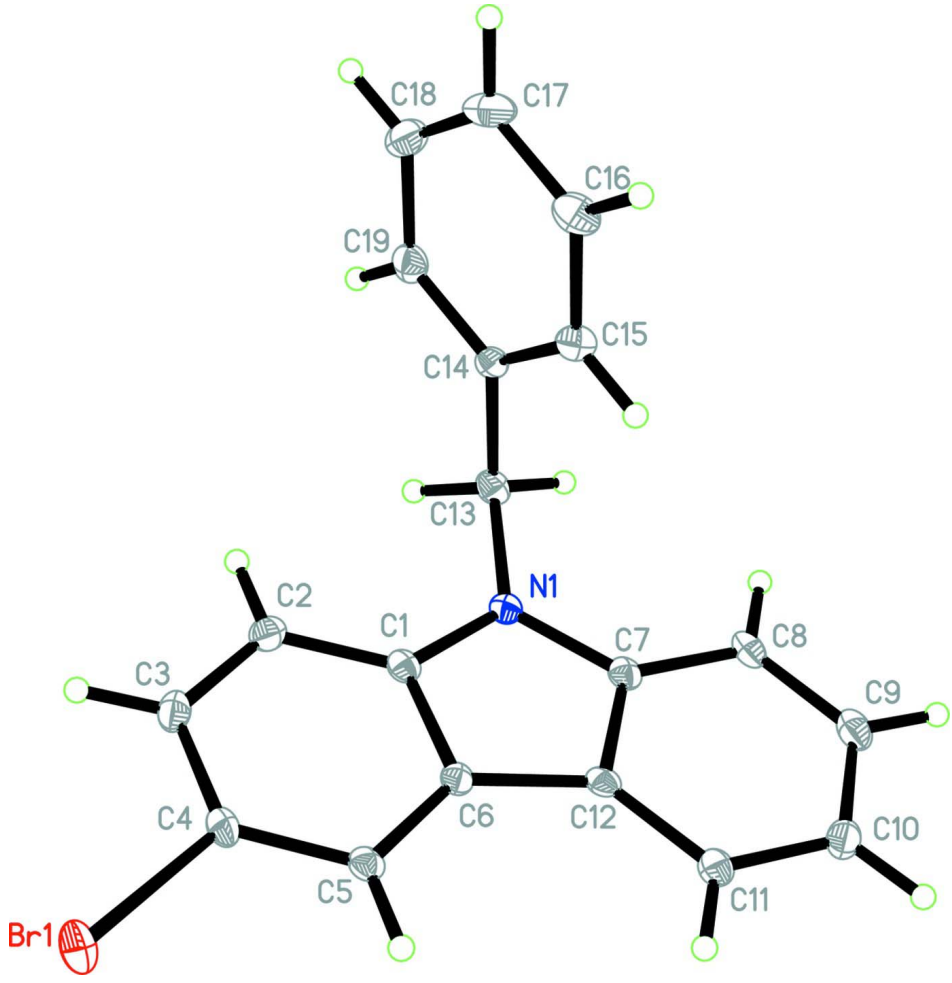

Figure 1

Molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level. H atoms are presented as spheres of arbitrary radius.

9-Benzyl-3-bromo-9*H*-carbazole

Crystal data

$C_{19}H_{14}BrN$
$M_r = 336.22$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 17.629\ (3)$ Å
$b = 14.666\ (2)$ Å
$c = 5.6420\ (8)$ Å
$V = 1458.7\ (4)$ Å^3
$Z = 4$
$F(000) = 680$
$D_x = 1.531$ Mg m^{-3}
Melting point = 392–394 K
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 3798 reflections
$\theta = 1.8$–$27.9°$
$\mu = 2.81$ mm^{-1}
$T = 113$ K
Block, colorless
0.14 × 0.12 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
Radiation source: rotating anode
Confocal multilayer X-ray optic monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.682, T_{max} = 0.755
14426 measured reflections
3441 independent reflections
2801 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.9°, θ_{min} = 1.8°
h = −23→23
k = −19→19
l = −7→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.069
S = 0.98
3441 reflections
191 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0148 (7)
Absolute structure: Flack (1983), 1521 Friedel pairs
Absolute structure parameter: −0.005 (10)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.257493 (13)	0.192950 (18)	0.66598 (14)	0.02943 (11)
N1	0.53686 (13)	0.19508 (14)	0.0539 (4)	0.0196 (5)
C1	0.46874 (12)	0.20289 (15)	0.1699 (6)	0.0180 (5)
C2	0.40547 (16)	0.25415 (17)	0.1164 (5)	0.0229 (7)
H2	0.4049	0.2918	−0.0206	0.027*
C3	0.34289 (16)	0.25037 (19)	0.2638 (5)	0.0231 (7)
H3	0.2988	0.2849	0.2278	0.028*
C4	0.34503 (16)	0.19535 (18)	0.4663 (5)	0.0206 (7)
C5	0.40726 (15)	0.14351 (19)	0.5264 (5)	0.0191 (6)
H5	0.4072	0.1064	0.6643	0.023*
C6	0.47028 (15)	0.14744 (17)	0.3781 (5)	0.0176 (6)
C7	0.58394 (13)	0.13641 (16)	0.1792 (6)	0.0191 (6)

C8	0.65823 (14)	0.10891 (17)	0.1344 (6)	0.0228 (7)
H8	0.6848	0.1303	−0.0013	0.027*
C9	0.69198 (16)	0.0502 (2)	0.2913 (5)	0.0269 (7)
H9	0.7424	0.0303	0.2617	0.032*
C10	0.65424 (18)	0.0186 (2)	0.4947 (5)	0.0260 (7)
H10	0.6794	−0.0215	0.6010	0.031*
C11	0.58048 (16)	0.04587 (18)	0.5403 (5)	0.0222 (7)
H11	0.5547	0.0246	0.6774	0.027*
C12	0.54435 (15)	0.10506 (18)	0.3825 (5)	0.0179 (6)
C13	0.56053 (16)	0.25418 (18)	−0.1405 (5)	0.0224 (7)
H13A	0.5185	0.2588	−0.2563	0.027*
H13B	0.6042	0.2258	−0.2223	0.027*
C14	0.58274 (15)	0.34943 (19)	−0.0620 (5)	0.0197 (6)
C15	0.62312 (14)	0.36493 (17)	0.1461 (6)	0.0241 (6)
H15	0.6360	0.3154	0.2470	0.029*
C16	0.64439 (15)	0.4530 (2)	0.2054 (6)	0.0307 (8)
H16	0.6726	0.4631	0.3464	0.037*
C17	0.6255 (2)	0.5257 (2)	0.0643 (6)	0.0344 (9)
H17	0.6402	0.5858	0.1077	0.041*
C18	0.58455 (17)	0.5108 (2)	−0.1427 (7)	0.0336 (8)
H18	0.5713	0.5605	−0.2424	0.040*
C19	0.56306 (16)	0.42221 (19)	−0.2030 (6)	0.0261 (7)
H19	0.5345	0.4120	−0.3432	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01928 (15)	0.03967 (17)	0.02934 (18)	0.00396 (12)	0.0029 (2)	−0.0045 (2)
N1	0.0176 (13)	0.0205 (12)	0.0208 (13)	−0.0014 (10)	0.0012 (11)	0.0036 (11)
C1	0.0175 (12)	0.0180 (12)	0.0184 (14)	−0.0031 (10)	−0.002 (2)	−0.0038 (16)
C2	0.0249 (15)	0.0199 (14)	0.024 (2)	−0.0015 (12)	−0.0055 (13)	0.0013 (13)
C3	0.0202 (16)	0.0211 (15)	0.0279 (17)	0.0034 (13)	−0.0056 (13)	−0.0036 (13)
C4	0.0152 (15)	0.0237 (16)	0.0228 (16)	0.0004 (12)	0.0026 (13)	−0.0038 (13)
C5	0.0179 (15)	0.0189 (14)	0.0204 (16)	−0.0040 (12)	−0.0021 (12)	−0.0011 (12)
C6	0.0166 (15)	0.0150 (14)	0.0213 (15)	−0.0022 (11)	−0.0031 (13)	−0.0029 (12)
C7	0.0185 (12)	0.0173 (12)	0.0214 (14)	−0.0035 (10)	−0.0027 (18)	−0.0048 (16)
C8	0.0159 (13)	0.0259 (14)	0.0268 (19)	−0.0044 (11)	0.0002 (14)	−0.0051 (15)
C9	0.0186 (16)	0.0258 (17)	0.0364 (19)	−0.0017 (13)	−0.0015 (15)	−0.0078 (15)
C10	0.0228 (17)	0.0225 (15)	0.0326 (18)	0.0020 (13)	−0.0053 (14)	0.0002 (14)
C11	0.0201 (16)	0.0231 (15)	0.0233 (16)	−0.0031 (12)	−0.0031 (13)	−0.0015 (13)
C12	0.0178 (15)	0.0140 (13)	0.0217 (16)	−0.0042 (11)	0.0010 (13)	−0.0034 (12)
C13	0.0195 (16)	0.0267 (16)	0.0209 (15)	−0.0024 (12)	0.0024 (13)	0.0004 (14)
C14	0.0170 (15)	0.0208 (14)	0.0215 (17)	0.0003 (12)	0.0076 (13)	0.0035 (14)
C15	0.0272 (14)	0.0229 (14)	0.0222 (16)	−0.0034 (11)	0.0000 (18)	0.0000 (17)
C16	0.0311 (16)	0.0336 (17)	0.028 (2)	−0.0080 (13)	0.0013 (15)	−0.0054 (16)
C17	0.039 (2)	0.0210 (16)	0.043 (2)	−0.0068 (15)	0.0162 (16)	−0.0033 (16)
C18	0.0319 (19)	0.0247 (16)	0.044 (2)	0.0040 (14)	0.0113 (18)	0.0080 (16)
C19	0.0213 (16)	0.0324 (17)	0.0244 (17)	0.0004 (13)	0.0045 (14)	0.0051 (14)

Geometric parameters (Å, º)

Br1—C4	1.911 (3)	C9—H9	0.9500
N1—C1	1.373 (3)	C10—C11	1.385 (4)
N1—C7	1.389 (3)	C10—H10	0.9500
N1—C13	1.459 (3)	C11—C12	1.397 (4)
C1—C2	1.379 (3)	C11—H11	0.9500
C1—C6	1.429 (4)	C13—C14	1.517 (4)
C2—C3	1.382 (4)	C13—H13A	0.9900
C2—H2	0.9500	C13—H13B	0.9900
C3—C4	1.399 (4)	C14—C19	1.376 (4)
C3—H3	0.9500	C14—C15	1.392 (4)
C4—C5	1.377 (4)	C15—C16	1.385 (4)
C5—C6	1.392 (4)	C15—H15	0.9500
C5—H5	0.9500	C16—C17	1.373 (4)
C6—C12	1.446 (3)	C16—H16	0.9500
C7—C8	1.393 (3)	C17—C18	1.390 (5)
C7—C12	1.419 (4)	C17—H17	0.9500
C8—C9	1.371 (4)	C18—C19	1.395 (4)
C8—H8	0.9500	C18—H18	0.9500
C9—C10	1.405 (4)	C19—H19	0.9500
C1—N1—C7	109.4 (2)	C9—C10—H10	120.0
C1—N1—C13	124.0 (2)	C10—C11—C12	119.3 (3)
C7—N1—C13	125.4 (2)	C10—C11—H11	120.4
N1—C1—C2	130.5 (3)	C12—C11—H11	120.4
N1—C1—C6	109.1 (2)	C11—C12—C7	119.5 (2)
C2—C1—C6	120.4 (3)	C11—C12—C6	133.6 (3)
C1—C2—C3	119.5 (3)	C7—C12—C6	106.9 (2)
C1—C2—H2	120.3	N1—C13—C14	113.7 (2)
C3—C2—H2	120.3	N1—C13—H13A	108.8
C2—C3—C4	119.5 (3)	C14—C13—H13A	108.8
C2—C3—H3	120.2	N1—C13—H13B	108.8
C4—C3—H3	120.2	C14—C13—H13B	108.8
C5—C4—C3	122.8 (3)	H13A—C13—H13B	107.7
C5—C4—Br1	119.2 (2)	C19—C14—C15	119.3 (3)
C3—C4—Br1	118.1 (2)	C19—C14—C13	118.7 (3)
C4—C5—C6	117.7 (3)	C15—C14—C13	121.9 (2)
C4—C5—H5	121.2	C16—C15—C14	119.6 (3)
C6—C5—H5	121.2	C16—C15—H15	120.2
C5—C6—C1	120.2 (2)	C14—C15—H15	120.2
C5—C6—C12	133.8 (3)	C17—C16—C15	121.3 (3)
C1—C6—C12	106.0 (2)	C17—C16—H16	119.4
N1—C7—C8	130.4 (3)	C15—C16—H16	119.4
N1—C7—C12	108.6 (2)	C16—C17—C18	119.4 (3)
C8—C7—C12	121.0 (3)	C16—C17—H17	120.3
C9—C8—C7	118.2 (3)	C18—C17—H17	120.3
C9—C8—H8	120.9	C17—C18—C19	119.5 (3)

C7—C8—H8	120.9	C17—C18—H18	120.2
C8—C9—C10	121.9 (3)	C19—C18—H18	120.2
C8—C9—H9	119.0	C14—C19—C18	120.9 (3)
C10—C9—H9	119.0	C14—C19—H19	119.6
C11—C10—C9	120.1 (3)	C18—C19—H19	119.6
C11—C10—H10	120.0		

C7—N1—C1—C2	178.6 (3)	C8—C9—C10—C11	0.7 (4)
C13—N1—C1—C2	10.5 (4)	C9—C10—C11—C12	−0.1 (4)
C7—N1—C1—C6	−0.3 (3)	C10—C11—C12—C7	−0.3 (4)
C13—N1—C1—C6	−168.5 (2)	C10—C11—C12—C6	−178.6 (3)
N1—C1—C2—C3	−179.9 (3)	N1—C7—C12—C11	−179.0 (2)
C6—C1—C2—C3	−1.1 (4)	C8—C7—C12—C11	0.1 (4)
C1—C2—C3—C4	0.7 (4)	N1—C7—C12—C6	−0.2 (3)
C2—C3—C4—C5	−0.4 (4)	C8—C7—C12—C6	178.9 (2)
C2—C3—C4—Br1	179.5 (2)	C5—C6—C12—C11	−1.5 (5)
C3—C4—C5—C6	0.5 (4)	C1—C6—C12—C11	178.5 (3)
Br1—C4—C5—C6	−179.48 (19)	C5—C6—C12—C7	180.0 (3)
C4—C5—C6—C1	−0.8 (4)	C1—C6—C12—C7	0.0 (3)
C4—C5—C6—C12	179.2 (3)	C1—N1—C13—C14	73.6 (3)
N1—C1—C6—C5	−179.8 (2)	C7—N1—C13—C14	−92.7 (3)
C2—C1—C6—C5	1.2 (4)	N1—C13—C14—C19	−141.7 (3)
N1—C1—C6—C12	0.2 (3)	N1—C13—C14—C15	39.1 (4)
C2—C1—C6—C12	−178.9 (2)	C19—C14—C15—C16	−1.5 (4)
C1—N1—C7—C8	−178.7 (3)	C13—C14—C15—C16	177.7 (3)
C13—N1—C7—C8	−10.7 (4)	C14—C15—C16—C17	0.9 (4)
C1—N1—C7—C12	0.3 (3)	C15—C16—C17—C18	−0.4 (5)
C13—N1—C7—C12	168.3 (2)	C16—C17—C18—C19	0.3 (5)
N1—C7—C8—C9	179.3 (3)	C15—C14—C19—C18	1.5 (4)
C12—C7—C8—C9	0.4 (4)	C13—C14—C19—C18	−177.7 (3)
C7—C8—C9—C10	−0.8 (4)	C17—C18—C19—C14	−0.9 (4)