(3,6-Dibromo-9*H*-carbazol-9-yl)(phenyl)methanone

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Key indicators

Single-crystal X-ray study
$T = 294$ K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.116
Data-to-parameter ratio = 13.3

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

The title compound, $C_{19}H_{11}Br_2NO$, was synthesized by *N*-alkylation of benzoyl chloride with 3,6-dibromo-9*H*-carbazole. The carbazole ring system is essentially planar and makes a dihedral angle of 62.2 (1)° with the plane of the benzene ring. Weak C—H⋯Br hydrogen bonding occurs in the crystal structure.

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). We present here the structure of the title carbazole derivative, (I).
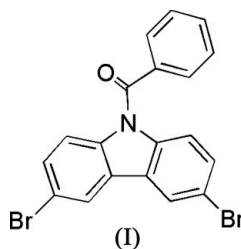
The molecular structure of (I) is shown in Fig. 1. The carbazole ring system is essentially planar, the mean atomic deviation being 0.033 Å. This is consistent with the situation found in similar compounds (Huang *et al.*, 2005; Duan *et al.*, 2005). The dihedral angle between the carbazole ring system and the benzene ring is 62.2 (1)°.

Weak intermolecular C—H⋯Br hydrogen bonding occurs in the crystal structure of (I) (Table 1).
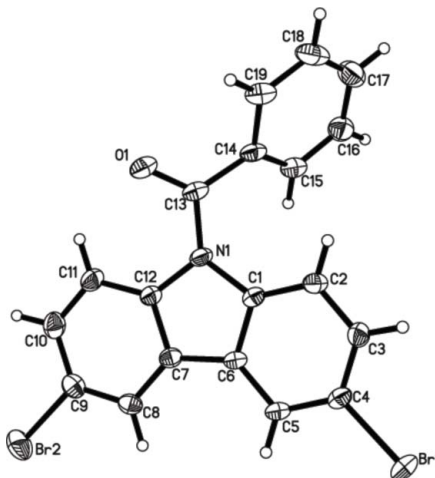

Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Experimental

3,6–9H-Dibromocarbazole (6.50 g, 20 mmol) was dissolved in a dimethylformamide solution (50 ml) of potassium hydroxide (7.0 g). The mixture was stirred for 40 min. A dimethylformamide solution (50 ml) of benzoyl chloride (4.22 g, 30 mmol) 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 and washed with cold water. Fine crystals of (I) were obtained by crystallization from an ethanol solution (yield 6.87 g, 80.1%; m.p. 483–484 K). Single crystals of (I) were obtained by recrystallization from a mixed solution of chloroform and ethanol (v/v 5:4).

Crystal data

$C_{19}H_{11}Br_2NO$
$M_r = 429.11$
Triclinic, $P\bar{1}$
$a = 7.398$ (2) Å
$b = 11.223$ (3) Å
$c = 11.431$ (4) Å
$\alpha = 61.384$ (4)°
$\beta = 80.036$ (5)°
$\gamma = 72.641$ (5)°
$V = 794.7$ (4) Å^3

$Z = 2$
$D_x = 1.793$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1944 reflections
$\theta = 2.9–25.0°$
$\mu = 5.10$ mm^{-1}
$T = 294$ (2) K
Block, colourless
$0.30 \times 0.26 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 1997)
$T_{min} = 0.242$, $T_{max} = 0.362$
4061 measured reflections

2780 independent reflections
2170 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.116$
$S = 1.04$
2780 reflections
209 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$
     where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: 0.081 (4)

Table 1
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C11—H11$\cdots$Br1^i	0.93	2.82	3.600 (6)	143

Symmetry code: (i) $x, y-1, z$.

H atoms were placed in calculated positions and refined using a riding model with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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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