

## 9-[4-(4-Bromostyryl)phenyl]-9H-carbazole

Lin Li, Lin Kong\* and  
Chen-Hao ZhuDepartment of Chemistry Anhui University, Hefei  
230039, People's Republic of China

Correspondence e-mail: ahu\_linli@163.com

## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.041  
 $wR$  factor = 0.113  
Data-to-parameter ratio = 14.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

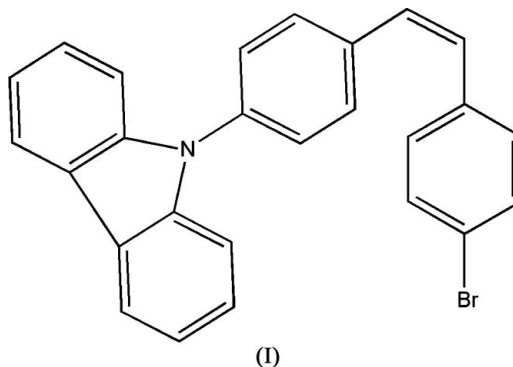
The title molecule,  $\text{C}_{26}\text{H}_{18}\text{BrN}$ , adopts the *Z* configuration and shows normal values of bond lengths and angles. The crystal packing is stabilized by van der Waals forces.

Received 14 February 2006

Accepted 26 February 2006

## Comment

Carbazole is a conjugated unit that has interesting optical and electronic properties such as photoconductivity and photo-refractivity. A number of carbazole derivatives, which can be used in organic light-emitting devices, have been designed and synthesized (Thomas *et al.*, 2001; Hwang *et al.*, 2003). Carbazole derivatives may also be used as materials for hole-transporting layers, utilizing the high charge mobility (Kimoto *et al.*, 2004), and as light-emitting layers because they are thermally stable and show blue photo- and electro-luminescence due to the large band gap of the biphenyl unit and planarity improved by the bridging N atom. We report here the crystal structure of the title compound, (I), a carbazole derivative.



The molecule of (I) adopts the *Z* configuration (Fig. 1). Bond lengths and angles (Table 1) are in agreement with the values reported in the literature (Allen *et al.*, 1987). The C13–C18 benzene ring makes dihedral angles of 53.6 (2) and 55.9 (2)° with the N1/C1/C6/C7/C12 and C21–C26 rings, respectively. The carbazole unit is almost planar; the two benzene rings make a dihedral angle of 1.7 (2)°. The crystal packing (Fig. 2) is stabilized by van der Waals forces.

## Experimental

For the preparation of 4-(9H-carbazol-9-yl)benzaldehyde, carbazole (8.35 g, 50 mmol), 4-fluorobenzaldehyde (6.20 g, 50 mmol), fresh potassium *tert*-butoxide (11.2 g, 100 mmol) and redistilled *N,N*-dimethylformamide (150 ml) under nitrogen were added to a three-necked flask equipped with a magnetic stirrer, a reflux condenser and a nitrogen input tube. The reaction mixture was refluxed for 72 h and

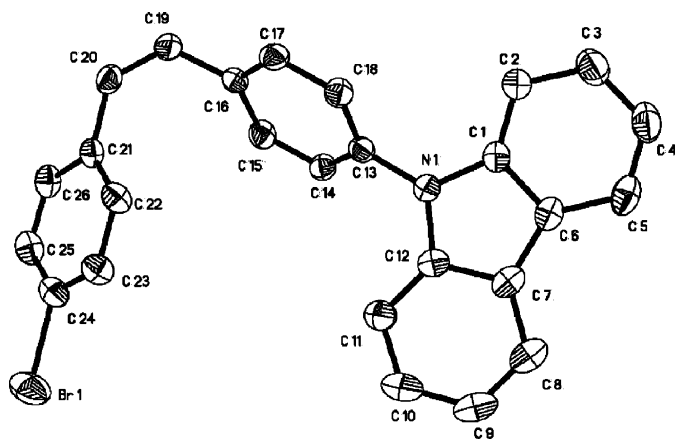


Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering. H atoms have been omitted for clarity.

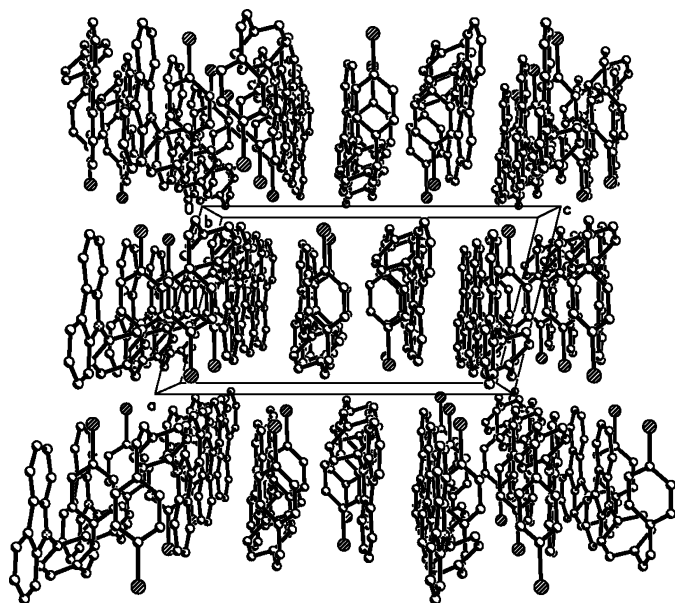


Figure 2

Packing of the title compound, viewed along the *b* axis. H atoms have been omitted for clarity.

then poured into ice water. After vigorously stirring for half an hour, a yellow solid was filtered off and air-dried. The product was recrystallized in acetone from give 10.84 g (yield 80%).

For the preparation of (4-bromobenzyl)terphenylphosphonium bromide, a flask was charged with a mixture 1-bromo-4-methylbenzene (8.55 g, 50 mmol), *N*-bromosuccinimide (NBS) (9.2 g, 51 mmol) and a catalytic amount of benzoyl peroxide, which was vigorously stirred in tetrachloromethane (150 ml) and refluxed for 5 h. The reaction was monitored by thin-layer chromatography. After completion of the reaction, the mixture was cooled to room temperature and extracted with chloroform several times. The organic layer was washed with water and saturated brine, then the organic extracts were dried over  $MgSO_4$ . After removing the solvent under reduced pressure, the residue was collected and dried *in vacuo*. This intermediate was added to triphenylphosphine (13.1 g,

50 mmol) in benzene (150 ml), and the resulting solution was refluxed for 4 h. After cooling to room temperature, a white solid was collected by filtration and air-dried to give 16.1 g of the product (yield 63%).

For the preparation of 9-(4-(4-bromostyryl)phenyl)-9*H*-carbazole, 4-(9*H*-carbazol-9-yl)benzaldehyde (4.07 g, 15 mmol), (4-bromobenzyl)terphenylphosphonium bromide (7.9 g, 15 mmol) and powdered NaOH (2.4 g, 60 mmol) were crushed together with a pestle and mortar for 2 h (Yang *et al.*, 2005). The mixture was extracted three times with dichloromethane. The organic layer was washed with saturated brine and the organic extracts were dried over  $MgSO_4$ . After removing the solvent under reduced pressure, the residue was purified by flash column chromatography to give the product as a yellow solid. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane/2-propanol (3:1) solution.

#### Crystal data

$C_{26}H_{18}BrN$   
 $M_r = 424.32$   
 Monoclinic,  $P2_1/c$   
 $a = 9.323$  (2) Å  
 $b = 13.051$  (3) Å  
 $c = 17.241$  (4) Å  
 $\beta = 104.035$  (3)°  
 $V = 2035.2$  (8) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.385$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 2737 reflections  
 $\theta = 2.3$ –22.1°  
 $\mu = 2.03$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, pale yellow  
 0.48 × 0.45 × 0.41 mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.393$ ,  $T_{max} = 0.435$   
 10492 measured reflections

3590 independent reflections  
 2257 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.038$   
 $\theta_{max} = 25.0^\circ$   
 $h = -11 \rightarrow 10$   
 $k = -15 \rightarrow 10$   
 $l = -18 \rightarrow 20$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.113$   
 $S = 1.00$   
 3590 reflections  
 253 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2 + 0.4676P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.64$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Br1—C24	1.899 (3)	N1—C13	1.426 (4)
N1—C12	1.391 (3)	C19—C20	1.327 (4)
N1—C1	1.396 (4)		
C12—N1—C1	108.6 (2)	N1—C1—C6	108.7 (3)
C12—N1—C13	125.8 (2)	C20—C19—C16	126.5 (3)
C1—N1—C13	125.5 (2)	C19—C20—C21	128.7 (3)
C2—C1—N1	129.3 (3)		

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and  $U_{iso} = 1.2U_{eq}(C)$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The authors thank the National Natural Science Foundation of China (grant Nos. 50532030 and 50335050) and Foundation of Anhui Province (grant No. 2002Z021). We also thank Professor D.-Q. Wang of Liao Cheng University for his assistance in the X-ray crystal structure determinations.

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