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9-[4-(6-Bromo-4-phenylnaphthalen-2-yl)-phenyl]-9*H*-carbazole

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Key indicators

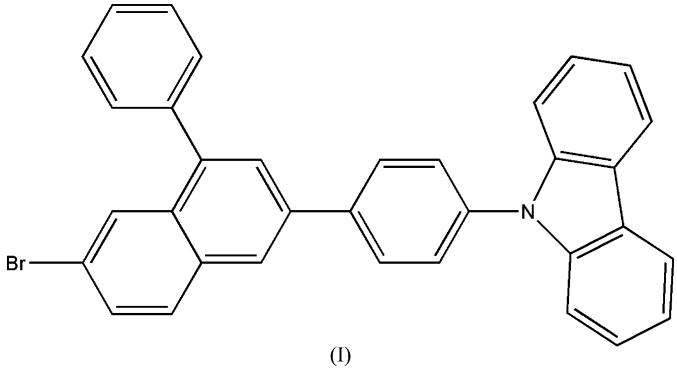
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.043
wR factor = 0.096
Data-to-parameter ratio = 15.0

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

The title compound, $C_{34}H_{22}BrN$, was synthesized by *N*-alkylation of 7-bromo-3-(4-bromophenyl)-1-phenylnaphthalene with 9*H*-carbazole. The carbazole ring system is essentially planar and makes a dihedral angle of 48.63 (9)° with the plane of the adjacent benzene ring.

Comment

A remarkable series of derivatives of carbazole has been investigated because of their diverse photophysical behavior (Adachi *et al.*, 2001). Previously, the most quantitative attention has been focused on the hole-transporting (HT) properties for organic light-emitting devices (Li *et al.*, 2005; Wong *et al.*, 2005). In recent years, much interest has been paid to their crystal structures (Chen *et al.*, 2005; Cui *et al.*, 2006; Huang *et al.*, 2005). In this research work, our idea is to synthesize a new derivative of carbazole with excellent HT ability and luminescent properties. Here, we report the crystal structure of the title compound, (I).



(I)

Selected bond lengths and angles for (I) are given in Table 1. The carbazole ring system is essentially planar and makes a dihedral angle of 48.63 (9)° with the plane of the adjacent C13–C18 benzene ring. The dihedral angles formed by the C13–C18 and C29–C34 benzene rings with the naphthalene system are 16.15 (8) and 49.29 (12)°, respectively (Fig. 1).

There are no supramolecular interactions, such as hydrogen bonds or π–π stacking forces, in the crystal structure of (I).

Experimental

Carbazole (1.0 mmol, 167.2 mg) and sodium hydroxide (10.0 mmol, 400.0 mg) were dissolved in dimethylformamide (DMF, 40 ml). After stirring at room temperature for 30 min, a solution of 7-bromo-3-(4-bromophenyl)-1-phenylnaphthalene (437.8 mg, 1.0 mmol) in DMF was added dropwise with stirring. The mixture was refluxed with

stirring for 3.5 h to obtain a clear yellow solution, which was then distilled under reduced pressure. The yellow solid residue was purified by column chromatography on silica gel using petrol ether/ethyl acetate (10:3 *v*/*v*) as eluent. Fine colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of the eluent at 298 K (yield 90%).

Crystal data

$C_{34}H_{22}BrN$
M_r = 524.44
Orthorhombic, *Pbcn*
a = 15.9337 (11) Å
b = 10.8421 (8) Å
c = 28.542 (2) Å
V = 4930.7 (6) Å^3
Z = 8
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 292 (2) K
Block, colourless
0.40 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.656, T_{max} = 0.815
26417 measured reflections
4871 independent reflections
2184 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.096
S = 0.78
4871 reflections
325 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C9—N	1.401 (4)	C13—N	1.421 (4)
C12—N	1.397 (4)	C23—Br	1.893 (3)
C14—C13—N	118.7 (3)	C12—N—C13	125.1 (3)
C18—C13—N	121.5 (3)	C9—N—C13	126.6 (3)

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

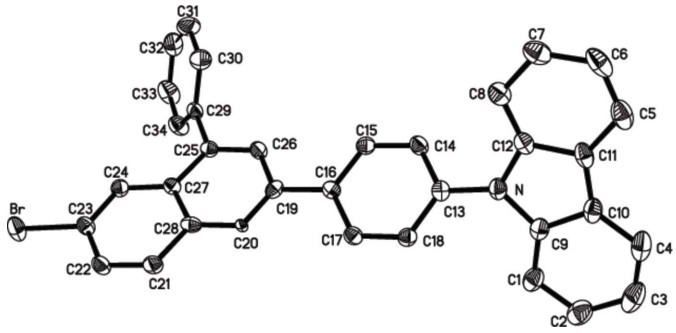


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Adachi, C., Baldo, M. A., Forrest, S. R., Lamansky, S., Thompson, M. E. & Kwomg, R. C. (2001). *Appl. Phys. Lett.* **78**, 1622–1624.
Bruker (1998). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, L.-Q., Yang, C.-L., Meng, X.-G. & Qin, J.-G. (2005). *Acta Cryst.* E**61**, o3073–o3075.
Cui, J.-L., Huang, P.-M. & Guo, W.-L. (2006). *Acta Cryst.* E**62**, o143–o144.
Huang, P.-M., Li, J.-S., Duan, X.-M., Zeng, T. & Yan, X.-L. (2005). *Acta Cryst.* E**61**, o2366–o2367.
Li, J., Liu, D., Li, Y., Lee, C.-S., Kwong, H.-L. & Lee, S. (2005). *Chem. Mater.* **17**, 1208–1212.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wong, K.-T., Chen, Y.-M., Lin, Y.-T., Su, H.-C. & Wu, C.-C. (2005). *Org. Lett.* **7**, 5361–5364.