

## 9-(4-Ethynylphenyl)-9H-carbazole

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In the title compound,  $C_{20}H_{13}N$ , the carbazole moiety is essentially planar, with the two benzene rings twisted by  $5.44(8)^\circ$ . The dihedral angle between the central five-membered ring and the ethynylphenyl ring is  $47.10(5)^\circ$ . The molecular packing in the crystal structure is stabilized by van der Waals forces.

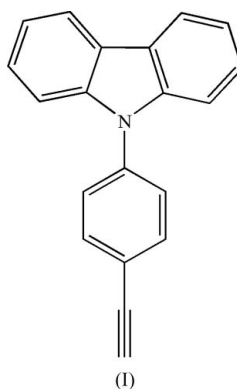
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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(C-C) = 0.002$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 13.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Comment

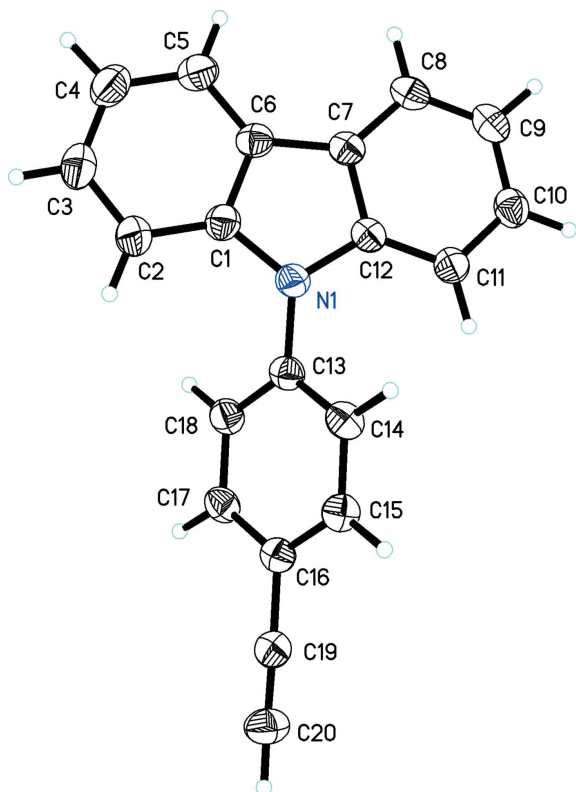
Carbazole–pyrene-based molecules can be used as organic emitters for organic light-emitting display (OLED) technology. In our earlier article (Xing *et al.*, 2005), we described how some carbazole-based compounds were synthesized and characterized. The title compound, (I), selected and attached to pyrene for its sufficiently high triplet energy and the hole-transport property, was synthesized through a Sonogashira coupling reaction between 9-(4-iodophenyl)-9H-carbazole and 2-methylbut-3-yn-2-ol, followed by decomposition under base conditions. An X-ray crystal-structure determination of (I) was undertaken in order to elucidate the conformation, and the results are presented here.



A perspective view of (I) with the atom-labeling scheme is shown in Fig. 1. The bond lengths and angles in the carbazole fragment are in good agreement with those observed for a closely related structure (Duan *et al.*, 2004). The carbazole group is essentially planar, the dihedral angle between the two benzene rings being  $5.44(8)^\circ$ . The central five-membered ring and the C13–C18 benzene ring are not coplanar; the dihedral angle between them is  $47.10(5)^\circ$ . The interplanar distance between two carbazole planes is  $3.875(2)$  Å along the  $b$  axis.

## Experimental

The starting materials were purchased from Acros and used without purification. The intermediate 9-(4-iodophenyl)carbazole and (I)



**Figure 1**  
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

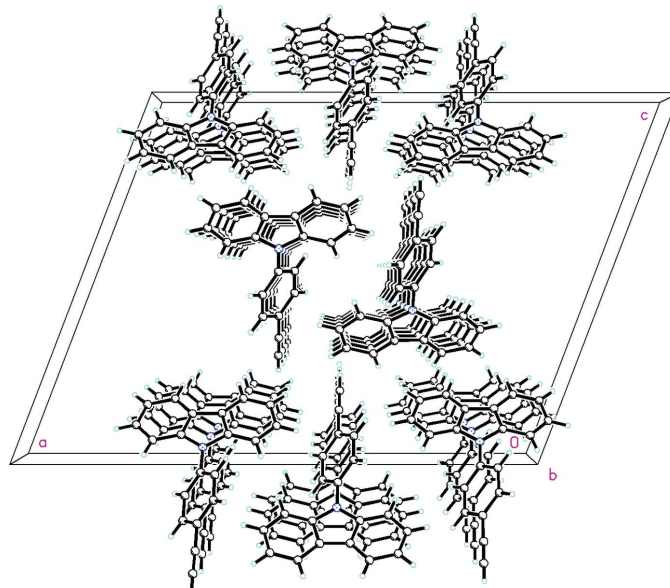
were synthesized according to the method described previously by Sanda *et al.* (2003) and characterized by IR,  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and elemental analysis. Compound (I),  $^1\text{H}$  NMR (500 MHz,  $\delta$  in p.p.m.,  $\text{CDCl}_3$ ): 3.18 (1H, s), 7.25–8.20 (12H, Ar).  $^{13}\text{C}$  NMR (125 MHz,  $\delta$  in p.p.m.,  $\text{CDCl}_3$ ): 78.1, 82.9, 109.8, 120.4, 120.5, 121.0, 123.5, 126.1, 126.8, 133.8, 138.1, 140.6. IR (KBr,  $\text{cm}^{-1}$ ): 3266, 2102, 1600, 1556, 1452, 1230, 839, 755, 723. Analysis calculated for  $\text{C}_{20}\text{H}_{13}\text{N}$ : C 89.86, H 4.90, N 5.24%; found: C 89.79, H 5.00, N 5.21%. The crystal used for the data collection was obtained by slow evaporation of a saturated hexane–dichloromethane solution of (I) at room temperature.

#### Crystal data

$\text{C}_{20}\text{H}_{13}\text{N}$	$D_x = 1.228 \text{ Mg m}^{-3}$
$M_r = 267.31$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 2387 reflections
$a = 26.753 (3) \text{ \AA}$	$\theta = 6.3\text{--}50.8^\circ$
$b = 5.7309 (6) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$c = 20.185 (2) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 110.868 (2)^\circ$	Block, colorless
$V = 2891.8 (5) \text{ \AA}^3$	$0.54 \times 0.52 \times 0.43 \text{ mm}$
$Z = 8$	

#### Data collection

Bruker SMART CCD area-detector diffractometer	3153 independent reflections
$\varphi$ and $\omega$ scans	2104 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.060$
$T_{\text{min}} = 0.7291$ , $T_{\text{max}} = 0.970$	$\theta_{\text{max}} = 27.0^\circ$
8078 measured reflections	$h = -34 \rightarrow 32$
	$k = -7 \rightarrow 7$
	$l = -25 \rightarrow 20$



**Figure 2**  
The molecular packing in the structure of (I), viewed along the  $b$  axis.

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 0.90$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
3153 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
243 parameters	Extinction correction: SHELXL97
All H-atom parameters refined	Extinction coefficient: 0.0108 (7)

All H atoms, located in a difference Fourier map, were refined freely. C–H distances are in the range 0.924 (16)–0.990 (14)  $\text{\AA}$ .

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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