

## 3,5-Bis[(carbazol-9-yl)methyl]-1-methoxybenzene

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## Key indicators

Single-crystal X-ray study

T = 100 K

Mean  $\sigma(\text{C}-\text{C}) = 0.001 \text{ \AA}$ 

R factor = 0.048

wR factor = 0.135

Data-to-parameter ratio = 32.4

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

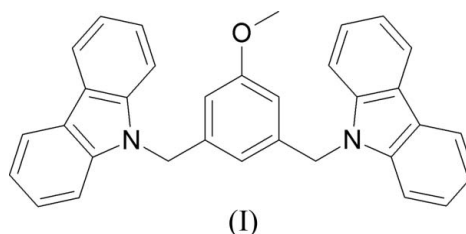
In the title compound,  $\text{C}_{33}\text{H}_{26}\text{N}_2\text{O}$ , the two carbazole ring systems are almost planar and form dihedral angles of  $77.17(2)$  and  $83.67(2)^\circ$  with the plane of the central benzene ring. The molecules are connected *via*  $\text{C}-\text{H}\cdots\pi$  interactions into a three-dimensional framework.

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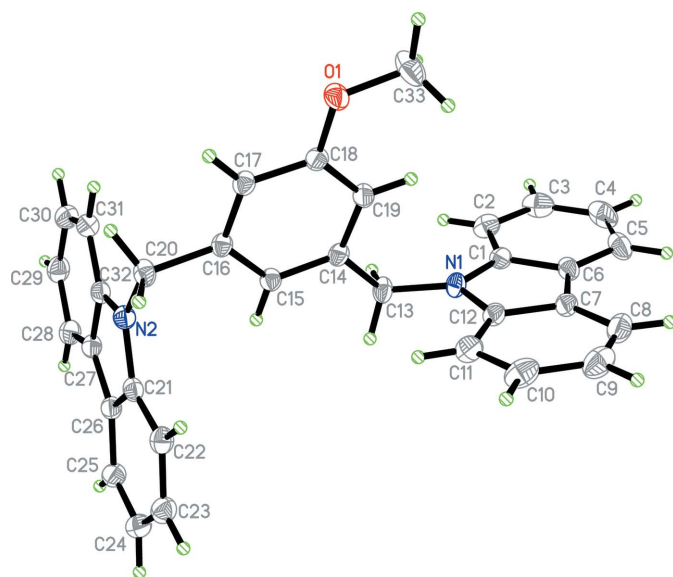
## Comment

Carbazole compounds are used as host materials for blue phosphorescent organic light-emitting diodes (OLEDs) and green and red phosphorescent OLEDs (Shih *et al.*, 2006; Wong *et al.*, 2005). Carbazole derivatives have been found to exhibit antitumor (Leon *et al.*, 1988; Routier *et al.*, 2005; Martin *et al.*, 2002), antimycobacterial (Sunthitikawinsakul *et al.*, 2003), antifungal (Segall *et al.*, 2003) and potent anti-HIV (Yan *et al.*, 2005; Hirata *et al.*, 1999) activities. The structure determination of the title compound, (I), was undertaken as part of our investigations of carbazole derivatives.

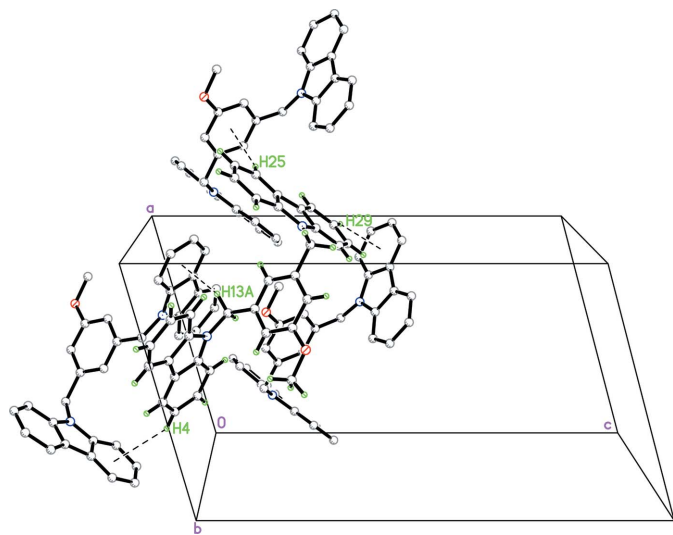


The molecular structure of (I) is illustrated in Fig. 1. Both carbazole ring systems are almost planar, with an r.m.s. deviation of  $0.034 \text{ \AA}$  in each case. One benzene ring in each carbazole ring system (C7–C12 and C21–C26) is slightly bent away from the central five-membered ring, with torsion angles of  $-1.30(12)^\circ$  (C8–C7–C12–C11) and  $3.03(12)^\circ$  (C22–C21–C26–C25). Bond distances and angles in the carbazole rings are in agreement with each other, as well as with those reported for other carbazole derivatives (Duan *et al.*, 2006; Cui *et al.*, 2006; Wang *et al.*, 2006). The  $\text{N1}-\text{C13}-\text{C14}$  [ $114.34(7)^\circ$ ] and  $\text{N2}-\text{C20}-\text{C16}$  [ $113.68(7)^\circ$ ] angles deviate significantly from the ideal tetrahedral angle. The planes of the  $\text{N1}/\text{C1}-\text{C12}$  and  $\text{N2}/\text{C21}-\text{C32}$  carbazole ring systems form dihedral angles of  $77.17(2)$  and  $83.67(2)^\circ$ , respectively, with the plane of the central  $\text{C14}-\text{C19}$  benzene ring.

The crystal packing reveals that molecules related by a center of inversion are linked *via* intermolecular  $\text{C}-\text{H}\cdots\pi$  interactions (Table 1) involving the C21–C26 (centroid  $\text{Cg1}$ ) and C1–C6 (centroid  $\text{Cg2}$ ) benzene rings to form a dimer. Adjacent glide-related dimers are linked by another set of  $\text{C}-\text{H}\cdots\pi$  interactions (Table 1) involving the C14–C19 (centroid



**Figure 1**  
The molecular structure of (I), showing 60% probability displacement ellipsoids and the atomic numbering.



**Figure 2**  
Part of the C—H... $\pi$  hydrogen-bonded (dashed lines) network in (I). Only the H atoms involved in hydrogen bonding are shown.

Cg3) and C1–C6 benzene rings, leading to the formation of a three-dimensional network (Fig. 2).

## Experimental

Carbazole (3.00 mmol) was added to a suspension of NaH (12 mmol) in dry DMF (10 ml) under nitrogen. The mixture was stirred for 15 min, after which time 3,5-bis(bromomethyl)methoxybenzene (1.50 mmol) in dry DMF (10 ml) was added dropwise over a period of 30 min. The reaction mixture was refluxed overnight and then the addition of water (100 ml) caused precipitation of the crude product; the solid was filtered off and extracted with chloroform (100 ml), washed with water (2  $\times$  100 ml) and brine (150 ml), and dried over

anhydrous Na<sub>2</sub>SO<sub>4</sub>. The solvent was removed *in vacuo* and the residue was subjected to column chromatography (SiO<sub>2</sub>) using hexane–chloroform (3:2 *v/v*). The compound was recrystallized from chloroform by slow evaporation.

## Crystal data

C<sub>33</sub>H<sub>26</sub>N<sub>2</sub>O  
*M<sub>r</sub>* = 466.56  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.3729 (1) Å  
*b* = 13.1360 (2) Å  
*c* = 18.3410 (2) Å  
 $\beta$  = 105.573 (1)°  
*V* = 2407.37 (5) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.287 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation  
 $\mu$  = 0.08 mm<sup>-1</sup>  
*T* = 100 (2) K  
 Block, colorless  
 0.65  $\times$  0.41  $\times$  0.25 mm

## Data collection

Bruker SMART APEX2 CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
*T<sub>min</sub>* = 0.953, *T<sub>max</sub>* = 0.981

63553 measured reflections  
 10571 independent reflections  
 8546 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.037  
 $\theta_{\max}$  = 35.0°

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.048  
*wR*(*F*<sup>2</sup>) = 0.135  
*S* = 1.03  
 10571 reflections  
 326 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0739P)^2 + 0.4533P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.47 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...Cg1 <sup>i</sup>	0.95	3.00	3.8376 (11)	148
C13—H13A...Cg2 <sup>i</sup>	0.99	2.52	3.3705 (10)	144
C25—H25...Cg3 <sup>ii</sup>	0.95	2.74	3.5736 (10)	147
C29—H29...Cg2 <sup>iii</sup>	0.95	2.96	3.7578 (10)	142

Symmetry codes: (i)  $-x + 1, -y, -z$ ; (ii)  $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (iii)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ .

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances of 0.95 (aromatic), 0.98 (methyl) and 0.99 Å (methylene). The *U*<sub>iso</sub>(H) values were set equal to 1.5 (methyl) or 1.2 (other H atoms) times *U*<sub>eq</sub> of the carrier atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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