

9-(*p*-Tolylsulfonyl)-9*H*-carbazoleNing Li,<sup>a\*</sup> Peng-Mian Huang,<sup>b</sup>  
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## Key indicators

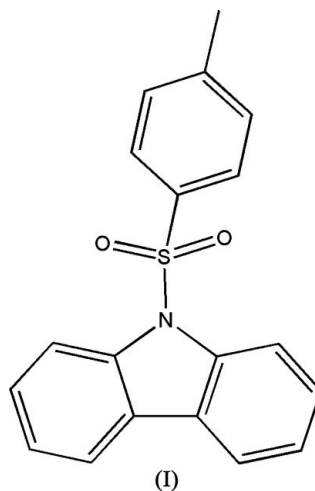
Single-crystal X-ray study  
*T* = 294 K  
Mean  $\sigma$ (C–C) = 0.004 Å  
*R* factor = 0.043  
*wR* factor = 0.125  
Data-to-parameter ratio = 13.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Two independent molecules constitute the asymmetric unit of the title compound, C<sub>19</sub>H<sub>15</sub>NO<sub>2</sub>S, which was synthesized by *N*-alkylation of 4-methylbenzenesulfonyl chloride with carbazole. The carbazole ring system is essentially planar and forms a dihedral angle with the benzene ring of 85.1 (7)° [83.9 (7)° for the second molecule]. In the crystal structure, weak C–H···O interactions are observed.

Received 10 March 2006  
Accepted 16 March 2006

## Comment

Carbazole derivatives substituted by *N*-alkylation exhibit useful pharmaceutical properties (Buu-Hoi & Royer, 1950; Harfenist & Joyner, 1983; Caulfield *et al.*, 2002; Harper *et al.*, 2002). In this paper, the structure of 9-(*p*-tolylsulfonyl)-9*H*-carbazole, (I), synthesized by *N*-alkylation of 4-methylbenzenesulfonyl chloride with carbazole, is reported.



The asymmetric unit of (I) contains two independent but similar molecules (Fig. 1). The carbazole ring systems in each are essentially planar, with mean deviations of 0.015 and 0.022 Å, consistent with recent determinations of similar structures (Huang *et al.*, 2005; Duan *et al.*, 2005). The dihedral angle formed between the carbazole ring system and the plane through the pendent benzene ring is 85.1 (7)° [83.9 (7)° for the second molecule]. There are C–H···O interactions, as shown in Fig. 2 and detailed in Table 1.

## Experimental

The title compound was prepared according to the procedure of Chakrabarti *et al.* (1989). Carbazole (1 g) dissolved in dimethylformamide (25 ml) and benzene (25 ml) was treated with sodium hydride (0.168 g) in an ice bath for 30 min. To the cold stirred solu-

tion, 4-methylbenzenesulfonyl chloride (1.12 g) was added and the mixture stirred at room temperature for a further 4 h. The resulting mixture was then poured into water (40 ml) and extracted with benzene (100 ml). After drying the benzene extracts over anhydrous sodium sulfate, filtration and concentration, the solid product was recrystallized from EtOH, giving crystals of (I) (yield 0.90 g, 96%; m.p. 393–394 K). Compound (I) (40 mg) was dissolved in a mixture of chloroform (6 ml) and ethanol (2 ml) and the solution was kept at room temperature for 10 d. Natural evaporation of the solution gave colourless crystals suitable for X-ray analysis.

Crystal data

C<sub>19</sub>H<sub>15</sub>NO<sub>2</sub>S  
*M<sub>r</sub>* = 321.38  
 Triclinic, *P*1̄  
*a* = 10.0889 (18) Å  
*b* = 10.8104 (19) Å  
*c* = 15.884 (3) Å  
 $\alpha$  = 77.896 (3)°  
 $\beta$  = 72.353 (3)°  
 $\gamma$  = 84.459 (3)°  
*V* = 1613.1 (5) Å<sup>3</sup>  
*Z* = 4  
*D<sub>x</sub>* = 1.323 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 2826 reflections  
 $\theta$  = 2.6–26.3°  
 $\mu$  = 0.21 mm<sup>-1</sup>  
*T* = 294 (2) K  
 Block, colourless  
 0.30 × 0.26 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 1997)  
*T<sub>min</sub>* = 0.940, *T<sub>max</sub>* = 0.971  
 8234 measured reflections  
 5640 independent reflections  
 3776 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.023  
 $\theta_{max}$  = 25.0°  
*h* = -11 → 9  
*k* = -10 → 12  
*l* = -18 → 18

Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.043  
*wR*(*F*<sup>2</sup>) = 0.125  
*S* = 1.05  
 5640 reflections  
 418 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.16886P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.002$   
 $\Delta\rho_{max} = 0.21 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.29 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0131 (14)

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>
C29—H29...O1	0.93	2.55	3.448 (4)	163

All H atoms were included in the riding model approximation, with C—H distances of 0.93 (aromatic) and 0.96 Å (methyl), and with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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*.

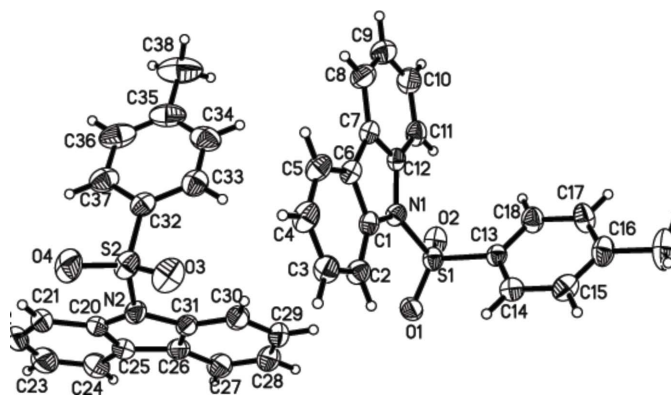


Figure 1  
 The asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level.

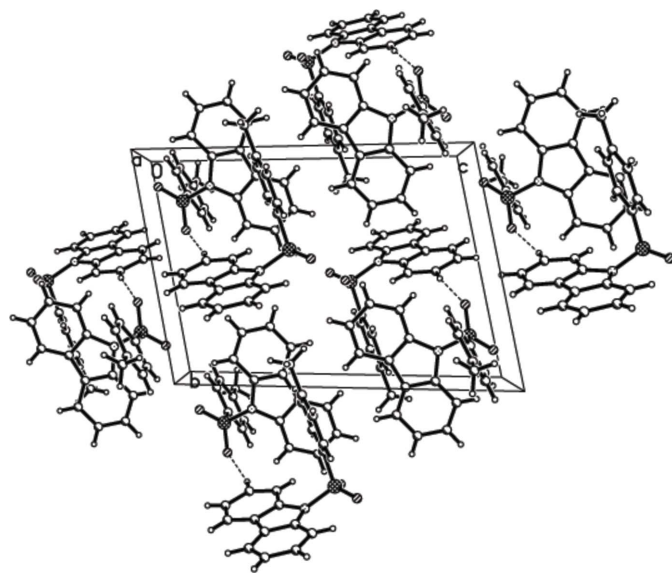


Figure 2  
 Part of the packing of the title compound, viewed down the *a*-axis direction. Dashed lines indicate hydrogen bonds.

References

Bruker (1997). *SADABS* (Version 2.0), *SMART* (Version 5.10), *SAINTE* (Version 5.10) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Buu-Hoi, N. P. & Royer, R. (1950). *J. Org. Chem.* **15**, 123–130.  
 Caulfield, T., Cherrier, M. P., Combeau, C. & Mailliet, P. (2002). European Patent No. 1253141.  
 Chakrabarti, A., Goutam, K. B. & Chakraborty, D. P. (1989). *Tetrahedron*, **45**, 5059–5064.  
 Duan, X.-M., Huang, P.-M., Zheng, P.-W. & Li, J.-S. (2005). *Acta Cryst.* **E61**, o3361–o3363.  
 Harfenist, M. & Joyner, C. T. (1983). US Patent No. 4 379 160.  
 Harper, R. W., Lin, H. S. & Richett, M. E. (2002). World Patent No. 02079154.  
 Huang, P.-M., Li, J.-S., Duan, X.-M., Zeng, T. & Yan, X.-L. (2005). *Acta Cryst.* **E61**, o2366–o2367.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.