

***N*-[4-(Dimethylamino)benzylidene]-4-methylbenzene-sulfonamide****Li-Ping Deng and Yong-Zhou Hu\***

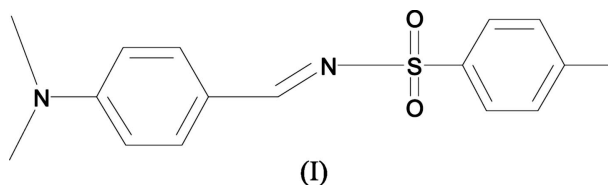
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huyz@zjuem.zju.edu.cn**Key indicators**Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.055  
 $wR$  factor = 0.152  
Data-to-parameter ratio = 16.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The molecule of the title compound,  $\text{C}_{16}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$ , consists of essentially planar 4-(dimethylamino)benzylidene and 4-tolyl fragments bonded through a sulfone S atom, which is approximately coplanar with both fragments. The mean planes of the  $\text{MeC}_6\text{H}_4\text{S}$  and  $\text{Me}_2\text{NC}_6\text{H}_4\text{CH}=\text{NS}$  groups are roughly orthogonal and form a dihedral angle of  $101.28$  ( $9$ )°.

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*N*-Sulfonylaldimines attract the attention of organic chemists because of their use as synthetic reagents (Love *et al.*, 1994). As electron-deficient imines, they find elegant application in inverse electron demand Diels–Alder chemistry (Boger *et al.*, 1991), as well as enophiles in stereochemically controlled ene reactions (Melnick *et al.*, 1988). Sulfonylaldimines have also been shown to possess thrombin inhibitor activity (Supuran *et al.*, 2000). Our interest in sulfonylaldimine derivatives is driven both by their biological and by their synthetic capabilities. The title compound, (I), has been prepared and studied in order to obtain a better understanding of its reactivity.



The molecular structure of the title compound is shown in Fig. 1. All non-H atoms of its molecule, with the exception of sulfone atoms O1 and O2, belong to one of the two almost planar fragments,  $\text{MeC}_6\text{H}_4\text{S}$  or  $\text{Me}_2\text{NC}_6\text{H}_4\text{CH}=\text{NS}$ , which share the sulfone S1 atom. The mean planes of the two groups are roughly orthogonal; they form a dihedral angle of  $78.72$  ( $9$ )°.

**Experimental**

4-Dimethylaminobenzaldehyde oxime (1 mmol) was refluxed in ethanol (20 ml) with sodium chloro(*p*-tosyl)amide (chloramine-T; 1.2 mmol) for 4 h, and the reaction mixture was then cooled to room temperature. After removal of the solvent, a yellow solid product was obtained, which was washed with water (30 ml) and extracted with dichloromethane (30 ml). The extracts were dried over anhydrous sodium sulfate and concentrated in a vacuum, and the residue was recrystallized from ethanol to give the title compound. Diffraction quality crystals were obtained by slow evaporation of an acetone/ethanol solution at room temperature.

## Crystal data

C<sub>16</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>SM<sub>r</sub> = 302.39Monoclinic, P2<sub>1</sub>/c

a = 17.1543 (4) Å

b = 8.3835 (2) Å

c = 10.9679 (3) Å

β = 105.976 (1)°

V = 1516.41 (6) Å<sup>3</sup>

Z = 4

D<sub>x</sub> = 1.324 Mg m<sup>-3</sup>

Mo Kα radiation

Cell parameters from 9315

reflections

θ = 1.2–27.5°

μ = 0.22 mm<sup>-1</sup>

T = 295 (1) K

Prism, yellow

0.30 × 0.22 × 0.20 mm

## Data collection

Rigaku R-Axis RAPID

diffractometer

ω scans

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

T<sub>min</sub> = 0.911, T<sub>max</sub> = 0.957

9646 measured reflections

3458 independent reflections

1718 reflections with I &gt; 2σ(I)

R<sub>int</sub> = 0.054θ<sub>max</sub> = 27.5°

h = -20 → 22

k = -10 → 10

l = -14 → 13

## Refinement

Refinement on F<sup>2</sup>R[F<sup>2</sup> > 2σ(F<sup>2</sup>)] = 0.055wR(F<sup>2</sup>) = 0.152

S = 1.00

3176 reflections

191 parameters

H-atom parameters constrained

w = 1/[0.0012F<sub>o</sub><sup>2</sup> + 1.0σ(F<sub>o</sub><sup>2</sup>)]/(4F<sub>o</sub><sup>2</sup>)(Δ/σ)<sub>max</sub> < 0.001Δρ<sub>max</sub> = 0.48 e Å<sup>-3</sup>Δρ<sub>min</sub> = -0.39 e Å<sup>-3</sup>

Extinction correction: Larson

(1970), equation 22

Extinction coefficient: 88 (2)

Table 1

Selected geometric parameters (Å, °).

S1–O1	1.435 (2)	N1–C8	1.289 (4)
S1–O2	1.426 (2)	N2–C12	1.355 (4)
S1–N1	1.645 (2)	N2–C15	1.447 (4)
S1–C5	1.755 (2)	N2–C16	1.435 (3)
O2–S1–O1	118.6 (1)	C5–S1–O2	109.0 (1)
N1–S1–O1	112.2 (1)	C5–S1–N1	101.6 (1)
C5–S1–O1	108.4 (1)	S1–N1–C8	117.3 (2)
N1–S1–O2	105.6 (1)	S1–C5–C4	119.9 (2)
O1–S1–N1–C8	17.4 (2)	O1–S1–C5–C6	164.4 (2)
O2–S1–N1–C8	148.0 (2)	O2–S1–C5–C4	-149.5 (2)
C5–S1–N1–C8	-98.2 (2)	N1–S1–C5–C6	-77.2 (2)
O1–S1–C5–C4	-19.1 (3)	S1–N1–C8–C9	179.8 (2)

All H atoms were positioned geometrically. The methyl H atoms were then constrained to an ideal geometry, with C–H distances of

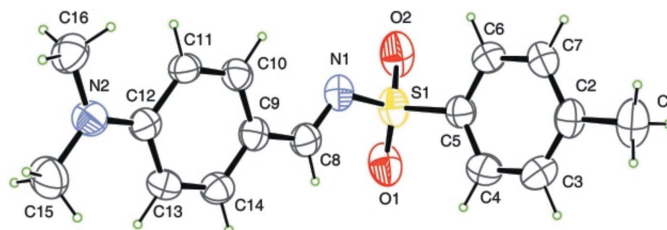


Figure 1

View of the molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , but each group was allowed to rotate freely about its C–C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances of 0.98 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . For the refinement, only data with  $\theta > 27^\circ$  was used.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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