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N-(4-Methylbenzyl)-*N*-(6-methyl-2-pyridyl)-benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.065
wR factor = 0.163
Data-to-parameter ratio = 15.9

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

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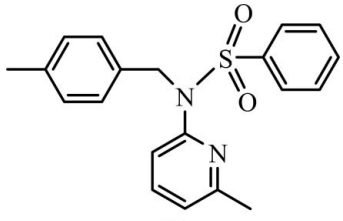
In the molecule of the title compound, $C_{20}H_{20}N_2O_2S$, with rings *A* (4-methylbenzyl aromatic ring), *B* (benzenesulfonamide aromatic ring) and *C* (pyridine), the dihedral angles are *A*/*B* = 71.12 (9), *A*/*C* = 80.50 (8) and *B*/*C* = 50.95 (7)°. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into centrosymmetric dimers, which may be effective in the stabilization of the structure.

Comment

Sulfonamides display a range of biological activities, making them attractive compounds to synthetic and medicinal chemists. For instance, an aromatic or heteroaromatic sulfonamide unit has been used as the primary recognition element necessary for small molecules to bind the active site of the carbonic anhydrase (CA) (Poulsen *et al.*, 2005). Zinc is an essential element for humans and plays an important role in biochemical and nutritional processes. Quinoline-based sulfonamides have therefore been employed to detect zinc (Fahrni & O'Halloran, 1999). Some heteroaromatic sulfonamide derivatives have been optimized as highly selective EP1 receptor antagonists (Naganawa *et al.*, 2006). *N*,*N*-Dialkyl sulfonamides have been used as antimycobacterial agents (Owen *et al.*, 2007). Sulfonamides have also been used in the treatment of bacterial infections, diabetes mellitus, edema, hypertension and gout. The present study was undertaken in order to ascertain the crystal structure of the title compound, (I).



(I)

The molecular structure of (I), is shown in Fig. 1. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987). For the individual rings [*A* (C2–C7), *B* (C8–C13) and *C* (N2/C14–18)] the dihedral angles are *A*/*B* = 71.12 (9), *A*/*C* = 80.50 (8) and *B*/*C* = 50.95 (7)°.

As can be seen from the packing diagram (Fig. 2), intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into dimers, which are stacked along the *b* axis and may be effective in the stabilization of the structure; van der Waals interactions are also effective in the molecular packing.

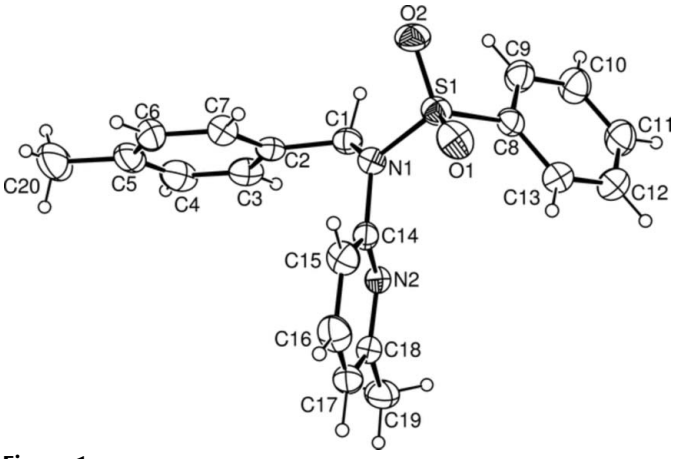


Figure 1
The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

The title compound, (I), was prepared from a mixture of *N*-(6-methyl-2-pyridyl)benzenesulfonamide (2.0 g, 8.05 mmol), 4-methylbenzyl bromide (1.5 g, 8.05 mmol) and potassium carbonate (1.1 g, 8.05 mmol) in dry dimethylformamide (25 ml), which was refluxed for 12 h under a nitrogen atmosphere. After cooling to room temperature, the solvent was removed. The residue was dissolved in chloroform and washed with hydrochloric acid (10%, 50 ml). The organic layer was dried with anhydrous magnesium sulfate and the solvent was evaporated. The residue was crystallized from methanol (yield 1.97 g, 69%; m.p. 405 K).

Crystal data

$C_{20}H_{20}N_2O_2S$
M_r = 352.45
Triclinic, $P\overline{1}$
a = 8.8386 (1) Å
b = 9.8790 (2) Å
c = 10.5647 (2) Å
α = 89.589 (5)°
β = 82.226 (6)°
γ = 81.737 (8)°
V = 904.44 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 294 (2) K
0.35 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.946, T_{max} = 0.971
3853 measured reflections
3646 independent reflections
2890 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.163
S = 1.18
3646 reflections
229 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O2^{i}	0.97	2.51	3.443 (2)	161

Symmetry code: (i) $-x, -y+1, -z$.

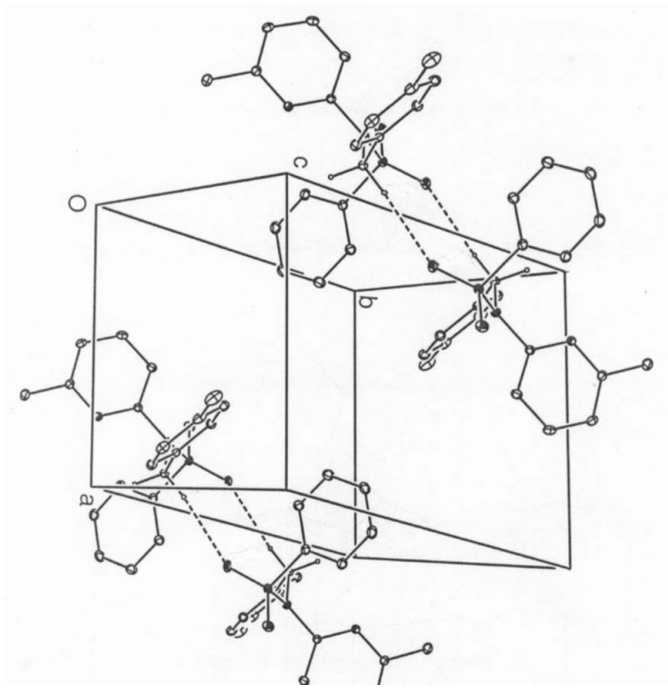


Figure 2
A partial packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and x = 1.2 for all other H atoms.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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