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N-Benzylidene-5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-amine

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The asymmetric unit of the title compound, $C_{16}H_{13}N_3OS$, contains two independent molecules. The dihedral angles between the planar rings differ in the two molecules. Weak intra- and intermolecular C—H···S and C—H···N hydrogen bonds may be effective in the stabilization of the crystal structure.

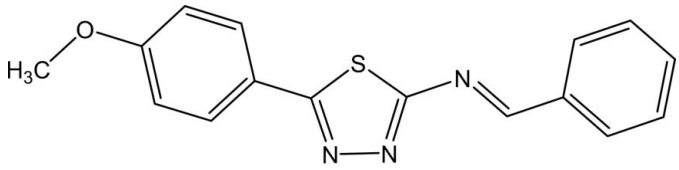
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.077
wR factor = 0.182
Data-to-parameter ratio = 14.6

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

Comment

1,3,4-Thiadiazole derivatives represent an interesting class of compounds possessing broad-spectrum biological activities (Nakagawa *et al.*, 1996; Wang *et al.*, 1999). These compounds are known to exhibit diverse biological effects, such as insecticidal and fungicidal activities (Wang *et al.*, 1999). We report here the crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The asymmetric unit contains two independent molecules. Rings *A* (atoms C1*A*–C6*A*), *B* (S1*A*/N2*A*/N3*A*/C8*A*/C9*A*), *C* (C10*A*–C15*A*) and *A*′ (C1*B*–C6*B*), *B*′ (S1*B*/N2*B*/N3*B*/C8*B*/C9*B*) and C′ (C10*B*–C15*B*) are, of course, planar and the dihedral angles between them are *A*/*B* = 33.76 (2), *A*/*C* = 22.81 (3), *B*/*C* = 12.78 (3) and *A*′/*B*′ = 37.17 (3), *A*′/*C*′ = 54.08 (2), *B*′/*C*′ = 17.26 (3)°.

Weak intramolecular C—H···S hydrogen bonds (Table 1) result in the formation of five-membered rings (Fig. 1), while weak intermolecular C—H···N hydrogen bonds (Table 1) may be effective in the stabilization of the crystal structure.

Experimental

5-(4-Methoxyphenyl)-1,3,4-thiadiazol-2-amine (5 mmol) and benzaldehyde (5 mmol) were added to toluene (50 ml). The water was removed by distillation for 5 h and the reaction mixture left to cool to room temperature. It was filtered, and the filter cake was crystallized from acetone to give the title compound (m.p. 408 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

Crystal data

$C_{16}H_{13}N_3OS$
M_r = 295.36
Monoclinic, $P2_1/n$
a = 7.4253 (7) Å
b = 11.5124 (11) Å
c = 33.0405 (19) Å
β = 93.10 (3)°
V = 2820.3 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.955, T_{max} = 0.977
5940 measured reflections
5517 independent reflections
2748 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.077
$wR(F^2)$ = 0.182
S = 1.04
5517 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7*A*—H7*A*···S1*A*	0.93	2.73	3.121 (5)	106
C7*B*—H7*B*···S1*B*	0.93	2.72	3.124 (5)	107
C16*A*—H16*B*···N3*A*^{i}	0.96	2.61	3.547 (7)	164

Symmetry code: (i) $-x-\frac{3}{2}, y-\frac{1}{2}, -z-\frac{1}{2}$.

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic 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 H and x = 1.2 for aromatic H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; 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: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

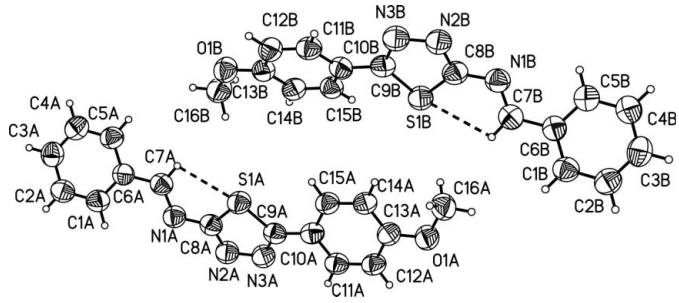


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

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