# organic papers

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**Key indicators**

# 4,5,6-Trimethyl-2-(phenylsulfonylamino)pyrimidine

In the crystal structure of the title compound, $C_{13}H_{15}N_3O_2S$, there are intermolecular N—H···O hydrogen-bond interactions and they give rise to dimers of the title compound. In the title molecule, the plane of the pyrimidine ring makes an angle of 81.90 (8)° with the plane of the benzene ring.

## Comment

Pyrimidine derivatives are very important molecules in biology and have many applications in the areas of pesticides and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely used anti-AIDS drug (Gilchrist, 1997). In the quest for further biologically active pyrimidine compounds, the title compound, (I), has been synthesized and its crystal structure determined (Fig. 1).



(I)
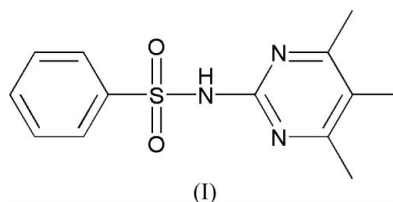
In (I), there are intermolecular N—H···O hydrogen-bond interactions, giving rise to dimers of the title compound (Fig. 2). The N1—H1···O1 distances and angle are 2.242 Å, 2.918 Å and 135.5°. In the crystal structure, the plane of the
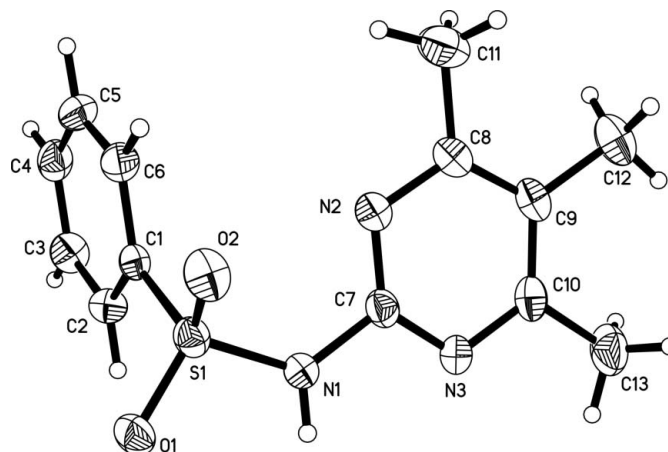


**Figure 1**
The asymmetric unit of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level.

pyrimidine ring makes an angle of 81.90 (8)° with the plane of the benzene ring.

## Experimental

Benzenesulfonyl chloride (0.37 g, 2.1 mmol) was added to a mixture of dry pyridine (4 ml) and 4,5,6-trimethylpyrimidin-2-amine(0.28 g, 2 mmol). The mixture was heated to 333 K slowly, and the temperature was maintained for 5 h. The solvent was evaporated *in vacuo* and the residue was added to water (5 ml). The mixture was filtered off and gave a brown solid, which was dissolved in ethanol (10 ml) and then decolourized with active carbon, giving the title compound (I) (0.23 g, 42% yield). The title compound was recrystallized from ethanol, yielding single crystals of (I) (m.p. 472–473 K).

*Crystal data*

| | |
|---|---|
| $C_{13}H_{15}N_3O_2S$ | $V = 682.0 (3)$ Å$^3$ |
| $M_r = 277.34$ | $Z = 2$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.351$ Mg m$^{-3}$ |
| $a = 7.7014 (19)$ Å | Mo $K\alpha$ radiation |
| $b = 8.831 (2)$ Å | $\mu = 0.24$ mm$^{-1}$ |
| $c = 10.849 (3)$ Å | $T = 294 (2)$ K |
| $\alpha = 83.894 (4)°$ | Prism, colorless |
| $\beta = 70.965 (4)°$ | $0.20 \times 0.18 \times 0.14$ mm |
| $\gamma = 78.118 (4)°$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3506 measured reflections |
| | 2399 independent reflections |
| $\varphi$ and $\omega$ scans | 1743 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (*SADABS*, Sheldrick, 1996) | $R_{int} = 0.018$ |
| $T_{min} = 0.954$, $T_{max} = 0.967$ | $\theta_{max} = 25.0°$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0691P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | $+ 0.0938P]$ |
| $wR(F^2) = 0.130$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.06$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 2399 reflections | $\Delta\rho_{max} = 0.27$ e Å$^{-3}$ |
| 175 parameters | $\Delta\rho_{min} = -0.27$ e Å$^{-3}$ |
| H-atom parameters constrained | |

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.
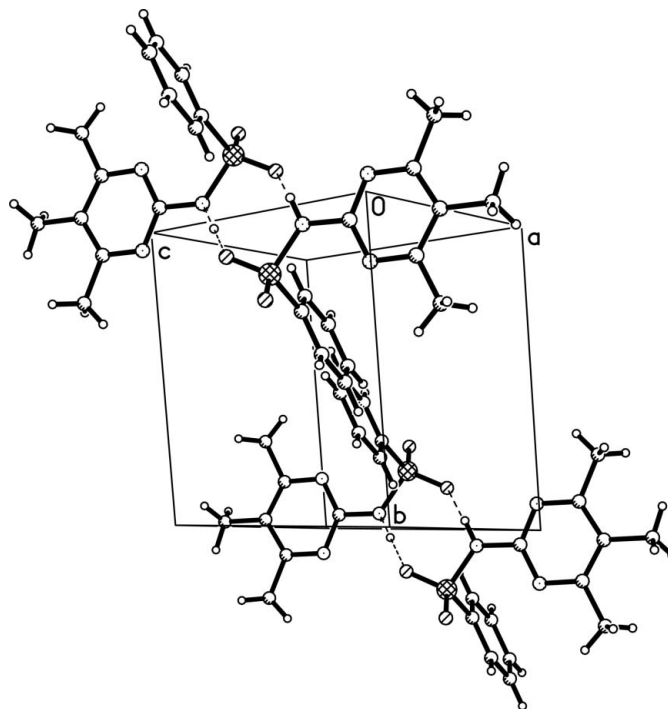


**Figure 2**
A view of the intermolecular N—H···O hydrogen-bond interactions (dashed lines) in (I).

## References

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