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Key indicators

 Single-crystal X-ray study
 $T = 150$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.053
 wR factor = 0.133
 Data-to-parameter ratio = 17.5

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

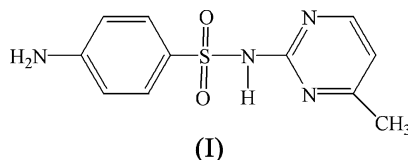
A new polymorph of sulfamerazine

 In the title compound, $\text{C}_{11}\text{H}_{12}\text{N}_4\text{O}_2\text{S}$, molecules are linked by
 intermolecular $\text{N}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds,
 forming a hydrogen-bonded network.

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Comment

 Two polymorphs of sulfamerazine were previously determined
 in the space groups *Pbca* (Acharya *et al.*, 1982) and *Pna2*₁
 (Caria & Mohamed, 1992). We have now obtained a new
 polymorph of sulfamerazine, (I), which crystallizes in the
 space group *P2*₁/*c* and its crystal structure is reported here.

 In the molecule of compound (I) (Fig. 1), the bond lengths
 and angles (Table 1) are in normal ranges (Allen *et al.*, 1987).
 The shortening of the C18–N14 [1.364 (3) Å], C15–S11
 [1.734 (2) Å] and S11–N11 [1.6530 (19) Å] bonds with
 respect to the expected single-bond distances are attributed to
 $d\pi-p\pi$ interactions, and are comparable with the corre-
 sponding values of 1.363 (12), 1.735 (7) and 1.654 (2) Å
 obtained by Acharya *et al.* (1982), and of 1.357 (7), 1.354 (7),
 1.736 (4) and 1.654 (2) Å obtained by Caria & Mohamed
 (1992). The endocyclic N12–C11–N13 angle of 127.5 (2)° is
 also comparable with the corresponding values in the other
 two polymorphs of sulfamerazine; these angles are consider-
 ably larger than the value usually observed for a pyrimidine
 ring.

 The planes of the benzene and pyrimidine rings are inclined
 to each other at 64.39 (2)°, which is comparable with the
 corresponding values of 71 (1)° (Acharya *et al.*, 1982) and
 61.5 (5) and 58.5 (5)° (Caria & Mohamed, 1992) in the other
 sulfamerazine polymorphs. These indicate that the molecules
 adopt a *gauche* conformation when viewed along the S–N
 vector. The tetrahedral geometry around atom S11 is
 distorted, as evidenced by the deviations of the bond angles
 around atom S11 atom from 109°.

 The crystal structure of (I) is stabilized by intermolecular
 $\text{N}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2), which
 result in the formation of a hydrogen-bonded network (Fig. 2).

Experimental

 Solid sulfamerazine was dissolved in dimethylformamide, filtered and
 left for crystallization by slow evaporation of the solvent at room

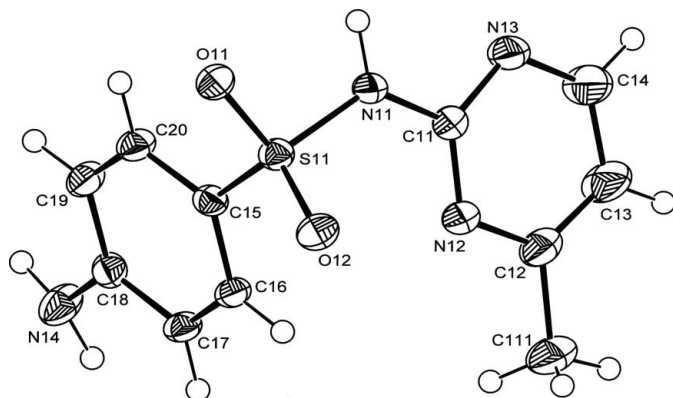


Figure 1

A drawing of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

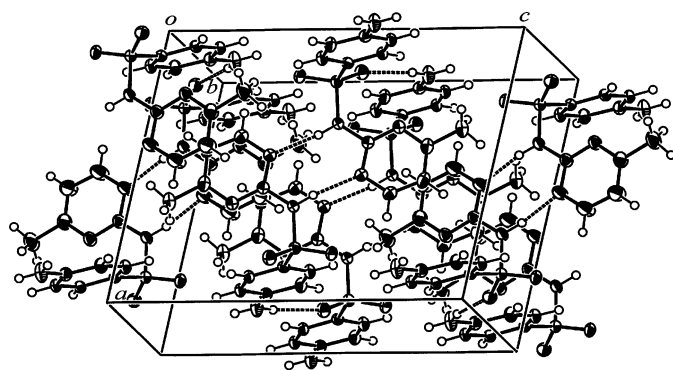


Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

temperature. Colourless block crystals were obtained after two weeks.

Crystal data

$C_{11}H_{12}N_4O_2S$
 $M_r = 264.31$
 Monoclinic, $P2_1/c$
 $a = 11.0966$ (5) Å
 $b = 8.3152$ (5) Å
 $c = 13.9640$ (7) Å
 $\beta = 99.327$ (4)°
 $V = 1271.43$ (11) Å³

$Z = 4$
 $D_x = 1.381$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.26$ mm⁻¹
 $T = 150$ (2) K
 Block, colourless
 $0.20 \times 0.15 \times 0.12$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.951$, $T_{\max} = 0.970$

11168 measured reflections
 2872 independent reflections
 2147 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.091$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.133$
 $S = 1.05$
 2872 reflections
 164 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.8661P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.28$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.55$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

S11—O11	1.4398 (16)	N12—C11	1.327 (3)
S11—O12	1.4293 (17)	N12—C12	1.345 (3)
S11—N11	1.6530 (19)	N13—C11	1.338 (3)
S11—C15	1.734 (2)	N13—C14	1.336 (3)
N11—C11	1.388 (3)	N14—C18	1.364 (3)
O11—S11—O12	119.28 (10)	N11—C11—N12	118.5 (2)
O11—S11—N11	102.31 (9)	N11—C11—N13	114.0 (2)
O12—S11—N11	109.06 (10)	N12—C11—N13	127.5 (2)
O11—S11—C15	109.20 (10)	N12—C12—C13	121.0 (2)
O12—S11—C15	109.54 (10)	N13—C14—C13	122.9 (3)
N11—S11—C15	106.59 (10)	C16—C15—S11	119.56 (17)
C11—N11—S11	126.20 (16)	C20—C15—S11	120.38 (18)
C11—N12—C12	116.2 (2)	N14—C18—C17	120.8 (2)
C11—N13—C14	114.6 (2)	N14—C18—C19	120.4 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N11—H11 ⁱ ⋯N13 ⁱ	0.88	2.08	2.912 (3)	158
N14—H14A ⁱⁱ ⋯O11 ⁱⁱ	0.88	2.43	3.089 (3)	132
N14—H14B ⁱⁱⁱ ⋯O12 ⁱⁱⁱ	0.88	2.14	2.985 (3)	160

Symmetry codes: (i) $-x + 1, -y, -z + 1$; (ii) $x, -y - \frac{1}{2}, z + \frac{1}{2}$; (iii) $x, y - 1, z$.

H atoms were positioned geometrically, with N—H = 0.88 Å (for NH and NH₂) and C—H = 0.95 and 0.98 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N})$, where $x = 1.5$ for methyl H and 1.2 for all other H.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; 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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