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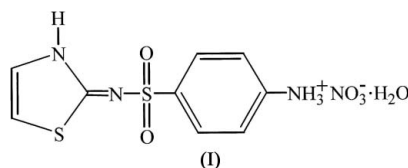
Key indicators

Single-crystal X-ray study
 $T = 120$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.038
 wR factor = 0.105
Data-to-parameter ratio = 14.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Sulfathiazolium nitrate monohydrate

The title compound, $\text{C}_9\text{H}_{10}\text{N}_3\text{O}_2\text{S}_2^+\cdot\text{NO}_3^-\cdot\text{H}_2\text{O}$, was obtained from a solution of sulfathiazole in dilute nitric acid at room temperature. The crystal structure is stabilized by a network of hydrogen bonds and van der Waals interactions.Received 16 March 2006
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Comment

Sulfathiazole has a remarkable solvate-forming ability with interesting structural and conformational properties. Many solvent-containing sulfathiazoles are known and a lot of them have been studied crystallographically (Bingham *et al.*, 2001).Shirovani *et al.* (1983) described three solvates of sulfathiazole and Caira *et al.* (1994) reported the crystal structure of the 1:1 complex of sulfathiazole and cyclodextrin, in which the molecules are hydrogen bonded with each other, forming a layer and these layers are linked by hydrogen bonds with water molecules.

The sulfathiazole molecule in the title complex, (I), is hydrogen bonded with a nitrate ion which is also hydrogen bonded with the water molecule. The sulfathiazole molecule is protonated on its terminal amino group.

The planes of the benzene and thiazole rings are inclined in a *gauche* conformation about the S12–N11 bond with a dihedral angle of $87.63(6)^\circ$. The crystal structure is stabilized by a network of hydrogen bonds and van der Waals interactions.

Experimental

Solid sulfathiazole (0.255 g; 1 mmol) was dissolved in 1M HNO_3 acid (50 ml) and stirred for 30 minutes, filtered off and the clear solution was left at room temperature for crystallization. Pale-yellow platelike crystals of sulfathiazole nitrate were obtained by slow evaporation of the solution.

Crystal data

 $\text{C}_9\text{H}_{10}\text{N}_3\text{O}_2\text{S}_2^+\cdot\text{NO}_3^-\cdot\text{H}_2\text{O}$
 $M_r = 336.35$
 Monoclinic, $P2_1/c$
 $a = 12.1917(2)$ Å
 $b = 7.6348(2)$ Å
 $c = 15.3895(2)$ Å
 $\beta = 107.4664(14)^\circ$
 $V = 1366.43(5)$ Å³
 $Z = 4$
 $D_x = 1.635$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 8182 reflections
 $\theta = 2.9\text{--}27.5^\circ$
 $\mu = 0.42$ mm⁻¹
 $T = 120(2)$ K
 Plate, pale yellow
 $0.34 \times 0.32 \times 0.05$ mm

Data collection

Nonius KappaCCD diffractometer
 ω scans
 Absorption correction: multi-scan
 (Blessing; 1995)
 $T_{\min} = 0.869$, $T_{\max} = 0.979$
 17799 measured reflections
 3117 independent reflections

2669 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.081$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -15 \rightarrow 15$
 $k = -9 \rightarrow 9$
 $l = -19 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.106$
 $S = 1.05$
 3117 reflections
 214 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.5659P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.47 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.61 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

S11—C11	1.7362 (17)	N13—C17	1.462 (2)
S11—C12	1.732 (2)	C12—C13	1.335 (3)
S12—O11	1.4566 (13)	C14—C15	1.381 (2)
S12—O12	1.4436 (13)	C14—C19	1.398 (2)
S12—N11	1.5824 (15)	C15—C16	1.392 (2)
S12—C14	1.7740 (17)	C16—C17	1.382 (2)
N11—C11	1.344 (2)	C17—C18	1.382 (2)
N12—C11	1.335 (2)	C18—C19	1.384 (3)
N12—C13	1.384 (2)		
C11—S11—C12	90.84 (8)	C13—C12—S11	111.26 (14)
O11—S12—O12	117.06 (8)	C12—C13—N12	112.90 (17)
O11—S12—N11	104.67 (8)	C15—C14—C19	121.33 (15)
O12—S12—N11	114.68 (8)	C15—C14—S12	120.22 (13)
O11—S12—C14	106.67 (8)	C19—C14—S12	118.45 (13)
O12—S12—C14	106.87 (8)	C14—C15—C16	119.52 (15)
N11—S12—C14	106.17 (8)	C15—C16—C17	118.86 (15)
C11—N11—S12	120.76 (13)	C16—C17—C18	121.95 (16)
C11—N12—C13	115.14 (15)	C16—C17—N13	119.15 (15)
N12—C11—N11	119.41 (15)	C18—C17—N13	118.90 (15)
N12—C11—S11	109.85 (12)	C17—C18—C19	119.43 (16)
N11—C11—S11	130.74 (14)	C14—C19—C18	118.90 (16)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N13—H13A \cdots O1	0.95 (1)	1.82 (1)	2.765 (2)	177 (2)
O4—H4A \cdots O2	0.95 (1)	1.87 (1)	2.8027 (19)	170 (2)
N12—H12A \cdots O4 ⁱ	0.95 (1)	2.00 (1)	2.9050 (19)	159 (2)
O4—H4B \cdots O11 ⁱ	0.95 (1)	1.97 (1)	2.8807 (18)	162 (2)
N13—H13C \cdots O11 ⁱⁱ	0.88 (3)	2.03 (3)	2.907 (2)	176 (2)
N13—H13B \cdots O4 ⁱⁱⁱ	0.95 (1)	1.91 (1)	2.857 (2)	175 (2)

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

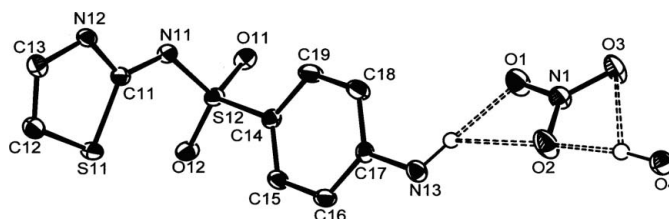


Figure 1

View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms not involved in hydrogen bonding (dashed lines) have been omitted.

C-bound H atoms were included in the riding model approximation with $C-H = 0.95 \text{ \AA}$, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms attached to N and O were located in an electron density map and refined isotropically with the N—H and O—H bond lengths restrained to $0.95 (5) \text{ \AA}$.

Data collection: COLLECT (Nonius, 1997–2000); cell refinement: HKL SCALEPACK (Otwinowski & Minor 1997); data reduction: HKL DENZO (Otwinowski & Minor 1997) and SCALEPACK; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); 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 publication routines (Farrugia, 1999).

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