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1,3,4-Thiadiazolium-2-thiolate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(N–C) = 0.002 Å
R factor = 0.021
wR factor = 0.056
Data-to-parameter ratio = 19.0

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

Molecules of the title compound, $C_2H_2N_2S_2$, exist in the crystal structure in the zwitterionic form with the thiol group deprotonated. Hydrogen bonds between the protonated N atoms and the thiolate S atoms link the molecules in a zigzag packing arrangement parallel to the *ac* plane.

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Comment

Thiadiazoles have attracted increasing attention because of their potential applications in pharmaceutical, agricultural, industrial, coordination and polymer chemistry (Coyanis *et al.*, 2002; Wang & Cao, 2005).

(I)

Molecules of the title compound, (I), exist in the crystal structure in a zwitterionic form, with the thiadiazole atom N1 protonated and the thiol substituent deprotonated (Fig. 1). The thiodiazole ring is planar, with a maximum deviation from the ring plane of 0.0082 (7) Å for atom N1. The thiolate atom S2 lies 0.018 (6) Å from that plane.

N1—H1···S2 hydrogen bonds link adjacent molecules in a zigzag network parallel to the *ac* plane (Figs. 2 and 3).

Experimental

Dilute hydrochloric acid (a few drops) was added to a solution of 2-mercapto-1,3,4-thiadiazole (1 g) in water (20 ml). Subsequent crystallization over 2 weeks gave colourless needle-like crystals of (I) suitable for X-ray diffraction analysis.

Crystal data

$C_2H_2N_2S_2$
M_r = 118.18
Orthorhombic, *Pbca*
a = 8.623 (2) Å
b = 8.249 (2) Å
c = 13.075 (3) Å
V = 930.0 (4) Å^3
Z = 8
D_x = 1.688 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4625 reflections
θ = 3.1–28.3°
μ = 0.97 mm^{-1}
T = 296 (2) K
Needle, colourless
0.32 × 0.13 × 0.13 mm

Data collection

Bruker APEX-2 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.747, T_{max} = 0.884
7289 measured reflections
1066 independent reflections
1000 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

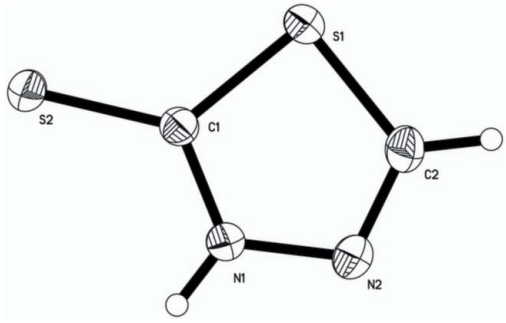

Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.056$
$S = 1.06$
1066 reflections
56 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 0.2499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.069 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···S2^{i}	0.86	2.40	3.2527 (13)	170

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

H atoms were treated as riding, with C—H = 0.93 Å and N—H = 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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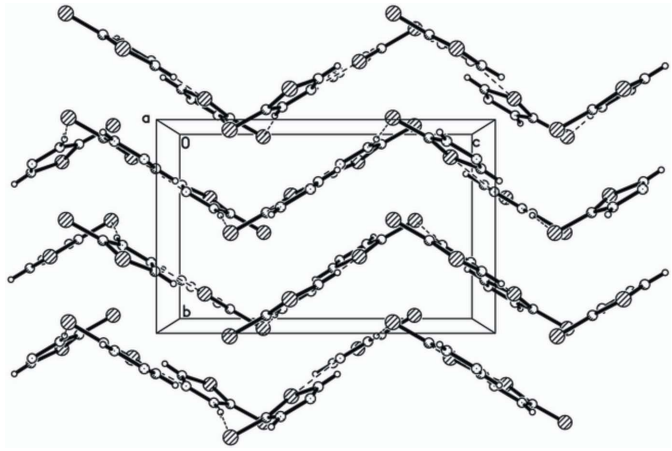

Figure 2
The one-dimensional chain structure of (I) formed by N—H···S hydrogen bonds (dashed lines) along the *c* axis.

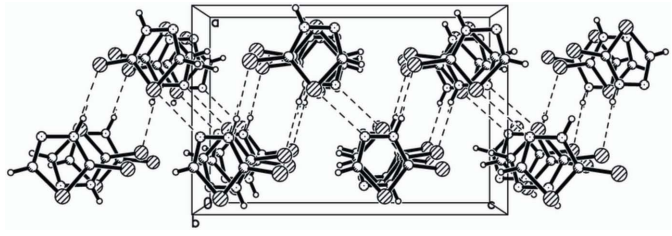

Figure 3
The zigzag packing arrangement of (I) in the *ac* plane. Hydrogen bonds are drawn as dashed lines.

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