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5-[(1*H*-1,2,4-Triazol-1-yl)methyl]-1,3,4-thiadiazole-2(3*H*)-thione

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Key indicators

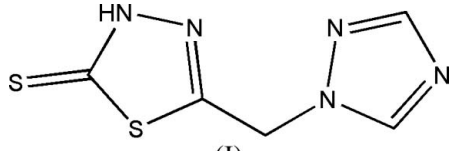
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.146
Data-to-parameter ratio = 17.7

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

In the title molecule, $C_5H_5N_5S_2$, the dihedral angle between the mean planes of the triazole and 1,3,4-thiadiazole-2(3*H*)-thione groups is 74.21 (3)°. In the crystal structure, intermolecular N—H···N hydrogen bonds link the molecules into zigzag linear chains extended along the *b* axis.

Comment

It has been found that 1,3,4-thiadiazoles possess a broad spectrum of biological activities and can be widely used as fungicides (Sharma & Bahel, 1982) and insecticides (Grasso, 1988). As an important type of fungicides, triazole compounds are highly efficient and have low toxicity (Xu *et al.*, 2002, 1998). The title compound, (I), contains the 1,3,4-thiadiazole and triazole fragments in one molecule (Fig. 1). We present its crystal structure here.



(I)

In the molecule of (I), the C1—N2 and C2—N3 bond lengths (Table 1) are close to the C=N double-bond length of 1.33 Å (John, 1998), showing that these two bonds have the features of unsaturated double bonds. Atoms S1, N4, N5, C3, C4 and C5 are essentially coplanar, the largest deviation from the least-squares plane being 0.016 (2) Å for atom C5. The dihedral angle between the mean planes of the triazole and 1,3,4-thiadiazole-2(3*H*)-thione rings is 74.21 (3)°.

An intermolecular N—H···N hydrogen bond (Table 2) links the molecules into zigzag linear chains extending along the *b* axis. The crystal packing (Fig. 2) is further stabilized by weak C—H···N interactions (Table 2).

Experimental

Potassium 1*H*-1,2,4-triazol-1-acetyldithiocarbazate (0.01 mol) in concentrated sulfuric acid (20 ml) was stirred for 10 h in an ice–water bath. The reaction mixture was then poured gradually on to crushed ice with stirring and the pH altered to 3–4 to afford the title compound, (I) (1.19 g, yield 60%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_5H_5N_5S_2$
M_r = 199.26
Monoclinic, $P2_1/n$
a = 7.0957 (14) Å
b = 13.152 (3) Å
c = 9.3478 (19) Å
β = 101.11 (3)°
V = 856.0 (3) Å^3
Z = 4
D_x = 1.546 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 293 (2) K
Block, colourless
0.51 × 0.42 × 0.37 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.759, T_{max} = 0.816
6862 measured reflections
1931 independent reflections
1346 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.146
S = 1.02
1931 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C4	1.740 (3)	N3—C2	1.329 (3)
S2—C5	1.662 (3)	N4—N5	1.364 (3)
N1—N3	1.363 (3)	N5—C5	1.342 (3)
N2—C1	1.358 (3)		
C4—S1—C5	89.47 (12)	C4—N4—N5	110.6 (2)
C1—N1—N3	102.3 (2)	N4—C4—C3	121.6 (2)
C2—N3—N1	109.9 (2)	N4—C4—S1	114.29 (18)
C2—N3—C3	131.1 (2)	S2—C5—S1	126.92 (16)
N1—N3—C3	119.0 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5A···N2^{i}	0.86	1.94	2.780 (3)	166
C2—H2B···N1^{ii}	0.93	2.41	3.331 (3)	169

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

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and N—H =0.86 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent).

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXL97*.

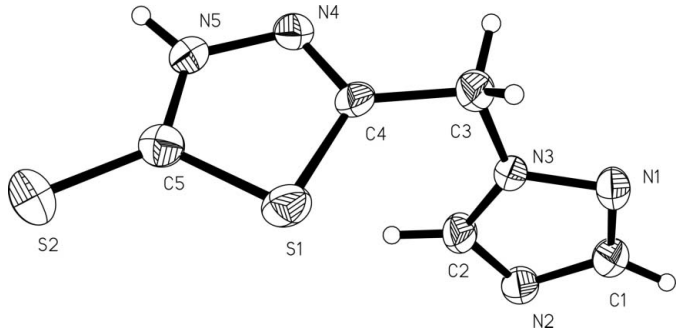


Figure 1
A view of (I), with displacement ellipsoids drawn at the 40% probability level.

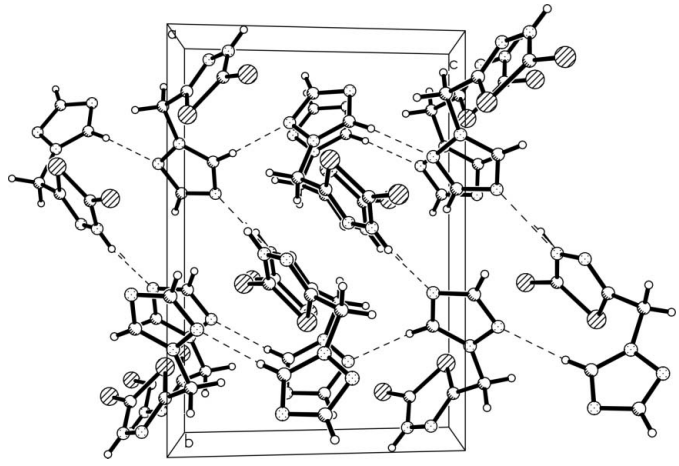


Figure 2
A packing diagram of the title compound, viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

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