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Synthesis, crystal structure and Hirshfeld surface analysis of 5-methyl-2-[(1,3-thiazol-2-yl)sulfanyl]-1,3,4-thiadiazole

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The title compound, $C_6H_5N_3S_3$, consists of two biologically relevant heterocyclic units, suggesting potential biological activity and possible use as a ligand in metal complexation. The compound crystallizes in the monoclinic space group $P2_1/c$ and features non-classical intermolecular $C-H \cdots N$ hydrogen bonds, along with $\pi-\pi$ stacking interactions that contribute to the crystal cohesion. Hirshfeld surface analysis highlights significant intermolecular interactions including, among others, $N \cdots H/H \cdots N$, $S \cdots H/H \cdots S$, and $S \cdots C/C \cdots S$ contacts.

1. Chemical context

Derivatives combining 1,3,4-thiadiazole and 1,3-thiazole moieties offer significant potential in medicinal chemistry due to their enhanced biological activity, pharmacokinetic profiles and structural versatility. This class of compounds is being actively explored in various therapeutic areas, including their use as antimicrobial (Booq *et al.*, 2021; Hussain *et al.*, 2022), anticancer (Shaikh *et al.*, 2024; Altuntop *et al.*, 2017; Dawood *et al.*, 2013), anti-inflammatory (Arshad *et al.*, 2022) and neuroprotective agents. With ongoing research into their SAR, bioavailability, and environmental impact, these derivatives are promising candidates for the next generation of drug development.

The structural fusion of 1,3,4-thiadiazole and 1,3-thiazole is expected to have synergistic biological effects due to their different modes of action. Thiadiazoles are often involved in enzyme inhibition and interaction with metal ions, while thiazoles enhance interactions with biological targets such as nucleic acids or proteins.

Herein, we report the synthesis and crystal structure of a new heterocyclic compound with combination of 1,3,4-thiadiazole and 1,3-thiazole fragments. This 2-thiazole-substituted derivative can act as a chelating ligand.





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Figure 1

A view of the molecular structure of 5-methyl-2-[(1,3-thiazol-2-yl) sulfanyl]-1,3,4-thiadiazole, showing the atom labeling and bond lengths. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The title compound (Fig. 1) crystallizes in the monoclinic system, space group $P2_1/c$. The molecular structure of the compound is shown in Fig. 1. The geometric parameters of the thiadiazole and thiazole rings are close to standard values and the values reported for related structures. (Renier et al., 2023; Luqman et al., 2016; Burnett et al., 2015; Dani et al., 2014; Weidner et al., 2008; Jumal et al., 2006; Kennedy et al., 2004; Hipler et al., 2003). The N-N and endocyclic C-S bonds are shorter than classical single bonds (1.4 and 1.81 Å), indicating partial double-bond character. At the same time, the C=N bonds are somewhat longer (~ 0.02 Å) than the corresponding double bond, as a result of conjugation within the ring systems. These facts confirm the aromaticity of both rings. The exocyclic C-S bond is shortened since it includes carbon atoms with sp^2 hybridization. Deviation of the bond angles from 120° in the 1,3,4-thiadiazole and 1,3-thiazole rings is a common feature in five-membered rings (Bharty et al., 2012). The C-S-C bond angles in the 1,3,4-thiadiazole and 1,3thiazole rings of the title compound are 86.62 (8) and $89.25 (9)^{\circ}$, respectively, and the C1-S2-C3 bond angle outside the ring is $103.82 (8)^{\circ}$. The thiadiazole and thiazole rings do not lie in the same plane, subtending a dihedral angle of 32.61 (10)°. No intramolecular hydrogen bonds are observed.

3. Supramolecular features and energy framework calculations

The crystal packing is consolidated by $C5-H5\cdots N3^{ii}$ hydrogen bonds [symmetry code: (ii) x + 1, y, z + 1], forming a six-membered R_2^2 (6) ring motif (Grabowski, 2020; Etter *et al.*, 1990). Along the *a*-axis direction, cohesion of the crystal packing is achieved by $C4-H4\cdots N2^i$ hydrogen bonds [symmetry code: (i) x + 1, y, z] between the methine group of the 1,3-thiazole ring and the nitrogen atom of the 1,3,4-thiadiazole ring of a nearby molecule. The geometrical parameters of intermolecular hydrogen bonds are shown in Table 1 and Fig. 2*a*.

In the supramolecular structure of the compound, weak π - π -stacking interactions are found (Fig. 2*b*) between thia-

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C4 - H4 \cdots N2^{i}$	0.93	2.55	3.472 (2)	169
$C5 - H5 \cdots N3^{ii}$	0.93	2.63	3.392 (3)	139

Symmetry codes: (i) x + 1, y, z; (ii) -x + 1, -y, -z + 1.

diazole rings (symmetry operation -x, 1 - y, 1 - z) with an intracentroid distance of 3.889 (9) Å and between thiazole rings (symmetry operation -x, -y, 1 - z) with a centroid-to-centroid distance of 3.809 (9) Å. Similarly, the structure also exhibits intermolecular chalcogen bond between C5 of the thiazole ring and the bridging S2 atom $[C5 \cdots S2(1 - x, -\frac{1}{2} + y, \frac{3}{2} - z) = 3.491$ (2) Å] (Fig. 2c).

The interaction energies of the hydrogen-bond system were calculated within the molecules using the B3LYP method (B3LYP/6-31G (d, p) in *CrystalExplorer 21.5* (Spackman *et al.*, 2021). The total energy (E_{tot}) is the sum of Coulombic (E_{ele}), polar (E_{pol}), dispersion (E_{dis}) and repulsive (E_{rep}) contributions. The four energy components were scaled in the total



Figure 2

(a) Overview of intermolecular C4-H4···N2 and C5-H5···N3 hydrogen bonds (shown in blue), (b) a view of the π - π stacking interactions (hydrogen bonds are shown in blue and π - π stacking interactions are shown in green). and (c) Highlight of S2···C5 chalcogen interactions (dashed lines) along the *b*-axis direction, with relevant atoms labeled.



Figure 3 View of the three-dimensional Hirshfeld surface of the molecule plotted over d_{norm} .

energy: $E_{tot} = 1.057 E_{ele} + 0.74 E_{pol} + 0.871 E_{dis} + 0.618 E_{rep}$. The interaction energies were investigated for a 3.8 Å cluster around the reference molecule. The results give a total interaction energy of -141 kJ mol^{-1} involving electrostatic ($-74.3 \text{ kJ mol}^{-1}$), polarization ($-12.2 \text{ kJ mol}^{-1}$), dispersion ($-146.9 \text{ kJ mol}^{-1}$) and repulsion (125 kJ mol^{-1}) components.

4. Hirshfeld surface analysis

To further investigate the intermolecular interactions present in the title compound, a Hirshfeld surface analysis was performed, and the two-dimensional (2D) fingerprint plots were generated with *CrystalExplorer17* (Spackman *et al.*, 2021). Fig. 3 shows the three-dimensional (3D) Hirshfeld surface of the complex plotted over d_{norm} (normalized contact distance). The hydrogen-bond interactions given in Table 1 play a key role in the molecular packing of the complex. The overall 2D fingerprint plot and those divided into interatomic interactions are shown in Fig. 4. The Hirshfeld surface analysis shows that 24.3% of the intermolecular interactions are from $N \cdots H/H \cdots N$ contacts, 21.1% from $S \cdots H/H \cdots S$ contacts, 17.7% from $H \cdots H$ contacts and 9.7% are from $S \cdots C/C \cdots S$ contacts, while other contributions are from $C \cdots H/H \cdots C$, $S \cdots C/C \cdots S$ and $S \cdots N/N \cdots S$ contacts (Fig. 4).

5. Database survey

A survey of the Cambridge Structural Database performed using ConQuest software (CSD, Version 5.46, last updated November 2024; Groom et al., 2016) revealed that 122 crystal structures have been reported for the 2-methyl-1,3,4-thiadiazole-5-thiol fragment; among them, 73 structures are related to organometallic compounds. There are mostly organic thiol-substituted compounds reported, because of the good reactivity of the thiol group. In addition, there are three organic structures based on the 2-methyl-1,3,4-thiadiazole-5thiol fragment (CILHAI, Dani et al., 2013; GEXWOY, Zhao et al., 2010; XICMOO, Cabral et al., 2018), which can bind in a bidentate manner with metal atoms to form six-membered rings. Similar to C₆H₅N₃S₃, chalcogen-bonding interactions were observed in both structures. In CILHAI, S-N chalcogen interactions occur where both nitrogen atoms of the thiadiazole ring interact with the bridging sulfur atom and the sulfur atom of an adjacent thiadiazole ring. In XICMOO, a chalcogen interaction is present between a sulfur atom and a carbon atom of a neighboring benzene ring.



Figure 4

The full two-dimensional fingerprint plot for the title compound, showing all interactions, and those delineated into separate interactions with the percentage contributions of various interatomic contacts occurring in the crystal.

research communications

Table 2

Experimental details.

Crystal data	
Chemical formula	$C_6H_5N_3S_3$
M _r	215.31
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	10.6463 (2), 7.7151 (2), 11.1774 (3)
β (°)	103.272 (1)
$V(Å^3)$	893.56 (4)
Ζ	4
Radiation type	Μο Κα
$\mu (\mathrm{mm}^{-1})$	0.77
Crystal size (mm)	$0.13 \times 0.1 \times 0.06$
Dete sellestica	
Data collection	
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTON II CPAD
Absorption correction	Multi-scan (SADABS; Krause et al., 2015)
No. of measured, independent and	18027, 2296, 1988
observed $[I > 2\sigma(I)]$ reflections	
R _{int}	0.052
$(\sin \theta / \lambda)_{\rm max} ({\rm \AA}^{-1})$	0.677
Refinement	
$R[F^2 > 2\sigma(F^2)] = wR(F^2)$ S	0.034 0.088 1.05
No of reflections	2296
No of parameters	110
H-atom treatment	H-atom parameters constrained
$\Delta \rho_{\text{max}} \Delta \rho_{\text{min}} (e \text{ Å}^{-3})$	0.500.48
$E \prod a \lambda = E \prod \prod \lambda = \frac{1}{2} + \frac{1}{2}$	· · · · · · · · · · · · · · · · · · ·

Computer programs: APEX2 and SAINT (Bruker, 2016), SHELXT2014/5 (Sheldrick, 2015a), SHELXL2016/6 (Sheldrick, 2015b) and OLEX2 (Dolomanov et al., 2009).

6. Synthesis and crystallization

A solution of 5-methyl-1,3,4-thiadiazole-2-thiol (0.01 mol) and 2-bromothiazole (0.01 mol) in DMF (10 ml) in presence of cesium carbonate was stirred for 5 h at 413 K. DMF was distilled off with a rotary evaporator. The resulting brown concentrate was dissolved in DCM/MeOH and separated by flash column chromatography. The synthesized amorphous product 2-methyl-5-(1,3-thiazol-2-ylsulfanyl)-1,3,4-thiadiazole was light yellow in color (m.p. 327 K). Further recrystallization gave crystals suitable for X-ray diffraction (yield: 60%).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically (C-H = 0.93–0.96 Å) and refined as riding with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm C}$ -methyl).

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Computing details

5-Methyl-2-[(1,3-thiazol-2-yl)sulfanyl]-1,3,4-thiadiazole

Crystal data

C₆H₅N₃S₃ $M_r = 215.31$ Monoclinic, $P2_1/c$ a = 10.6463 (2) Å b = 7.7151 (2) Å c = 11.1774 (3) Å $\beta = 103.272$ (1)° V = 893.56 (4) Å³ Z = 4

Data collection

Bruker D8 VENTURE Kappa Duo PHOTON II CPAD diffractometer φ and ω scans Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)

18027 measured reflections

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.088$ S = 1.052296 reflections 110 parameters 0 restraints F(000) = 440 $D_x = 1.600 \text{ Mg m}^{-3}$ Mo K α radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 8027 reflections $\theta = 3.5-28.7^{\circ}$ $\mu = 0.77 \text{ mm}^{-1}$ T = 296 KBlock, colourless $0.13 \times 0.1 \times 0.06 \text{ mm}$

2296 independent reflections 1988 reflections with $I > 2\sigma(I)$ $R_{int} = 0.052$ $\theta_{max} = 28.7^{\circ}, \ \theta_{min} = 3.6^{\circ}$ $h = -13 \rightarrow 14$ $k = -10 \rightarrow 10$ $l = -15 \rightarrow 15$

Primary atom site location: structure-invariant direct methods Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 0.4384P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} = 0.001$ $\Delta\rho_{max} = 0.50$ e Å⁻³ $\Delta\rho_{min} = -0.48$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

	x	у	Z	$U_{\rm iso}$ */ $U_{\rm eq}$
S1	0.18439 (4)	0.24766 (7)	0.46938 (4)	0.04704 (14)
S2	0.34737 (4)	0.41561 (7)	0.71120 (4)	0.04642 (14)
S3	0.61254 (5)	0.45960 (7)	0.67293 (6)	0.05644 (16)
N1	0.10297 (15)	0.3506 (3)	0.65446 (15)	0.0558 (4)
N2	-0.00530 (15)	0.2958 (3)	0.56825 (16)	0.0591 (5)
N3	0.46784 (15)	0.2117 (2)	0.57237 (16)	0.0497 (4)
C1	0.20708 (15)	0.3340 (2)	0.61488 (15)	0.0384 (3)
C2	0.02170 (17)	0.2417 (3)	0.46812 (17)	0.0449 (4)
C3	0.47049 (15)	0.3452 (2)	0.64267 (14)	0.0358 (3)
C4	0.67326 (17)	0.3165 (3)	0.58452 (17)	0.0460 (4)
H4	0.756109	0.320593	0.570753	0.055*
C5	0.58447 (17)	0.1979 (3)	0.53809 (18)	0.0479 (4)
Н5	0.599905	0.110958	0.485673	0.058*
C6	-0.07813 (19)	0.1783 (4)	0.3609 (2)	0.0606 (6)
H6A	-0.089445	0.261709	0.295572	0.091*
H6B	-0.158370	0.162416	0.384862	0.091*
H6C	-0.050886	0.069815	0.333151	0.091*

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

Atomic displacement parameters $(Å^2)$

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0320 (2)	0.0677 (3)	0.0452 (2)	-0.00771 (18)	0.01673 (17)	-0.0140 (2)
S2	0.0357 (2)	0.0601 (3)	0.0451 (2)	-0.00303 (18)	0.01261 (17)	-0.0143 (2)
S3	0.0371 (2)	0.0589 (3)	0.0750 (4)	-0.0130 (2)	0.0165 (2)	-0.0186 (3)
N1	0.0346 (7)	0.0911 (13)	0.0452 (8)	-0.0027 (8)	0.0164 (6)	-0.0116 (9)
N2	0.0312 (7)	0.0991 (14)	0.0502 (9)	-0.0052 (8)	0.0160 (7)	-0.0104 (9)
N3	0.0372 (7)	0.0557 (9)	0.0591 (9)	-0.0067 (7)	0.0175 (7)	-0.0144 (8)
C1	0.0336 (7)	0.0455 (9)	0.0382 (8)	0.0005 (6)	0.0128 (6)	0.0004 (7)
C2	0.0313 (8)	0.0600 (11)	0.0456 (9)	-0.0036 (7)	0.0131 (7)	-0.0005 (8)
C3	0.0292 (7)	0.0421 (8)	0.0354 (7)	0.0000 (6)	0.0058 (6)	0.0023 (6)
C4	0.0319 (8)	0.0571 (11)	0.0507 (10)	0.0024 (7)	0.0131 (7)	0.0058 (8)
C5	0.0387 (9)	0.0568 (11)	0.0512 (10)	0.0035 (8)	0.0163 (8)	-0.0054 (8)
C6	0.0377 (9)	0.0926 (17)	0.0509 (11)	-0.0108 (10)	0.0087 (8)	-0.0101 (11)

Geometric parameters (Å, °)

S1—C1	1.7222 (17)	N3—C3	1.292 (2)
S1—C2	1.7295 (17)	N3—C5	1.385 (2)
S2—C1	1.7460 (17)	C2—C6	1.490 (3)

supporting information

S2—C3	1.7496 (16)	C4—H4	0.9300
S3—C3	1.7162 (16)	C4—C5	1.332 (3)
S3—C4	1.705 (2)	С5—Н5	0.9300
N1—N2	1.388 (2)	С6—Н6А	0.9600
N1—C1	1.291 (2)	С6—Н6В	0.9600
N2—C2	1.287 (2)	С6—Н6С	0.9600
C1—S1—C2	86 62 (8)	N3—C3—S3	115 16 (12)
C1 - S2 - C3	103.82 (8)	S3-C4-H4	125.0
C4 - S3 - C3	89 25 (9)	C5-C4-S3	109.93(13)
C1—N1—N2	111.92 (15)	C5—C4—H4	125.0
C2—N2—N1	112.76 (15)	N3—C5—H5	121.9
C3—N3—C5	109.47 (15)	C4—C5—N3	116.16 (17)
S1—C1—S2	129.53 (9)	С4—С5—Н5	121.9
N1—C1—S1	114.64 (13)	С2—С6—Н6А	109.5
N1—C1—S2	115.66 (14)	С2—С6—Н6В	109.5
N2—C2—S1	114.04 (14)	С2—С6—Н6С	109.5
N2—C2—C6	123.05 (17)	H6A—C6—H6B	109.5
C6—C2—S1	122.91 (14)	H6A—C6—H6C	109.5
S3—C3—S2	117.96 (10)	H6B—C6—H6C	109.5
N3—C3—S2	126.86 (13)		
S2 C4 C5 N2	-1.7(2)	C^2 S1 C1 S2	-172 80 (14)
$S_{3} - C_{4} - C_{3} - N_{3}$	-1.7(2)	$C_2 = S_1 = C_1 = S_2$	-1/5.00(14)
N1 = N2 = C2 = C6	1.5(3)	$C_2 = S_1 = C_1 = S_1$	1.12(17) 12.27(15)
N1 - N2 - C2 - C6	-1/9.1(2)	$C_3 = S_2 = C_1 = S_1$	-13.37(15)
$N_2 - N_1 - C_1 - S_1$	-0.7(2)	$C_3 = S_2 = C_1 = N_1$	1/1./5(15)
$N_2 - N_1 - C_1 - S_2$	1/4.98 (15)	$C_3 = S_3 = C_4 = C_5$	1.02(15)
CI = SI = C2 = N2	-1.35(1/)	$C_3 - N_3 - C_5 - C_4$	1.6 (3)
C1 = S1 = C2 = C6	1/9.1 (2)	C4 = S3 = C3 = S2	1/8.5/(11)
C1 = S2 = C3 = S3	156.31 (10)	C4 - S3 - C3 - N3	-0.16 (15)
C1—S2—C3—N3	-25.35 (18)	C5—N3—C3—S2	-179.10 (14)
C1-N1-N2-C2	-0.4 (3)	C5—N3—C3—S3	-0.7 (2)

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	D····A	<i>D</i> —H··· <i>A</i>
C4—H4···N2 ⁱ	0.93	2.55	3.472 (2)	169
C5—H5····N3 ⁱⁱ	0.93	2.63	3.392 (3)	139

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) –*x*+1, –*y*, –*z*+1.