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2-[(5-Methyl-1,3,4-thiadiazol-2-yl)sulfanyl]-*N*′-(4-nitrobenzylidene)acetohydrazide monohydrate

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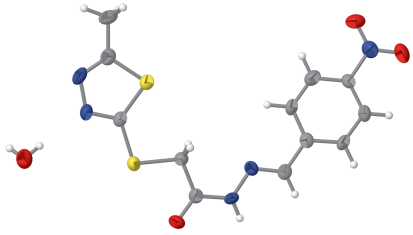
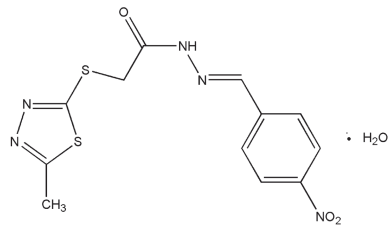
Structural data: full structural data are available from iucrdata.iucr.org

In the title hydrate, $C_{12}H_{11}N_5O_3S_2\cdot H_2O$, the dihedral angle between the aromatic rings is 9.6 (3)°. In the crystal, N—H···O and O—H···N hydrogen bonds link the components into $(10\bar{1})$ sheets.

3D view



Chemical scheme



Structure description

1,3,4-Thiadiazole derivatives exhibit various biological activities such as cytotoxic (Janowska *et al.*, 2020), anticancer (Hekal *et al.*, 2023), anticonvulsant (Luszczki *et al.*, 2015), anti-epileptic (Anthwal & Nain, 2022), antinociceptive (Altıntop *et al.*, 2016), antitubercular (Jain *et al.*, 2013), antimicrobial, antifungal and anthelmintic activities (Bhinge *et al.*, 2015). As part of the ongoing studies in this area, the present work describes the synthesis and structure of the title hydrate, $C_{12}H_{11}N_5O_3S_2\cdot H_2O$ (**I**) (Fig. 1 and scheme).

The dihedral angle between the C2/C5/N3/N4/S1 1,3,4-thiadiazole ring and the C10–C15 benzylidene ring is 9.6 (3)°. The torsion angles O1—C8—N1—N2, C7—C8—N1—N2 and C8—N1—N2—C9 are 177.1 (5), −2.5 (8) and 174.6 (5)°, respectively. The first and third of these indicate that the molecule adopts a near-planar *trans* conformation. The small value for the second appears to minimize steric hindrance and maintains overall near-planarity. The bond angles for the hydrazide nitrogen atoms (N1 and N2) are close to 120°, indicative of the expected sp^2 hybridization (Mohan *et al.*, 2011). Overall, the organic molecule is close to planar (r.m.s. deviation for the non-hydrogen atoms = 0.139 Å).

In the crystal, the components are linked by N—H···O_w and O_w—H···N (w = water) hydrogen bonds (Table 1), generating infinite $(10\bar{1})$ sheets. Various supramolecular

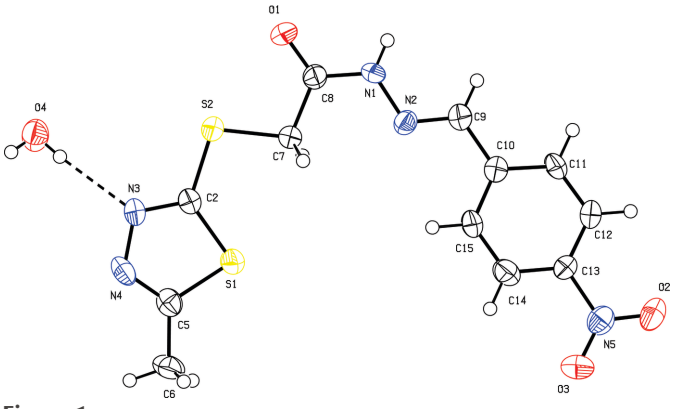


Figure 1
The molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level.

assemblies arise from this connectivity including $R_4^4(10)$ $R_2^2(24)$, $R_3^3(17)$, $R_4^4(10)$, $R_3^3(17)$ and $R_2^2(24)$ loops (Fig. 2). Two weak C—H···O interactions also occur.

The quantitative contribution of each type interaction to the Hirshfeld surface is provided in the two-dimensional finger print plots and it is supported by the HS mapped with d_{norm}. The O···H/H···O contacts provide a maximum contribution (28.4%) through strong hydrogen bonding, followed by H···H (25.2%), and a significant role is played by N···H/H···N (9.2%) contacts. The other contact types S···H/H···S (7.7%), C···H/H···C (8.6%) O···C/C···O (5.4%) N···C/C···N (3.9%) and S···O/O···S (3.4%) presumably play a minor role on the crystal packing of (**I**) (see Figs. S1 and S2 in the supporting information).

Synthesis and crystallization

The title compound was synthesized by mixing 20 mL of an ethanolic solution of (5-methyl-[1,3,4]lthiadiazol-2-ylsulfanyl) acetic acid hydrazide (0.25 mmol) and ethanol:water mixture (3:1 *v*/*v*) 4-nitrobenzaldehyde (0.25 mmol). The resulting mixture was refluxed under basic conditions for approximately 2 h. The resultant product was dissolved in 20 mL of ethanol, and the solution was allowed to crystallize *via* slow evaporation at room temperature, from which golden crystals of the title compound were harvested.

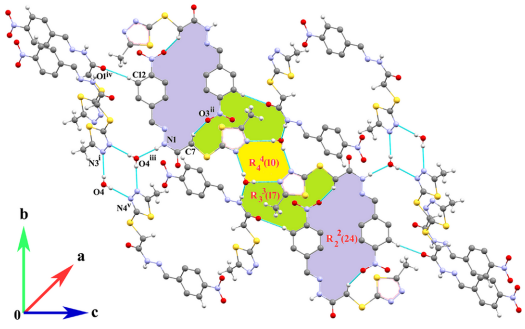


Figure 2
Part of a supramolecular layer in the crystal of (**I**) showing various supramolecular motifs. Symmetry codes (i) $-1+x, y, z$; (ii) $-x, -y, -z$; (iii) $\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (iv) $-\frac{3}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z$; (v) $1-x, -y, 1-z$].

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.82 (4)	2.08 (4)	2.900 (8)	176 (5)
O4—H4A···N4^{ii}	0.72 (9)	2.32 (9)	3.037 (8)	175 (10)
O4—H4B···N3	0.75 (8)	2.15 (9)	2.898 (8)	176 (13)
C7—H7B···O3^{iii}	0.97	2.51	3.400 (7)	153
C12—H12···O1^{iv}	0.93	2.46	3.349 (6)	159

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{11}N_5O_3S_2·H_2O$
M_r	355.39
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	273
a, b, c (Å)	4.9431 (3), 18.3181 (11), 17.2223 (9)
β (°)	95.557 (2)
V (Å^3)	1552.12 (16)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.37
Crystal size (mm)	0.14 × 0.10 × 0.04
Data collection	
Diffractometer	Bruker D8 Quest
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7776, 2857, 1703
R_{int}	0.098
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.090, 0.155, 1.22
No. of reflections	2857
No. of parameters	221
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.35

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *PLATON* (Spek, 2020), *Mercury* (Macrae *et al.*, 2020), *POVRay* (Cason, 2004) and *publCIF* (Westrip, 2010).

Refinement

The crystal data, data collection and structure refinement details for the compound are summarized in Table 2.

Acknowledgements

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full crystallographic data

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2-[(5-Methyl-1,3,4-thiadiazol-2-yl)sulfanyl]-*N*′-(4-nitrobenzylidene)acetohydrazide monohydrate

Murugan Nidhishree, Sundaramoorthy Gomathi, Jeyaraman Selvaraj Nirmalram and Logesh Mathivathanan

2-[(5-Methyl-1,3,4-thiadiazol-2-yl)sulfanyl]-*N*′-(4-nitrobenzylidene)acetohydrazide monohydrate

Crystal data

$C_{12}H_{11}N_5O_3S_2·H_2O$
M_r = 355.39
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 4.9431 (3) Å
b = 18.3181 (11) Å
c = 17.2223 (9) Å
β = 95.557 (2)°
V = 1552.12 (16) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.521 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2857 reflections
θ = 2.5–26.3°
μ = 0.37 mm^{-1}
T = 273 K
Trapezoid, gold
0.14 × 0.10 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
7776 measured reflections
2857 independent reflections
1703 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 26.3°, θ_{min} = 2.5°
h = −5→5
k = −22→19
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.090
$wR(F^2)$ = 0.155
S = 1.22
2857 reflections
221 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
W = 1/[$\Sigma^2(FO^2)$ + 5.0708P] WHERE P = (FO^2 + 2FC^2)/3
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.
The nitrogen- and oxygen-bound hydrogen atoms (H1, H14A & H14B) were located from the difference-Fourier map and refined freely. All other H atoms were positioned geometrically and refined *via* a riding model.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.3438 (3)	0.03917 (9)	0.27832 (9)	0.0388 (5)
S2	0.7558 (3)	0.16604 (9)	0.27385 (9)	0.0406 (6)
O1	0.8363 (9)	0.2756 (2)	0.1699 (2)	0.0502 (17)
O2	−0.8321 (10)	0.0733 (3)	−0.2101 (3)	0.0619 (17)
O3	−0.7278 (10)	−0.0085 (2)	−0.1227 (3)	0.0576 (17)
N1	0.5049 (11)	0.2563 (3)	0.0730 (3)	0.0344 (17)
N2	0.2957 (10)	0.2128 (3)	0.0442 (3)	0.0329 (17)
N3	0.7537 (10)	0.0603 (3)	0.3767 (3)	0.0419 (17)
N4	0.6281 (11)	−0.0020 (3)	0.4009 (3)	0.0423 (17)
N5	−0.6936 (11)	0.0505 (3)	−0.1527 (3)	0.0421 (19)
C2	0.6256 (12)	0.0873 (3)	0.3140 (3)	0.033 (2)
O4	1.1824 (13)	0.1213 (3)	0.4840 (4)	0.0509 (19)
C5	0.4153 (12)	−0.0206 (3)	0.3560 (4)	0.038 (2)
C6	0.2509 (12)	−0.0867 (3)	0.3681 (4)	0.049 (3)
C7	0.5363 (12)	0.1752 (3)	0.1848 (3)	0.039 (2)
C8	0.6405 (13)	0.2400 (3)	0.1429 (3)	0.034 (2)
C9	0.1601 (12)	0.2331 (3)	−0.0185 (3)	0.035 (2)
C10	−0.0591 (11)	0.1862 (3)	−0.0527 (3)	0.0319 (19)
C11	−0.2248 (12)	0.2078 (3)	−0.1184 (3)	0.038 (2)
C12	−0.4307 (12)	0.1647 (3)	−0.1523 (3)	0.039 (2)
C13	−0.4703 (11)	0.0975 (3)	−0.1198 (3)	0.032 (2)
C14	−0.3105 (13)	0.0738 (3)	−0.0551 (4)	0.044 (2)
C15	−0.1059 (13)	0.1177 (3)	−0.0217 (4)	0.042 (2)
H1	0.557 (9)	0.292 (2)	0.050 (3)	0.006 (13)*
H6A	0.29906	−0.10554	0.41958	0.0740*
H6B	0.28606	−0.12305	0.33019	0.0740*
H6C	0.06142	−0.07423	0.36230	0.0740*
H7A	0.35003	0.18331	0.19596	0.0460*
H7B	0.54276	0.13154	0.15321	0.0460*
H9	0.19963	0.27696	−0.04217	0.0420*
H11	−0.19521	0.25314	−0.14028	0.0460*
H12	−0.54010	0.18052	−0.19606	0.0460*
H14	−0.34078	0.02823	−0.03384	0.0530*
H15	0.00261	0.10145	0.02197	0.0500*
H4A	1.231 (18)	0.092 (5)	0.509 (5)	0.10 (4)*
H4B	1.070 (16)	0.104 (5)	0.458 (5)	0.09 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0353 (9)	0.0392 (9)	0.0406 (10)	−0.0011 (8)	−0.0025 (7)	0.0083 (8)
S2	0.0422 (10)	0.0379 (9)	0.0388 (10)	−0.0074 (8)	−0.0111 (8)	0.0063 (8)
O1	0.056 (3)	0.048 (3)	0.044 (3)	−0.026 (2)	−0.009 (2)	0.004 (2)
O2	0.060 (3)	0.064 (3)	0.056 (3)	−0.010 (3)	−0.023 (3)	0.000 (3)
O3	0.067 (3)	0.041 (3)	0.064 (3)	−0.018 (3)	0.002 (3)	0.007 (3)
N1	0.043 (3)	0.028 (3)	0.032 (3)	−0.010 (3)	0.002 (3)	0.007 (2)
N2	0.033 (3)	0.035 (3)	0.030 (3)	−0.003 (2)	0.000 (2)	−0.003 (2)
N3	0.045 (3)	0.043 (3)	0.035 (3)	−0.003 (3)	−0.010 (3)	0.010 (3)
N4	0.046 (3)	0.045 (3)	0.036 (3)	0.006 (3)	0.005 (3)	0.017 (3)
N5	0.045 (3)	0.044 (4)	0.037 (3)	−0.001 (3)	0.003 (3)	−0.010 (3)
C2	0.035 (4)	0.033 (3)	0.030 (4)	0.003 (3)	0.002 (3)	0.003 (3)
O4	0.061 (4)	0.043 (3)	0.046 (3)	0.006 (3)	−0.009 (3)	−0.004 (3)
C5	0.033 (4)	0.039 (4)	0.041 (4)	0.009 (3)	0.005 (3)	0.005 (3)
C6	0.040 (4)	0.044 (4)	0.065 (5)	−0.005 (3)	0.010 (4)	0.020 (4)
C7	0.043 (4)	0.035 (4)	0.036 (4)	−0.010 (3)	−0.006 (3)	0.007 (3)
C8	0.042 (4)	0.027 (3)	0.031 (4)	0.000 (3)	−0.001 (3)	−0.004 (3)
C9	0.037 (4)	0.037 (4)	0.031 (4)	0.002 (3)	0.002 (3)	0.001 (3)
C10	0.029 (3)	0.037 (4)	0.030 (3)	0.003 (3)	0.004 (3)	−0.002 (3)
C11	0.041 (4)	0.034 (3)	0.038 (4)	0.003 (3)	−0.004 (3)	0.014 (3)
C12	0.039 (4)	0.045 (4)	0.030 (4)	0.000 (3)	−0.006 (3)	0.002 (3)
C13	0.028 (4)	0.034 (4)	0.032 (4)	−0.002 (3)	0.001 (3)	−0.003 (3)
C14	0.048 (4)	0.038 (4)	0.046 (4)	0.000 (3)	0.003 (3)	0.011 (3)
C15	0.041 (4)	0.042 (4)	0.040 (4)	0.001 (3)	−0.010 (3)	0.014 (3)

Geometric parameters (Å, º)

S1—C2	1.712 (6)	C10—C15	1.392 (8)
S1—C5	1.738 (7)	C10—C11	1.389 (8)
S2—C2	1.749 (6)	C11—C12	1.373 (8)
S2—C7	1.799 (6)	C12—C13	1.374 (8)
O1—C8	1.221 (7)	C13—C14	1.372 (8)
O2—N5	1.220 (7)	C14—C15	1.374 (9)
O3—N5	1.217 (7)	O4—H4A	0.72 (9)
N1—N2	1.361 (8)	O4—H4B	0.75 (8)
N1—C8	1.353 (8)	C6—H6C	0.9600
N2—C9	1.270 (7)	C6—H6A	0.9600
N3—N4	1.383 (8)	C6—H6B	0.9600
N3—C2	1.296 (7)	C7—H7B	0.9700
N4—C5	1.290 (8)	C7—H7A	0.9700
N5—C13	1.470 (8)	C9—H9	0.9300
N1—H1	0.82 (4)	C11—H11	0.9300
C5—C6	1.484 (8)	C12—H12	0.9300
C7—C8	1.506 (8)	C14—H14	0.9300
C9—C10	1.461 (8)	C15—H15	0.9300

C2—S1—C5	87.2 (3)	N5—C13—C14	118.7 (5)
C2—S2—C7	101.5 (3)	N5—C13—C12	119.9 (5)
N2—N1—C8	119.3 (5)	C12—C13—C14	121.4 (5)
N1—N2—C9	117.3 (5)	C13—C14—C15	119.8 (5)
N4—N3—C2	111.6 (5)	C10—C15—C14	120.7 (6)
N3—N4—C5	113.7 (5)	H4A—O4—H4B	103 (10)
O2—N5—O3	123.9 (6)	C5—C6—H6B	109.00
O2—N5—C13	117.0 (5)	C5—C6—H6C	109.00
O3—N5—C13	119.1 (5)	C5—C6—H6A	109.00
C8—N1—H1	117 (3)	H6A—C6—H6C	110.00
N2—N1—H1	124 (3)	H6B—C6—H6C	109.00
S1—C2—N3	114.7 (4)	H6A—C6—H6B	109.00
S2—C2—N3	118.4 (4)	S2—C7—H7B	111.00
S1—C2—S2	126.9 (3)	C8—C7—H7A	110.00
N4—C5—C6	123.9 (6)	C8—C7—H7B	110.00
S1—C5—N4	112.9 (4)	H7A—C7—H7B	109.00
S1—C5—C6	123.3 (5)	S2—C7—H7A	111.00
S2—C7—C8	106.0 (4)	C10—C9—H9	121.00
N1—C8—C7	115.9 (5)	N2—C9—H9	121.00
O1—C8—C7	122.3 (5)	C10—C11—H11	119.00
O1—C8—N1	121.8 (5)	C12—C11—H11	119.00
N2—C9—C10	118.7 (5)	C13—C12—H12	121.00
C11—C10—C15	117.6 (5)	C11—C12—H12	121.00
C9—C10—C11	121.1 (5)	C13—C14—H14	120.00
C9—C10—C15	121.3 (5)	C15—C14—H14	120.00
C10—C11—C12	122.5 (5)	C10—C15—H15	120.00
C11—C12—C13	118.1 (5)	C14—C15—H15	120.00

C5—S1—C2—S2	178.8 (4)	O2—N5—C13—C14	179.8 (6)
C5—S1—C2—N3	0.1 (5)	O3—N5—C13—C12	−179.2 (5)
C2—S1—C5—N4	0.5 (5)	O3—N5—C13—C14	−1.3 (8)
C2—S1—C5—C6	−178.4 (5)	S2—C7—C8—O1	−0.4 (7)
C7—S2—C2—S1	−4.9 (5)	S2—C7—C8—N1	179.2 (4)
C7—S2—C2—N3	173.8 (5)	N2—C9—C10—C11	175.9 (5)
C2—S2—C7—C8	−177.1 (4)	N2—C9—C10—C15	−5.5 (8)
C8—N1—N2—C9	174.6 (5)	C9—C10—C11—C12	179.4 (5)
N2—N1—C8—O1	177.1 (5)	C15—C10—C11—C12	0.7 (8)
N2—N1—C8—C7	−2.5 (8)	C9—C10—C15—C14	−179.1 (6)
N1—N2—C9—C10	177.6 (5)	C11—C10—C15—C14	−0.5 (9)
C2—N3—N4—C5	1.0 (7)	C10—C11—C12—C13	−0.6 (9)
N4—N3—C2—S1	−0.6 (6)	C11—C12—C13—N5	178.1 (5)
N4—N3—C2—S2	−179.5 (4)	C11—C12—C13—C14	0.3 (8)
N3—N4—C5—S1	−1.0 (7)	N5—C13—C14—C15	−177.9 (6)
N3—N4—C5—C6	177.9 (5)	C12—C13—C14—C15	−0.1 (9)
O2—N5—C13—C12	1.9 (8)	C13—C14—C15—C10	0.2 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O4^{i}	0.82 (4)	2.08 (4)	2.900 (8)	176 (5)
O4—H4*A*···N4^{ii}	0.72 (9)	2.32 (9)	3.037 (8)	175 (10)
O4—H4*B*···N3	0.75 (8)	2.15 (9)	2.898 (8)	176 (13)
C7—H7*B*···O3^{iii}	0.97	2.51	3.400 (7)	153
C12—H12···O1^{iv}	0.93	2.46	3.349 (6)	159

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*, −*y*, −*z*; (iv) *x*−3/2, −*y*+1/2, *z*−1/2.