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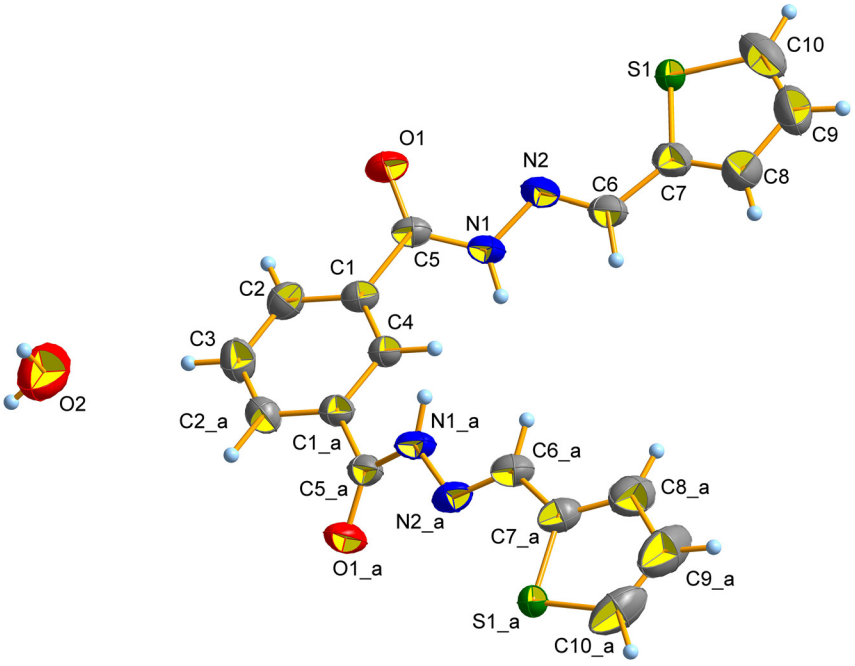
The crystal structure of N'^{1},N'^{3}-bis((*E*)-thiophen-2-ylmethylene)isophthalohydrazide monohydrate, $C_{18}H_{16}N_4O_3S_2$



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Abstract

$C_{18}H_{16}N_4O_3S_2$, monoclinic, $C2/c$ (no. 15), a = 19.694(4) Å, b = 11.450(2) Å, c = 8.3382(16) Å, β = 91.820 (2)°, V = 1879.3(6) Å^3, Z = 4, $R_{gt}(F)$ = 0.0408, $wR_{ref}(F^2)$ = 0.1206, T = 296(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Block
Size:	0.42 × 0.39 × 0.31 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.31 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8713, 1649, 0.015
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 1489
$N(param)_{refined}$:	127
Programs:	Bruker [1], SHELX [2,3]

1 Source of material

Isophthalohydrazide (194 mg, 1 mmol) and thiophene-2-carbaldehyde (224 mg, 2 mmol) were dissolved in ethanol (15 mL) and the mixture was refluxed for 6 h. The target compound (351 mg, yield 92 %) was collected by filtration and washed with ethanol. Single crystals of the product can be obtained by recrystallization from ethanol.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.46045 (8)	0.66797 (14)	0.63606 (18)	0.0377 (4)
C2	0.46145 (9)	0.78919 (17)	0.6358 (2)	0.0470 (4)
H2	0.436088	0.830127	0.558403	0.056*
C3	0.500000	0.8494 (2)	0.750000	0.0535 (7)
H3	0.499999	0.930580	0.750001	0.064*
C4	0.500000	0.6073 (2)	0.750000	0.0356 (5)
H4	0.499999	0.526108	0.750001	0.043*
C5	0.41976 (8)	0.60213 (15)	0.51155 (18)	0.0392 (4)
C6	0.35943 (9)	0.31999 (17)	0.4990 (2)	0.0466 (4)
H6	0.377051	0.301597	0.600649	0.056*
C7	0.32880 (10)	0.22840 (17)	0.4024 (2)	0.0488 (5)
C8	0.33478 (14)	0.1118 (2)	0.4330 (3)	0.0723 (7)
H8	0.358641	0.081174	0.521367	0.087*
C9	0.30095 (17)	0.0431 (3)	0.3164 (4)	0.0940 (10)
H9	0.300422	−0.038114	0.318823	0.113*
C10	0.26960 (14)	0.1061 (3)	0.2015 (3)	0.0824 (8)
H10	0.244392	0.074101	0.116097	0.099*
N1	0.39507 (7)	0.49969 (13)	0.56020 (15)	0.0433 (4)
H1	0.398906	0.480115	0.659652	0.052*
N2	0.36323 (7)	0.42481 (13)	0.45023 (16)	0.0432 (4)
O1	0.41189 (7)	0.63889 (12)	0.37323 (14)	0.0541 (4)
O2	0.500000	1.1683 (4)	0.750000	0.1592 (19)
H2A	0.503396	1.228051	0.690264	0.239*
H2B	0.463308	1.172206	0.800742	0.239*
S1	0.28134 (3)	0.25195 (5)	0.23017 (7)	0.0639 (3)

2 Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The U_{iso} values of the methyl groups, phenolic hydroxyl and water were set to $1.5U_{eq}$(C), and the U_{iso} values of all other hydrogen atoms were set to $1.2U_{eq}$(C).

3 Comment

Hydrazone is a Schiff base constructed by hydrazide and carbonyl compounds. It has attracted much attention due to its biological activities [4,5]. The structure of hydrazone compounds has always been the focus of research [6–11].

A compound containing thiophene ring was synthesized from isophthalohydrazide with thiophene-2-carbaldehyde and characterized by single-crystal X-ray diffraction [1–3]. In the crystal, the molecule exhibits crystallographic C_2 axial symmetry (C3, C4 and O2). The title molecule is V-shaped. The dihedral angle between rings C1–C4 and C7–S1 is 5.6°, and the dihedral angle between rings C7–S1 and C7-a–S1-a is 3.7°. The bond lengths of C(1)–C(5), C(5)–N(1), N(1)–N(2), N(2)–C(6), C(6)–C(7), C(7)–S(1) and S(1)–C(10) are 1.338(2), 1.3902(19), 1.270(2), 1.443(3), 1.710(2) and 1.702(3) Å respectively.

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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