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N′-[1-(2-Thienyl)ethylidene]acetohydrazide

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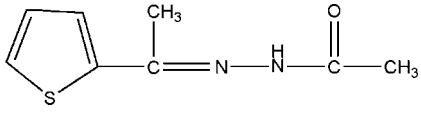
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.132; data-to-parameter ratio = 16.2.

The title compound, $C_8H_{10}N_2OS$, was prepared by the reaction of 1-(thiophen-2-yl)ethanone and acetohydrazide. The molecules form a dimer, in which two N—H···O hydrogen bonds generate an intermolecular $R_2^2(8)$ ring. There is also an intermolecular C—H···O hydrogen-bonding interaction.

Related literature

For related literature, see: Cimerman *et al.* (1997); Sutherland & Hoy (1968); Tucker *et al.* (1975);



Experimental

Crystal data

$C_8H_{10}N_2OS$
M_r = 182.24
Monoclinic, $P2_1/n$
a = 5.2903 (11) Å
b = 9.788 (2) Å
c = 17.435 (4) Å
β = 94.102 (3)°
V = 900.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 294 (2) K
0.24 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.929, T_{max} = 0.958
5012 measured reflections
1847 independent reflections
1435 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.132
S = 1.06
1847 reflections
114 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.89 (2)	2.10 (2)	2.978 (3)	169 (3)
C6—H6A···O1^{i}	0.96	2.46	3.279 (3)	143

Symmetry code: (i) $-x+2, -y, -z$.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2295).

References

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supplementary materials

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N'-[1-(2-Thienyl)ethylidene]acetohydrazide

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Comment

Schiff bases have received considerable attention in the literature. They are attractive from several points of view, such as the possibility of analytical application (Cimerman, *et al.*, 1997). As part of our search for new schiff base compounds we synthesized the title compound (I), and describe its structure here.

The molecular structure of the title compund (I) is shown in Fig. 1. The values of all the geometric parameters in (I) are normal. The structure is stabilized by the N—H···O hydrogen bonds form a dimer structure, generating an intermolecular $R_2^2(8)$ ring, and intramolecular C—H···O hydrogen bonding interactions.

Experimental

A mixture of the 1-(thiophen-2-yl)ethanone (0.1 mol), and acetohydrazide (0.1 mol) was stirred in refluxing ethanol (30 ml) for 5 h to afford the title compound (0.087 mol, yield 87%). Single crystals (I) of suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

NH H atom was found from difference Fourier map and refined freely. H atoms bonded to C atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H = 0.93 − 0.96 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

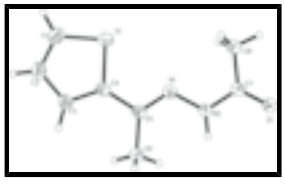

Fig. 1. An *ORTEP* view of the title compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N'-[1-(2-Thienyl)ethylidene]acetohydrazide

Crystal data

$C_8H_{10}N_2OS$	$Z = 4$
$M_r = 182.24$	$F_{000} = 384$
Monoclinic, $P2_1/n$	$D_x = 1.344$ Mg m^{-3}
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.2903$ (11) Å	$\theta = 2.3$–26.4°

b = 9.788 (2) Å	μ = 0.31 mm^{-1}
c = 17.435 (4) Å	T = 294 (2) K
β = 94.102 (3)º	Block, colourless
V = 900.5 (3) Å^3	0.24 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD area detector diffractometer	1847 independent reflections
Radiation source: fine-focus sealed tube	1435 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$h = -5 \rightarrow 6$
T_{min} = 0.929, T_{max} = 0.958	$k = -7 \rightarrow 12$
5012 measured reflections	$l = -21 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.044	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.132	$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.4879P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
1847 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
114 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.22200 (12)	0.44789 (7)	0.06956 (4)	0.0566 (3)
O1	0.8443 (4)	0.0201 (2)	−0.09105 (9)	0.0601 (5)
N1	0.5822 (3)	0.23827 (19)	0.03934 (10)	0.0405 (4)
N2	0.7406 (3)	0.1420 (2)	0.01056 (10)	0.0433 (5)
C1	0.0993 (5)	0.5464 (3)	0.13844 (17)	0.0590 (7)
H1	−0.0331	0.6078	0.1284	0.071*
C2	0.2152 (5)	0.5258 (3)	0.20932 (16)	0.0542 (6)
H2	0.1716	0.5718	0.2531	0.065*
C3	0.4117 (4)	0.4255 (2)	0.20935 (14)	0.0445 (5)
H3	0.5104	0.3982	0.2529	0.053*
C4	0.4369 (4)	0.3738 (2)	0.13575 (12)	0.0382 (5)
C5	0.6116 (4)	0.2692 (2)	0.11116 (12)	0.0363 (5)
C6	0.8019 (4)	0.2087 (3)	0.16943 (13)	0.0464 (6)
H6A	0.8417	0.1173	0.1545	0.070*
H6B	0.7325	0.2071	0.2188	0.070*
H6C	0.9532	0.2632	0.1723	0.070*
C7	0.7020 (4)	0.1030 (2)	−0.06398 (12)	0.0428 (5)
C8	0.4802 (5)	0.1646 (3)	−0.11048 (14)	0.0525 (6)
H8A	0.4804	0.1339	−0.1628	0.079*
H8B	0.4932	0.2624	−0.1089	0.079*
H8C	0.3256	0.1367	−0.0894	0.079*
H2A	0.871 (3)	0.104 (3)	0.0379 (14)	0.058 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0562 (4)	0.0665 (5)	0.0460 (4)	0.0183 (3)	−0.0035 (3)	0.0045 (3)
O1	0.0651 (11)	0.0742 (13)	0.0402 (9)	0.0259 (10)	−0.0033 (8)	−0.0083 (9)
N1	0.0392 (9)	0.0452 (11)	0.0365 (9)	0.0038 (8)	−0.0006 (7)	−0.0007 (8)
N2	0.0438 (10)	0.0493 (11)	0.0357 (10)	0.0107 (9)	−0.0042 (8)	−0.0010 (8)
C1	0.0520 (14)	0.0568 (16)	0.0684 (17)	0.0152 (12)	0.0066 (13)	0.0005 (13)
C2	0.0512 (14)	0.0573 (16)	0.0549 (15)	0.0008 (11)	0.0096 (11)	−0.0119 (12)
C3	0.0402 (11)	0.0487 (14)	0.0443 (12)	−0.0032 (10)	0.0008 (9)	−0.0083 (10)
C4	0.0344 (10)	0.0418 (12)	0.0377 (11)	−0.0032 (9)	−0.0022 (8)	0.0013 (9)
C5	0.0331 (10)	0.0401 (12)	0.0352 (10)	−0.0040 (9)	−0.0010 (8)	0.0013 (9)
C6	0.0456 (12)	0.0532 (14)	0.0394 (11)	0.0072 (10)	−0.0048 (9)	−0.0012 (10)
C7	0.0437 (11)	0.0475 (13)	0.0365 (11)	0.0027 (10)	−0.0020 (9)	0.0022 (10)
C8	0.0533 (14)	0.0624 (16)	0.0403 (12)	0.0073 (12)	−0.0079 (10)	−0.0002 (11)

Geometric parameters (Å, °)

S1—C1	1.704 (3)	C3—C4	1.394 (3)
S1—C4	1.721 (2)	C3—H3	0.9300
O1—C7	1.224 (3)	C4—C5	1.464 (3)
N1—C5	1.287 (3)	C5—C6	1.500 (3)

N1—N2	1.379 (3)	C6—H6A	0.9600
N2—C7	1.356 (3)	C6—H6B	0.9600
N2—H2A	0.889 (10)	C6—H6C	0.9600
C1—C2	1.355 (4)	C7—C8	1.504 (3)
C1—H1	0.9300	C8—H8A	0.9600
C2—C3	1.430 (3)	C8—H8B	0.9600
C2—H2	0.9300	C8—H8C	0.9600
C1—S1—C4	91.85 (12)	N1—C5—C6	126.5 (2)
C5—N1—N2	118.70 (18)	C4—C5—C6	119.00 (18)
C7—N2—N1	119.20 (18)	C5—C6—H6A	109.5
C7—N2—H2A	117.1 (18)	C5—C6—H6B	109.5
N1—N2—H2A	123.7 (18)	H6A—C6—H6B	109.5
C2—C1—S1	112.9 (2)	C5—C6—H6C	109.5
C2—C1—H1	123.6	H6A—C6—H6C	109.5
S1—C1—H1	123.6	H6B—C6—H6C	109.5
C1—C2—C3	112.6 (2)	O1—C7—N2	120.1 (2)
C1—C2—H2	123.7	O1—C7—C8	122.4 (2)
C3—C2—H2	123.7	N2—C7—C8	117.5 (2)
C4—C3—C2	111.5 (2)	C7—C8—H8A	109.5
C4—C3—H3	124.3	C7—C8—H8B	109.5
C2—C3—H3	124.3	H8A—C8—H8B	109.5
C3—C4—C5	128.82 (19)	C7—C8—H8C	109.5
C3—C4—S1	111.24 (17)	H8A—C8—H8C	109.5
C5—C4—S1	119.93 (15)	H8B—C8—H8C	109.5
N1—C5—C4	114.48 (18)		
C5—N1—N2—C7	176.3 (2)	N2—N1—C5—C4	179.08 (18)
C4—S1—C1—C2	0.3 (2)	N2—N1—C5—C6	−1.2 (3)
S1—C1—C2—C3	−0.4 (3)	C3—C4—C5—N1	177.0 (2)
C1—C2—C3—C4	0.4 (3)	S1—C4—C5—N1	−1.9 (3)
C2—C3—C4—C5	−179.1 (2)	C3—C4—C5—C6	−2.7 (3)
C2—C3—C4—S1	−0.2 (2)	S1—C4—C5—C6	178.39 (17)
C1—S1—C4—C3	−0.04 (19)	N1—N2—C7—O1	178.3 (2)
C1—S1—C4—C5	179.01 (19)	N1—N2—C7—C8	−2.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1^{i}	0.89 (2)	2.10 (2)	2.978 (3)	169 (3)
C6—H6A···O1^{i}	0.96	2.46	3.279 (3)	143

Symmetry codes: (i) −*x*+2, −*y*, −*z*.

Fig. 1