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# *N*′-[(3-Methyl-2-thienyl)carbonyl]-isonicotinohydrazide

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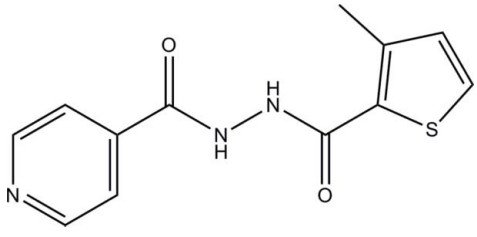
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.036; $wR$ factor = 0.097; data-to-parameter ratio = 26.4.

In the title compound, $C_{12}H_{11}N_3O_2S$, the pyridine ring is inclined to the thiophene ring, forming a dihedral angle of 34.96 (7)°. The mean plane through the hydrazide unit forms dihedral angles of 21.57 (8) and 53.08 (8)°, respectively, with the pyridine and thiophene rings. The two O atoms are twisted away from each other, as indicated by the C—N—N—C torsion angle of −81.27 (15)°. In the crystal structure, molecules are linked into an extended three-dimensional network by intermolecular N—H···N, N—H···O and C—H···O hydrogen bonds. The crystal structure also features a short S···O [3.2686 (10) Å] interaction and a weak intermolecular C—H···$\pi$ interaction.

## Related literature

For general background to and application of isoniazid derivatives, see: Janin (2007); Maccari *et al.* (2005); Slayden *et al.* (2000). For the preparation of the title compound, see: Besra *et al.* (1993). For bond-length data, see: Allen *et al.* (1987). For a closely related structure, see: Naveenkumar *et al.* (2009). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).




## Experimental

### *Crystal data*

$C_{12}H_{11}N_3O_2S$
$M_r$ = 261.30
Orthorhombic, $P2_12_12_1$
$a$ = 8.9206 (1) Å
$b$ = 10.7552 (2) Å
$c$ = 12.4934 (2) Å
$V$ = 1198.65 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 100 K
0.58 × 0.20 × 0.15 mm

### *Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.861, $T_{max}$ = 0.961
17333 measured reflections
4355 independent reflections
4078 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
$S$ = 1.05
4355 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$
Absolute structure: Flack (1983), 1856 Friedel pairs
Flack parameter: −0.04 (6)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H1*N2*···N1$^{i}$ | 0.86 | 2.14 | 2.9068 (17) | 149 |
| N3—H1*N3*···O2$^{ii}$ | 0.86 | 1.99 | 2.8034 (15) | 158 |
| C4—H4*A*···O1$^{iii}$ | 0.93 | 2.58 | 3.2047 (17) | 125 |
| C10—H10*A*···O2$^{iv}$ | 0.93 | 2.51 | 3.3928 (19) | 159 |
| C11—H11*A*···*Cg*1$^{v}$ | 0.93 | 2.80 | 3.3760 (17) | 121 |

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$; (iii) $-x+\frac{1}{2}, -y+1, z-\frac{1}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x, y+\frac{3}{2}, -z+\frac{1}{2}$. *Cg*1 is centroid of the C1/C2/N1/C3–C5 ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2451).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Besra, G. S., Minnikin, D. E., Wheeler, P. R. & Ratledge, C. (1993). *Chem. Phys. Lipids*, **66**, 23–34.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Janin, Y. L. (2007). *Bioorg. Med. Chem.* **15**, 2479–2513.

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§ Thomson Reuters ResearcherID: A-3561-2009.

Maccari, R., Ottanà, R. & Vigorita, M. G. (2005). *Bioorg. Med. Chem. Lett.* **15**, 2509–2513.
Naveenkumar, H. S., Sadikun, A., Ibrahim, P., Yeap, C. S. & Fun, H.-K. (2009). *Acta Cryst.* E**65**, o1912.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Slayden, R. A. & Barry, C. E. (2000). *Microbes Infect.* **2**, 659–669.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supplementary materials

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# *N*'-[(3-Methyl-2-thienyl)carbonyl]isonicotinohydrazide

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## Comment

In the search of new compounds, isoniazid derivatives have been found to possess potential tuberculostatic activity (Janin, 2007; Maccari *et al.*, 2005; Slayden *et al.*, 2000). As a part of a current work on synthesis of such derivatives, in this paper we present the crystal structure of the title compound, (I) which was synthesized in our lab.

In (I), the pyridine ring (C1/C2/N1/C3-C5) is inclined to the thiophene ring (C8-C11/S1), forming a dihedral angle of 34.96 (7)° (Fig. 1). The mean plane through the hydrazide unit (C7/N2/N3/O2) forms dihedral angles of 21.57 (8) and 53.08 (8)°, respectively, with the pyridine and thiophene rings. The O1 and O2 atoms are twisted away from each other as indicated by torsion angle C6–N2–N3–C7 [-81.27 (15)°]. The bond lengths (Allen *et al.*, 1987) and angles are comparable to a closely related structure (Naveenkumar *et al.*, 2009).

In the crystal structure (Fig. 2), the molecules are linked into an extended three-dimensional network by intermolecular C4—H4A···O1, C10—H10A···O2, N2—H1N2···N1 and N3—H1N3···O2 hydrogen bonds (Table 1). The crystal structure is further stabilized by short S1···O2 interactions of 3.2686 (10) Å [symmetry code: 1/2+x, 3/2-y, -z] and by weak intermolecular C11—H11A···*Cg*1 interactions (Table 1; *Cg*1 is the centroid of the pyridine ring).

## Experimental

Compound (I) was prepared following the procedure by literature (Besra *et al.*, 1993). Dry dichloromethane (30 ml) and 4-dimethylaminopyridine (4-DMAP) (1.2 eq) was added to 3-methylthiophene-2-carbonyl chloride followed by isoniazid (1.1 eq). The reaction mixture was kept in an ice bath for 1 h and then left stirring under nitrogen atmosphere overnight at room temperature. Dichloromethane (20 ml) was added to the reaction mixture, which was then washed with water, and the organic layer dried over anhydrous sodium sulphate. The solvent was removed under reduced pressure to afford the crude product which was purified by column chromatography and recrystallized from ethanol to afford colorless single crystals.

## Refinement

All the H atoms were placed in calculated positions, with N—H = 0.86 Å, $U_{iso}$(H) = 1.2 $U_{eq}$(N), C—H = 0.93 Å, $U_{iso}$(H) = 1.2 $U_{eq}$(C) for aromatic, and C—H = 0.96 Å, $U_{iso}$(H) = 1.5 $U_{eq}$(C) for methyl group. These H atoms were refined as riding on their parent atoms. A rotating group model was used for the methyl group.

## Figures

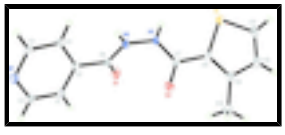

Fig. 1. The molecular structure of the (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen atoms are shown as spheres of arbitrary radius.

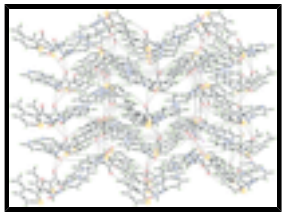

Fig. 2. Three dimensional extended network, viewed along the *b* axis. Intermolecular interactions are shown as dashed lines.

### *N′*-[(3-Methyl-2-thienyl)carbonyl]isonicotinohydrazide

*Crystal data*

| | |
|---|---|
| $C_{12}H_{11}N_3O_2S$ | $F_{000}$ = 544 |
| $M_r$ = 261.30 | $D_x$ = 1.448 Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 9634 reflections |
| $a$ = 8.9206 (1) Å | θ = 2.5–32.7º |
| $b$ = 10.7552 (2) Å | μ = 0.27 mm$^{-1}$ |
| $c$ = 12.4934 (2) Å | $T$ = 100 K |
| $V$ = 1198.65 (3) Å$^3$ | Block, colourless |
| $Z$ = 4 | 0.58 × 0.20 × 0.15 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 4355 independent reflections |
| Radiation source: fine-focus sealed tube | 4078 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.025 |
| $T$ = 100 K | $\theta_{max}$ = 32.7º |
| φ and ω scans | $\theta_{min}$ = 2.5º |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | $h$ = −13→13 |
| $T_{min}$ = 0.861, $T_{max}$ = 0.961 | $k$ = −14→16 |
| 17333 measured reflections | $l$ = −17→18 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | $w = 1/[\sigma^2(F_o^2) + (0.0542P)^2 + 0.3319P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.097 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.05 | $\Delta\rho_{max}$ = 0.79 e Å$^{-3}$ |
| 4355 reflections | $\Delta\rho_{min}$ = −0.43 e Å$^{-3}$ |
| 165 parameters | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 1856 Friedel pairs |

Secondary atom site location: difference Fourier map  Flack parameter: −0.04 (6)

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

**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.

**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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 | 0.26735 (4) | 0.98879 (3) | 0.04525 (3) | 0.01858 (8) |
| O1 | 0.29108 (13) | 0.48575 (10) | 0.02488 (8) | 0.0221 (2) |
| O2 | 0.01066 (11) | 0.69442 (9) | 0.07046 (8) | 0.01664 (19) |
| N1 | 0.03034 (14) | 0.21406 (11) | −0.25010 (10) | 0.0159 (2) |
| N2 | 0.18343 (13) | 0.62066 (10) | −0.09379 (9) | 0.0137 (2) |
| H1N2 | 0.1404 | 0.6288 | −0.1550 | 0.016* |
| N3 | 0.21647 (13) | 0.72506 (10) | −0.03274 (9) | 0.01367 (19) |
| H1N3 | 0.2954 | 0.7684 | −0.0458 | 0.016* |
| C1 | 0.11893 (17) | 0.29049 (12) | −0.08076 (11) | 0.0165 (2) |
| H1A | 0.1343 | 0.2764 | −0.0081 | 0.020* |
| C2 | 0.05396 (17) | 0.19936 (13) | −0.14457 (11) | 0.0174 (2) |
| H2A | 0.0255 | 0.1248 | −0.1128 | 0.021* |
| C3 | 0.07732 (15) | 0.32069 (12) | −0.29452 (11) | 0.0153 (2) |
| H3A | 0.0653 | 0.3306 | −0.3680 | 0.018* |
| C4 | 0.14288 (15) | 0.41719 (12) | −0.23723 (11) | 0.0143 (2) |
| H4A | 0.1741 | 0.4894 | −0.2716 | 0.017* |
| C5 | 0.16079 (15) | 0.40323 (12) | −0.12698 (10) | 0.0136 (2) |
| C6 | 0.21924 (14) | 0.50531 (11) | −0.05670 (10) | 0.0138 (2) |
| C7 | 0.12212 (14) | 0.75769 (11) | 0.04814 (11) | 0.0125 (2) |
| C8 | 0.15680 (15) | 0.87488 (12) | 0.10399 (11) | 0.0142 (2) |
| C9 | 0.10620 (16) | 0.91137 (14) | 0.20356 (11) | 0.0177 (2) |
| C10 | 0.15852 (18) | 1.03210 (14) | 0.23047 (13) | 0.0209 (3) |
| H10A | 0.1356 | 1.0716 | 0.2947 | 0.025* |
| C11 | 0.24567 (18) | 1.08445 (13) | 0.15288 (12) | 0.0214 (3) |
| H11A | 0.2883 | 1.1631 | 0.1581 | 0.026* |
| C12 | 0.0117 (2) | 0.83596 (16) | 0.27738 (13) | 0.0259 (3) |
| H12A | 0.0530 | 0.7538 | 0.2835 | 0.039* |
| H12B | −0.0884 | 0.8309 | 0.2496 | 0.039* |
| H12C | 0.0097 | 0.8745 | 0.3466 | 0.039* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.02092 (15) | 0.01399 (13) | 0.02083 (16) | −0.00198 (11) | 0.00366 (12) | −0.00283 (12) |
| O1 | 0.0302 (5) | 0.0186 (4) | 0.0176 (5) | 0.0033 (4) | −0.0104 (4) | −0.0021 (4) |
| O2 | 0.0134 (4) | 0.0166 (4) | 0.0200 (5) | −0.0026 (3) | 0.0000 (3) | 0.0000 (4) |
| N1 | 0.0187 (5) | 0.0131 (5) | 0.0160 (5) | −0.0004 (4) | −0.0017 (4) | −0.0018 (4) |
| N2 | 0.0177 (5) | 0.0113 (4) | 0.0120 (5) | −0.0003 (4) | −0.0028 (4) | −0.0031 (4) |
| N3 | 0.0150 (5) | 0.0122 (4) | 0.0138 (5) | −0.0024 (4) | 0.0005 (4) | −0.0046 (4) |
| C1 | 0.0229 (6) | 0.0140 (6) | 0.0125 (5) | 0.0003 (5) | −0.0015 (5) | 0.0011 (4) |
| C2 | 0.0226 (6) | 0.0123 (5) | 0.0173 (6) | −0.0006 (5) | −0.0006 (5) | 0.0004 (5) |
| C3 | 0.0182 (6) | 0.0163 (6) | 0.0114 (5) | −0.0001 (4) | 0.0005 (4) | −0.0028 (4) |
| C4 | 0.0172 (6) | 0.0127 (5) | 0.0131 (5) | −0.0014 (4) | −0.0001 (4) | −0.0011 (4) |
| C5 | 0.0158 (5) | 0.0123 (5) | 0.0128 (5) | 0.0014 (4) | −0.0015 (4) | −0.0018 (4) |
| C6 | 0.0159 (5) | 0.0133 (5) | 0.0122 (5) | 0.0008 (4) | −0.0012 (4) | −0.0018 (4) |
| C7 | 0.0129 (5) | 0.0123 (5) | 0.0124 (5) | 0.0012 (4) | −0.0020 (4) | 0.0002 (4) |
| C8 | 0.0139 (5) | 0.0128 (5) | 0.0160 (6) | 0.0008 (4) | −0.0015 (4) | −0.0016 (4) |
| C9 | 0.0180 (6) | 0.0188 (6) | 0.0165 (6) | 0.0005 (5) | −0.0001 (5) | −0.0021 (5) |
| C10 | 0.0230 (6) | 0.0194 (6) | 0.0205 (6) | 0.0026 (5) | −0.0022 (5) | −0.0084 (5) |
| C11 | 0.0246 (7) | 0.0152 (5) | 0.0245 (7) | −0.0008 (5) | −0.0006 (5) | −0.0079 (5) |
| C12 | 0.0299 (8) | 0.0246 (7) | 0.0234 (7) | −0.0028 (6) | 0.0019 (6) | −0.0040 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C11 | 1.7041 (14) | C3—C4 | 1.3898 (18) |
| S1—C8 | 1.7355 (14) | C3—H3A | 0.9300 |
| O1—C6 | 1.2222 (15) | C4—C5 | 1.3948 (19) |
| O2—C7 | 1.2367 (15) | C4—H4A | 0.9300 |
| N1—C3 | 1.3412 (18) | C5—C6 | 1.4994 (18) |
| N1—C2 | 1.3445 (18) | C7—C8 | 1.4736 (17) |
| N2—C6 | 1.3623 (16) | C8—C9 | 1.3803 (19) |
| N2—N3 | 1.3890 (14) | C9—C10 | 1.420 (2) |
| N2—H1N2 | 0.8600 | C9—C12 | 1.489 (2) |
| N3—C7 | 1.3611 (17) | C10—C11 | 1.364 (2) |
| N3—H1N3 | 0.8600 | C10—H10A | 0.9300 |
| C1—C2 | 1.3899 (19) | C11—H11A | 0.9300 |
| C1—C5 | 1.3940 (18) | C12—H12A | 0.9600 |
| C1—H1A | 0.9300 | C12—H12B | 0.9600 |
| C2—H2A | 0.9300 | C12—H12C | 0.9600 |
| C11—S1—C8 | 91.61 (7) | O1—C6—C5 | 123.00 (12) |
| C3—N1—C2 | 117.21 (12) | N2—C6—C5 | 112.71 (11) |
| C6—N2—N3 | 119.98 (11) | O2—C7—N3 | 121.52 (11) |
| C6—N2—H1N2 | 120.0 | O2—C7—C8 | 122.19 (12) |
| N3—N2—H1N2 | 120.0 | N3—C7—C8 | 116.25 (11) |
| C7—N3—N2 | 119.00 (11) | C9—C8—C7 | 126.96 (13) |
| C7—N3—H1N3 | 120.5 | C9—C8—S1 | 111.48 (10) |
| N2—N3—H1N3 | 120.5 | C7—C8—S1 | 121.53 (10) |

| | | | |
|---|---|---|---|
| C2—C1—C5 | 119.18 (12) | C8—C9—C10 | 111.46 (13) |
| C2—C1—H1A | 120.4 | C8—C9—C12 | 126.03 (14) |
| C5—C1—H1A | 120.4 | C10—C9—C12 | 122.50 (13) |
| N1—C2—C1 | 123.01 (13) | C11—C10—C9 | 113.35 (13) |
| N1—C2—H2A | 118.5 | C11—C10—H10A | 123.3 |
| C1—C2—H2A | 118.5 | C9—C10—H10A | 123.3 |
| N1—C3—C4 | 123.85 (12) | C10—C11—S1 | 112.10 (11) |
| N1—C3—H3A | 118.1 | C10—C11—H11A | 124.0 |
| C4—C3—H3A | 118.1 | S1—C11—H11A | 124.0 |
| C3—C4—C5 | 118.45 (12) | C9—C12—H12A | 109.5 |
| C3—C4—H4A | 120.8 | C9—C12—H12B | 109.5 |
| C5—C4—H4A | 120.8 | H12A—C12—H12B | 109.5 |
| C1—C5—C4 | 118.16 (12) | C9—C12—H12C | 109.5 |
| C1—C5—C6 | 119.18 (11) | H12A—C12—H12C | 109.5 |
| C4—C5—C6 | 122.64 (12) | H12B—C12—H12C | 109.5 |
| O1—C6—N2 | 124.29 (12) | | |
| C6—N2—N3—C7 | −81.27 (15) | N2—N3—C7—C8 | −175.15 (11) |
| C3—N1—C2—C1 | 2.3 (2) | O2—C7—C8—C9 | 21.3 (2) |
| C5—C1—C2—N1 | 0.6 (2) | N3—C7—C8—C9 | −161.26 (13) |
| C2—N1—C3—C4 | −2.5 (2) | O2—C7—C8—S1 | −156.60 (11) |
| N1—C3—C4—C5 | −0.2 (2) | N3—C7—C8—S1 | 20.83 (16) |
| C2—C1—C5—C4 | −3.4 (2) | C11—S1—C8—C9 | −0.12 (11) |
| C2—C1—C5—C6 | 175.06 (12) | C11—S1—C8—C7 | 178.09 (12) |
| C3—C4—C5—C1 | 3.2 (2) | C7—C8—C9—C10 | −178.07 (13) |
| C3—C4—C5—C6 | −175.20 (12) | S1—C8—C9—C10 | 0.02 (15) |
| N3—N2—C6—O1 | −6.2 (2) | C7—C8—C9—C12 | 3.3 (2) |
| N3—N2—C6—C5 | 173.77 (11) | S1—C8—C9—C12 | −178.58 (13) |
| C1—C5—C6—O1 | 32.1 (2) | C8—C9—C10—C11 | 0.12 (19) |
| C4—C5—C6—O1 | −149.49 (14) | C12—C9—C10—C11 | 178.78 (14) |
| C1—C5—C6—N2 | −147.86 (13) | C9—C10—C11—S1 | −0.21 (17) |
| C4—C5—C6—N2 | 30.54 (18) | C8—S1—C11—C10 | 0.19 (12) |
| N2—N3—C7—O2 | 2.30 (18) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H1N2···N1$^{i}$ | 0.86 | 2.14 | 2.9068 (17) | 149 |
| N3—H1N3···O2$^{ii}$ | 0.86 | 1.99 | 2.8034 (15) | 158 |
| C4—H4A···O1$^{iii}$ | 0.93 | 2.58 | 3.2047 (17) | 125 |
| C10—H10A···O2$^{iv}$ | 0.93 | 2.51 | 3.3928 (19) | 159 |
| C11—H11A···Cg1$^{v}$ | 0.93 | 2.80 | 3.3760 (17) | 121 |

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

**Fig. 1**

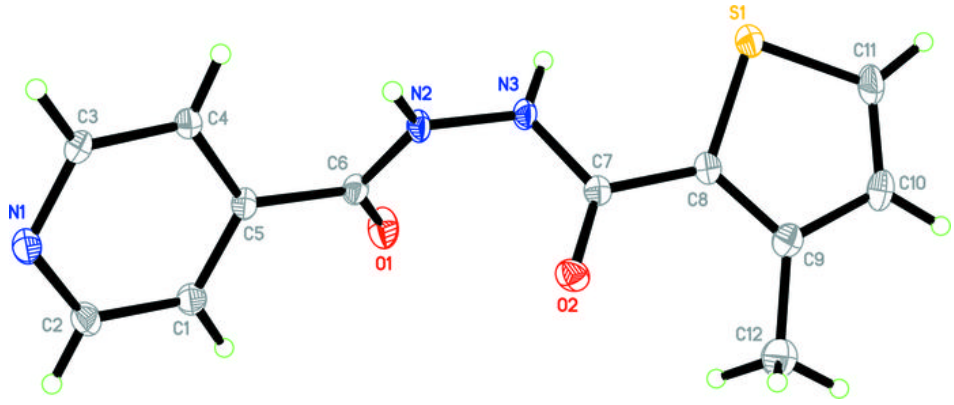

**Fig. 2**