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2-Methyl-1*H*-indole-3-carbaldehyde 2-thienoylhydrazone

Hapipah M. Ali,[a] Mohd Idris Najwa,[a] Ming-Jin Xie[b] and Seik Weng Ng[a]*

[a]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [b]School of Chemistry, Yunnan University, Kunming 650092, People's Republic of China

Correspondence e-mail: seikweng@um.edu.my

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Key indicators

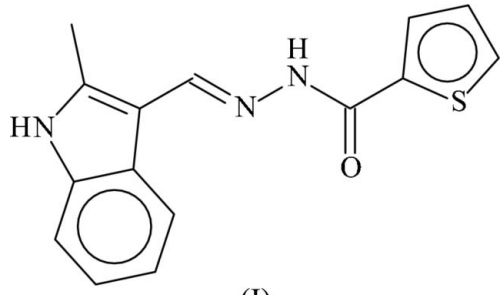
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.075
wR factor = 0.209
Data-to-parameter ratio = 16.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_{15}H_{13}N_3OS$, the amide H atom interacts with the amide O atom of an adjacent molecule [N···O = 3.027 (4) Å] to form a zigzag chain that runs along the c axis of the monoclinic unit cell.

Comment

This study continues our work on Schiff bases that are formed by condensing an aldehyde with thienoylhydrazide (Ali, Abdul Halim *et al.*, 2005; Ali, Puvaneswary *et al.*, 2005).



(I)

In the title compound, (I) (Fig. 1), the molecules interact through the amide N and carbonyl O atoms to form a zigzag chain (Table 1 and Fig. 2). The amine unit in the indolyl portion does not participate in hydrogen-bonding interactions.

Experimental

2-Methylindole-3-carbaldehyde (0.73 g, 4.6 mmol) and 2-thienoylhydrazide (0.66 g, 4.6 mmol) were heated in ethanol (100 ml) for 2 h. The solvent was removed and the product recrystallized from acetonitrile.

Crystal data

$C_{15}H_{13}N_3OS$
M_r = 283.34
Monoclinic, $P2_1/c$
a = 11.688 (2) Å
b = 11.546 (2) Å
c = 10.133 (2) Å
β = 94.694 (2)°
V = 1362.8 (4) Å^3
Z = 4
D_x = 1.381 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 295 (2) K
Block, yellow
0.24 × 0.23 × 0.20 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: none
11514 measured reflections
2793 independent reflections
1420 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.075$
$wR(F^2) = 0.209$
$S = 1.02$
2793 reflections
170 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0979P)^2 + 0.3022P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O1^{i}	0.86	2.27	3.027 (4)	147

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

The C-bound H atoms were placed at calculated positions (C—H = 0.93 and 0.96 Å), and were included in the refinement in the riding-model approximation with U_{iso}(H) set to 1.2–1.5 times U_{eq}(C). The amide and amine H atoms were similarly treated [N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N)]. The benzene ring was refined as a rigid hexagon in order to increase the data/parameter ratio as the crystal was not strongly diffracting.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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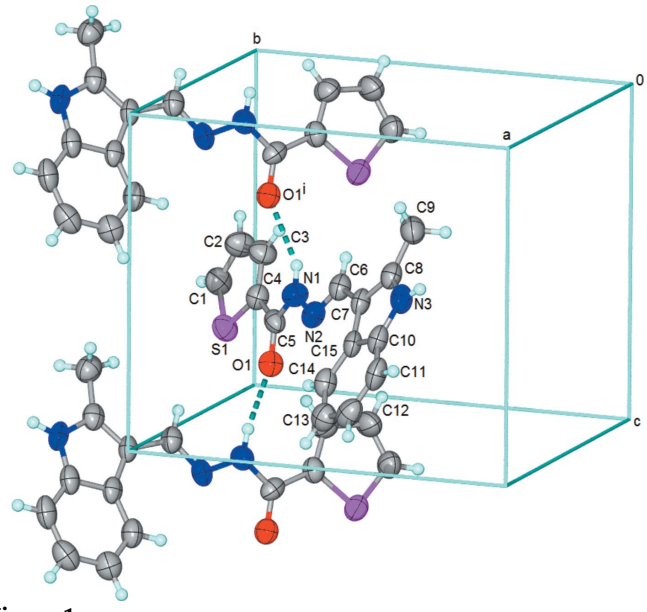

Figure 1
A partial packing diagram of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii. The dashed lines represent hydrogen bonds [symmetry code: (i) $x, \frac{3}{2}-y, -\frac{1}{2}+z$].

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