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N-Phenyl-*N*′-(2-thienylmethylene)hydrazine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.088
Data-to-parameter ratio = 13.7

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

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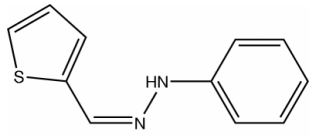
The title molecule, $C_{11}H_{10}N_2S$, is almost planar with normal bond lengths and angles. The crystal packing is stabilized by C—H···π and van der Waals interactions.

Comment

Thiophene-containing compounds are known as materials with potential applications in the flavor (Bertram *et al.*, 1993) and pharmaceutical industries (Press, 1991), in conducting polymer design (Bloor, 1995), as well as in non-linear optical materials (Nalwa, 1993). Moreover, thiophene derivatives are often used as intermediates in synthetic chemistry. The chemistry of hydrazones has been intensively investigated in recent years, owing to their coordinating capability, pharmacological activity, antibacterial and antifungal properties, and their use in analytical chemistry as highly selective extractants (Domino *et al.*, 1984; Sakamoto *et al.*, 1993; Li *et al.*, 1998).



(I)

We report here the crystal structure of the title compound, (I) (Fig. 1), synthesized by a condensation reaction of thiophene-2-carbaldehyde with phenylhydrazine. All bond lengths (Table 1) and angles in (I) are normal. The molecule is distorted from planarity; the dihedral angles of phenyl and thiophene rings with the plane formed by atoms C1/N1/N2/C7/C11 are 9.6 (3) and 9.82 (3)°, respectively. The crystal packing (Fig. 2) is mainly stabilized by van der Waals interactions. However, there is a short C7—H7···*Cg* (*Cg* is the centroid of the phenyl ring) contact (Table 2), which may be attributed to a C—H···π interaction.

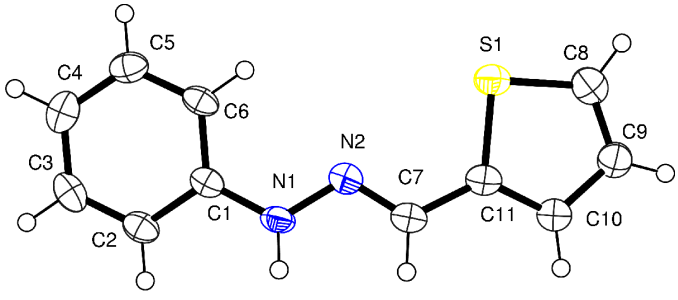


Figure 1
An *ORTEP*-3 (Farrugia, 1997) drawing of (I), showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

Experimental

Compound (I) was prepared according to the method described in the literature by Sarı & Gürkan (2003). A stirred mixture of phenylhydrazine (108 g, 1 mmol) and thiophene-2-carboxaldehyde (112 mg, 1 mmol) in methanolic media was refluxed for 6 h. After cooling, the precipitate was filtered off and was crystallized from methanol (yield 78%, m.p. 398 K).

Crystal data

$C_{11}H_{10}N_2S$
$M_r = 202.27$
Orthorhombic, $P2_12_12_1$
$a = 6.0473$ (6) Å
$b = 7.4417$ (7) Å
$c = 22.376$ (3) Å
$V = 1006.97$ (19) Å^3
$Z = 4$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12 880 reflections
$\theta = 1.8$–$25.8°$
$\mu = 0.28$ mm^{-1}
$T = 293$ (2) K
Plate, colorless
0.50 × 0.33 × 0.05 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{min} = 0.892$, $T_{max} = 0.986$
5892 measured reflections
1738 independent reflections
1403 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.0°$
$h = -6 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.088$
$S = 0.93$
1738 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: (Flack, 1983), 688 Friedel pairs
Flack parameter = 0.03 (12)

Table 1
Selected geometric parameters (Å, °).

N1—N2	1.363 (3)	N1—C1	1.381 (4)
S1—C8	1.709 (3)	N2—C7	1.272 (4)
S1—C11	1.721 (3)	C7—C11	1.445 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···Cg^{i}	0.93	2.68	3.461 (3)	142

Symmetry code: (i) $-x, y-\frac{1}{2}, \frac{1}{2}-z$. *Cg* is the centroid of the phenyl ring.

All H atoms were positioned geometrically (N—H = 0.86, C—H = 0.93 Å) and refined using a riding model. The U_{iso} values were assigned to $1.2U_{eq}$(C,N).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

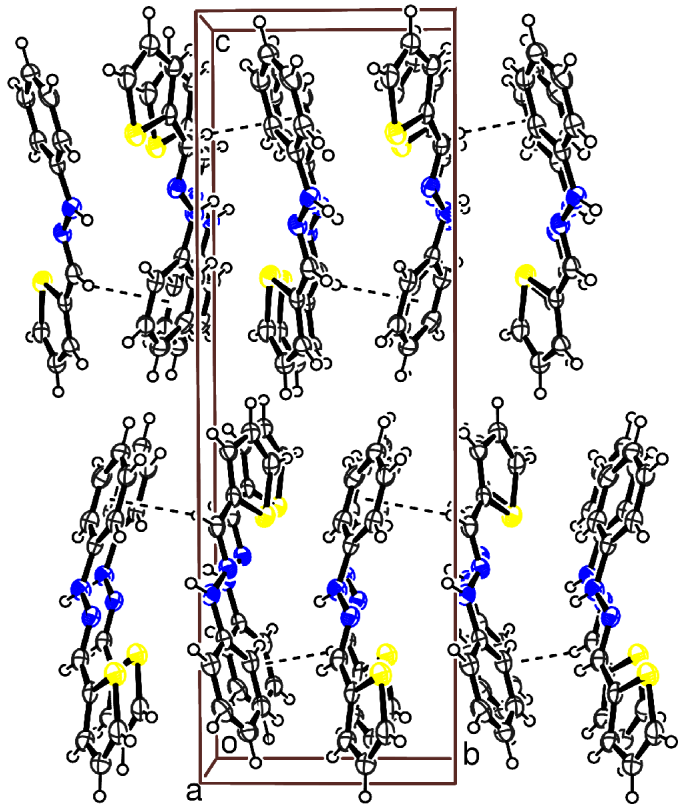


Figure 2
The packing (*ORTEP*-3; Farrugia, 1997) of (I). C—H···π interactions are indicated by dashed lines.

References

Bertram, H. J., Emberger, R., Güntrt, M., Sommer, H. & Werkhoff, P. (1993). *Recent Dev. Flavor Fragrance Chem.* **11**, 241–259.
Bloor, D. (1995). *Chem. Ber.* **31**, 385–387.
Domino, P., Pelizzi, C. & Predieri, G. (1984). *Polyhedron*, **3**, 281–286.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Li, X. R., Sun, Z. M. & Chang, J. C. (1998). *Synth. React. Inorg. Met. Org. Chem.* **18**, 657–665.
Nalwa, H. S. (1993). *Adv. Mater.* **5**, 341–358.
Press, J. B. (1991). *Chem. Heterocycl. Compd*, **44**, 397–502.
Sakamoto, H., Goto, H., Yokoshima, M., Dobashi, M., Ishikawa, J., Doi, K. & Otomo, M. (1993). *Bull. Chem. Soc. Jpn*, **66**, 2907–1914.
Sarı, N. & Gürkan, P. (2003). *Transition Met. Chem.* **28**, 687–693.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED*32 (Version 1.04). Stoe & Cie, Darmstadt, Germany.