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N′-(4-Hydroxybenzylidene)thiophene-2-carbohydrazide

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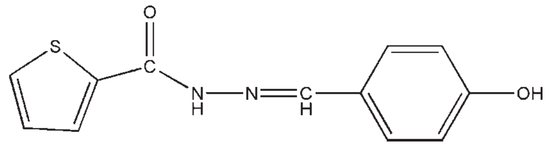
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.181; data-to-parameter ratio = 17.1.

In the title compound, $C_{12}H_{10}N_2O_2S$, the dihedral angle between the benzene and thiophene rings is 23.34 (16)°. In the crystal structure, molecules are linked by N—H⋯O and O—H⋯O hydrogen bonds, forming (100) sheets.

Related literature

For background to the pharmacological properties of Schiff bases, see: Ren *et al.* (2002). For a related structure, see: Li *et al.* (2009).



Experimental

Crystal data

$C_{12}H_{10}N_2O_2S$
M_r = 246.28
Monoclinic, $P2_1/c$
a = 9.5622 (19) Å
b = 12.404 (3) Å
c = 9.991 (2) Å
β = 104.40 (3)°
V = 1147.8 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
10889 measured reflections
2629 independent reflections
1501 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.181
S = 1.07
2629 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.27 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.38 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯O1$^{\rm i}$	0.86	2.09	2.887 (3)	154
O2—H2C⋯O1$^{\rm ii}$	0.82	2.10	2.913 (3)	174

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5483).

References

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supplementary materials

Acta Cryst. (2010). E**66**, o1719 [**doi:10.1107/S1600536810021483**]

N'-(4-Hydroxybenzylidene)thiophene-2-carbohydrazide

Y.-F. Li, J.-H. Jiang and **F.-F. Jian**

Comment

Schiff bases derivatives have attracted much attention due to their pharmacological activity (Ren *et al.*, 2002). As part of an investigation of the properties of Schiff bases functioning as ligands, we synthesized the title compound (I), and describe its structure here. The title compound contains two independent molecules in the unit. The dihedral angle between the aromatic rings is [23.33 (16)°]. In the crystal lattice, the N—H···O and O—H···O intramolecular hydrogen bonds which form the molecule structures.

Bond lengths and angles are comparable to those in a related compound (Li *et al.*, 2009).

Experimental

A mixture of 4-methylbenzaldehyde (0.1 mol), and thiophene-2-carbohydrazide (0.1 mol) was stirred in refluxing ethanol (20 ml) for 4 h to afford the title compound (0.092 mol, yield 92%). Colourless blocks of (I) were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances=0.97 Å, and with U_{iso}=1.2–1.5U_{eq}.

Figures

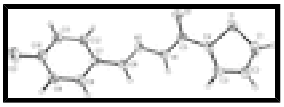

Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids.

N'-(4-Hydroxybenzylidene)thiophene-2-carbohydrazide

Crystal data

$C_{12}H_{10}N_2O_2S$	F(000) = 512
M_r = 246.28	D_x = 1.425 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1501 reflections
a = 9.5622 (19) Å	θ = 3.1–27.5°
b = 12.404 (3) Å	μ = 0.27 mm^{-1}
c = 9.991 (2) Å	T = 293 K
β = 104.40 (3)°	Block, colorless

$V = 1147.8$ (4) Å^3

$Z = 4$

0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer

Radiation source: fine-focus sealed tube

graphite

phi and ω scans

10889 measured reflections

2629 independent reflections

1501 reflections with $I > 2\sigma(I)$

$R_{\mathrm{int}} = 0.057$

$\theta_{\mathrm{max}} = 27.5°$, $\theta_{\mathrm{min}} = 3.1°$

$h = -12 \rightarrow 12$

$k = -16 \rightarrow 16$

$l = -11 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.181$

$S = 1.07$

2629 reflections

154 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\mathrm{max}} < 0.001$

$\Delta\rho_{\mathrm{max}} = 0.27$ e Å^{-3}

$\Delta\rho_{\mathrm{min}} = -0.38$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.89443 (10)	0.07271 (7)	0.19012 (8)	0.0713 (3)
N2	1.2232 (2)	0.37439 (19)	0.1118 (2)	0.0452 (6)
O1	1.1172 (2)	0.24125 (17)	0.27388 (17)	0.0548 (6)
N1	1.1217 (2)	0.29541 (19)	0.0602 (2)	0.0482 (6)
H1A	1.0911	0.2863	−0.0275	0.058*
C12	1.4377 (3)	0.5507 (2)	0.1730 (3)	0.0464 (6)

H12A	1.4518	0.4976	0.2407	0.056*
C4	0.9590 (3)	0.1566 (2)	0.0840 (2)	0.0435 (6)
C5	1.0717 (3)	0.2334 (2)	0.1475 (2)	0.0406 (6)
C7	1.3299 (3)	0.5378 (2)	0.0519 (2)	0.0430 (6)
C6	1.2339 (3)	0.4464 (2)	0.0230 (3)	0.0483 (7)
H6A	1.1759	0.4392	−0.0663	0.058*
C11	1.5235 (3)	0.6408 (2)	0.1941 (3)	0.0506 (7)
H11A	1.5936	0.6491	0.2767	0.061*
O2	1.5867 (3)	0.81085 (19)	0.1088 (2)	0.0816 (8)
H2C	1.6718	0.7957	0.1418	0.122*
C10	1.5063 (3)	0.7198 (2)	0.0930 (3)	0.0518 (7)
C8	1.3140 (3)	0.6189 (2)	−0.0471 (3)	0.0510 (7)
H8A	1.2427	0.6120	−0.1291	0.061*
C9	1.3999 (3)	0.7083 (2)	−0.0273 (3)	0.0569 (8)
H9A	1.3866	0.7613	−0.0951	0.068*
C3	0.8883 (4)	0.1398 (3)	−0.0502 (3)	0.0647 (9)
H3A	0.9077	0.1779	−0.1237	0.078*
C2	0.7834 (4)	0.0591 (3)	−0.0662 (3)	0.0756 (11)
H2B	0.7253	0.0377	−0.1512	0.091*
C1	0.7759 (4)	0.0163 (3)	0.0548 (3)	0.0765 (11)
H1B	0.7124	−0.0386	0.0632	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0791 (6)	0.0780 (6)	0.0592 (5)	−0.0243 (5)	0.0220 (4)	0.0166 (4)
N2	0.0506 (13)	0.0473 (14)	0.0398 (10)	−0.0127 (10)	0.0151 (10)	−0.0051 (9)
O1	0.0635 (13)	0.0682 (14)	0.0331 (9)	−0.0089 (10)	0.0129 (8)	0.0017 (8)
N1	0.0592 (15)	0.0545 (14)	0.0323 (10)	−0.0207 (11)	0.0138 (9)	−0.0059 (9)
C12	0.0476 (16)	0.0448 (15)	0.0466 (13)	−0.0047 (12)	0.0113 (12)	0.0066 (11)
C4	0.0461 (15)	0.0454 (15)	0.0416 (13)	−0.0069 (12)	0.0155 (11)	0.0010 (10)
C5	0.0446 (15)	0.0421 (14)	0.0374 (12)	−0.0003 (11)	0.0145 (10)	0.0003 (10)
C7	0.0485 (15)	0.0430 (15)	0.0398 (12)	−0.0050 (12)	0.0151 (11)	−0.0050 (10)
C6	0.0552 (17)	0.0510 (16)	0.0393 (13)	−0.0130 (13)	0.0129 (12)	−0.0049 (11)
C11	0.0465 (16)	0.0493 (17)	0.0514 (14)	−0.0048 (13)	0.0035 (12)	0.0062 (12)
O2	0.0694 (16)	0.0573 (15)	0.0975 (17)	−0.0248 (12)	−0.0184 (13)	0.0290 (12)
C10	0.0473 (16)	0.0409 (16)	0.0640 (17)	−0.0058 (13)	0.0078 (13)	0.0081 (12)
C8	0.0577 (18)	0.0497 (17)	0.0423 (13)	−0.0090 (14)	0.0064 (12)	0.0018 (11)
C9	0.063 (2)	0.0483 (18)	0.0543 (15)	−0.0072 (14)	0.0048 (14)	0.0120 (12)
C3	0.075 (2)	0.074 (2)	0.0457 (15)	−0.0327 (18)	0.0160 (15)	−0.0009 (14)
C2	0.079 (2)	0.085 (3)	0.0599 (18)	−0.041 (2)	0.0132 (17)	−0.0104 (16)
C1	0.073 (2)	0.071 (2)	0.088 (2)	−0.0361 (19)	0.0245 (19)	0.0017 (18)

Geometric parameters (Å, °)

S1—C1	1.685 (4)	C6—H6A	0.9300
S1—C4	1.707 (2)	C11—C10	1.387 (4)
N2—C6	1.281 (3)	C11—H11A	0.9300
N2—N1	1.385 (3)	O2—C10	1.354 (3)

O1—C5	1.233 (3)	O2—H2C	0.8200
N1—C5	1.337 (3)	C10—C9	1.375 (4)
N1—H1A	0.8600	C8—C9	1.364 (4)
C12—C11	1.371 (4)	C8—H8A	0.9300
C12—C7	1.390 (4)	C9—H9A	0.9300
C12—H12A	0.9300	C3—C2	1.398 (4)
C4—C3	1.360 (4)	C3—H3A	0.9300
C4—C5	1.461 (4)	C2—C1	1.339 (4)
C7—C8	1.392 (4)	C2—H2B	0.9300
C7—C6	1.443 (4)	C1—H1B	0.9300

C1—S1—C4	91.70 (14)	C12—C11—H11A	119.8
C6—N2—N1	113.9 (2)	C10—C11—H11A	119.8
C5—N1—N2	119.68 (19)	C10—O2—H2C	109.5
C5—N1—H1A	120.2	O2—C10—C9	117.6 (3)
N2—N1—H1A	120.2	O2—C10—C11	122.9 (3)
C11—C12—C7	120.9 (2)	C9—C10—C11	119.5 (3)
C11—C12—H12A	119.6	C9—C8—C7	121.9 (3)
C7—C12—H12A	119.6	C9—C8—H8A	119.1
C3—C4—C5	131.4 (2)	C7—C8—H8A	119.1
C3—C4—S1	110.6 (2)	C8—C9—C10	119.9 (3)
C5—C4—S1	118.01 (18)	C8—C9—H9A	120.0
O1—C5—N1	122.0 (2)	C10—C9—H9A	120.0
O1—C5—C4	122.1 (2)	C4—C3—C2	112.9 (3)
N1—C5—C4	115.9 (2)	C4—C3—H3A	123.5
C12—C7—C8	117.5 (3)	C2—C3—H3A	123.5
C12—C7—C6	124.2 (2)	C1—C2—C3	112.3 (3)
C8—C7—C6	118.3 (2)	C1—C2—H2B	123.9
N2—C6—C7	124.5 (2)	C3—C2—H2B	123.9
N2—C6—H6A	117.8	C2—C1—S1	112.6 (3)
C7—C6—H6A	117.8	C2—C1—H1B	123.7
C12—C11—C10	120.3 (3)	S1—C1—H1B	123.7

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1$^{\rm i}$	0.86	2.09	2.887 (3)	154
O2—H2C···O1$^{\rm ii}$	0.82	2.10	2.913 (3)	174

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

Fig. 1