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1-(4-Hydroxybenzylidene)-4-phenylthiosemicarbazide

Fang-Fang Jian* and Ying Li

New Materials & Function Coordination Chemistry Laboratory, Qingdao University of Science & Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: ffj2003@163169.net

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Key indicators

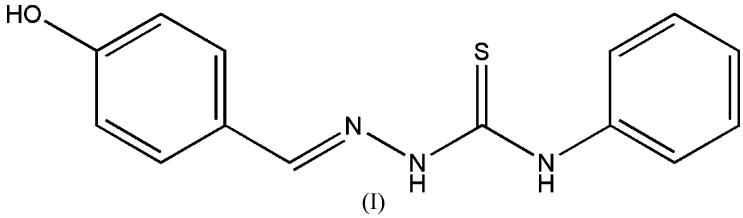
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.111
Data-to-parameter ratio = 17.1

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

The title compound, $C_{14}H_{13}N_3OS$, was prepared by the reaction of *p*-hydroxybenzaldehyde, hydrazine and phenyl isothiocyanate. The crystal packing is stabilized by C—H···π, N—H···S, C—H···O and O—H···S intermolecular interactions.

Comment

Thiourea (TU) is a very convenient and frequently employed nucleophile used to study ligand substitution reactions in coordination chemistry because of its good solubility, neutral character and high nucleophilicity (Schiessl *et al.*, 2005). Thiourea derivatives have been successfully screened for various biological activities (Antholine & Taketa, 1982). Furthermore, TU and its derivatives have also been screened for allergenic and carcinogenic factors. It has also been shown that their presence inhibits nitrification in soil and water (Spataru *et al.*, 2005). As TU and its derivatives have unique characteristics and pharmacutical potential, we have synthesized the title compound, (I), and describe its structure here.



(I)

In the title compound, bond lengths and angles are in usual ranges (Ji *et al.*, 2002). In (I), atoms S1, N1, N2, C6 and C7 are planar (plane *p*1); the intramolecular hydrogen bond N1—H1*B*···N3 (Table 1 and Fig. 1) contributes to the planarity. The other four atoms (N2, N3, C8, C9) are also coplanar (plane *p*2). The dihedral angle between the two aromatic rings is 83.51 (3)°. The dihedral angle between *p*1 and *p*2 is 12.30 (2)°.

The crystal packing is realised by O—H···S and N—H···S hydrogen bonds (Table 1 and Fig. 2). Molecules are involved in C—H···π interactions between C13–H13 and the centroid (*Cg*) of the C1–C6 ring at $(1+x, \frac{1}{2}-y, -\frac{1}{2}+z)$; C—H = 0.93 Å, H···*Cg* = 2.80 Å, C···*Cg* = 3.595 (2) Å and C—H···*Cg* = 144°.

Experimental

The title compound was prepared by the reaction of hydrazine (1.0 g, 20 mmol) and *p*-hydroxybenzaldehyde (2.4 g, 20 mmol) with phenyl isothiocyanate (2.7 g, 20 mmol). Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization

from an ethanol solution at room temperature. (yield 5.0 g, 92.3%; m.p. 481–484 K).

Crystal data

$C_{14}H_{13}N_3OS$
M_r = 271.34
Monoclinic, $P2_1/c$
a = 10.323 (2) Å
b = 12.697 (3) Å
c = 10.597 (2) Å
β = 95.57 (3)°
V = 1382.4 (5) Å^3
Z = 4
D_x = 1.304 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 293 (2) K
Block, yellow
0.30 × 0.25 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
3123 measured reflections
2999 independent reflections
1914 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 27.0°
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.02
2964 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.3594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0094 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···S1^{i}	0.82	2.43	3.159 (3)	149
N1—H1B···N3	0.86	2.18	2.594 (2)	109
N2—H2A···S1^{ii}	0.86	2.62	3.422 (2)	156

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

All H atoms were positioned geometrically (N—H = 0.86, C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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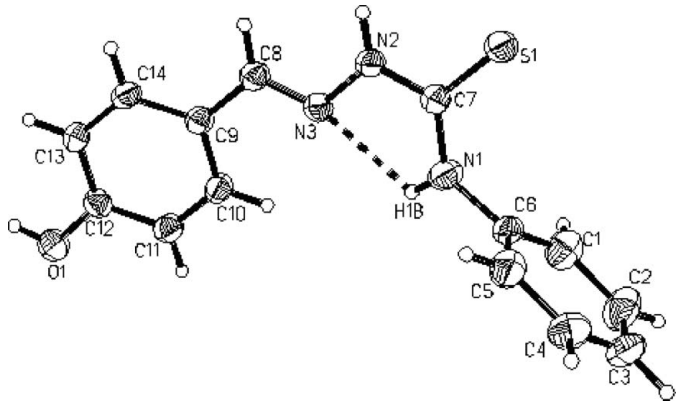

Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is indicated by a dashed line.

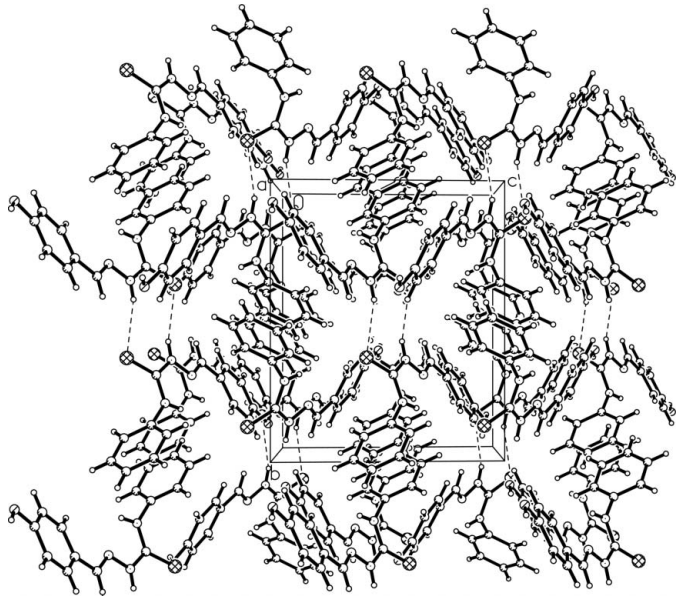

Figure 2
Crystal packing of (I). Hydrogen bonds are shown as dashed lines.

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