

De-Suo Yang

Department of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, Baoji 721007, People's Republic of China

Correspondence e-mail:
desuoyang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.045
wR factor = 0.117
Data-to-parameter ratio = 16.0

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

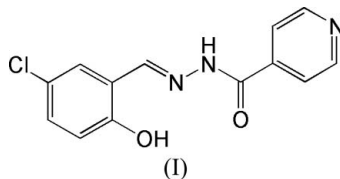
N'-[1-(5-Chloro-2-hydroxyphenyl)methylidene]-isonicotinohydrazide

The molecule of the title compound, $\text{C}_{13}\text{H}_{10}\text{ClN}_3\text{O}_2$, is approximately planar and displays a *trans* configuration with respect to the $\text{C}=\text{N}$ double bond. The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds, forming layers parallel to the *ab* plane.

Received 6 August 2006
Accepted 6 August 2006

Comment

Schiff base compounds play an important role in the development of coordination chemistry (Musie *et al.*, 2001; Bernardo *et al.*, 1996; Paul *et al.*, 2002). As an extension of our work on the structural characterization of such compounds (Yang, 2006*a,b,c*), the crystal structure of the title compound, (I), is reported here.



In (I) (Fig. 1), all the bond lengths are within normal ranges (Allen *et al.*, 1987), and comparable to those of the similar compounds (Qian *et al.*, 2006; Qiu, Xu *et al.*, 2006; Qiu, Fang, Liu & Zhu, 2006; Qiu, Fang, Yang *et al.*, 2006). The $\text{C}7-\text{N}1$ bond length of 1.267 (2) \AA conforms to the value for a double bond. The bond length of 1.357 (2) \AA between atoms $\text{C}8$ and $\text{N}2$ is intermediate between a $\text{C}-\text{N}$ single and double bond. The dihedral angle between the benzene ring and the pyridine ring is 10.6 (2) $^\circ$. The molecular structure is stabilized by an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond (Table 1). In the crystal structure, molecules are linked through intermolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 1), forming layers parallel to the *ab* plane (Fig. 2).

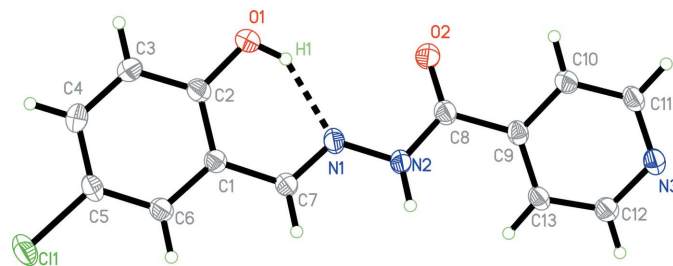


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and pyridine-4-carboxylic acid hydrazide (0.1 mmol, 13.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature to give a clear yellow solution. Crystals of the title compound were formed by gradual evaporation of the solvent over a period of about one week at room temperature. Analysis found: C 56.73, H 3.72, N 15.08%; calculated for C₁₃H₁₀ClN₃O₂: C 56.64, H 3.66, N 15.24%.

Crystal data

C₁₃H₁₀ClN₃O₂ Z = 4
 M_r = 275.69 D_x = 1.483 Mg m⁻³
 Monoclinic, P2₁/n Mo Kα radiation
 a = 8.617 (1) Å μ = 0.31 mm⁻¹
 b = 15.730 (2) Å T = 298 (2) K
 c = 9.285 (1) Å Block, yellow
 β = 101.219 (2)° 0.33 × 0.29 × 0.27 mm
 V = 1234.5 (3) Å³

Data collection

Bruker SMART CCD area-detector 10471 measured reflections
 diffractometer 2812 independent reflections
 ω scans 2007 reflections with I > 2σ(I)
 Absorption correction: multi-scan R_{int} = 0.036
 (SADABS; Sheldrick, 1996) θ_{max} = 27.5°
 T_{min} = 0.905, T_{max} = 0.921

Refinement

Refinement on F² w = 1/[σ²(F_o²) + (0.0507P)²
 R[F² > 2σ(F²)] = 0.045 + 0.1995P
 wR(F²) = 0.117 where P = (F_o² + 2F_c²)/3
 S = 1.02 (Δ/σ)_{max} < 0.001
 2812 reflections Δρ_{max} = 0.24 e Å⁻³
 176 parameters Δρ_{min} = -0.24 e Å⁻³
 H atoms treated by a mixture of independent and constrained refinement

Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
N2—H2...N3 ⁱ	0.897 (10)	2.127 (10)	3.017 (2)	172 (2)
O1—H1...N1	0.82	1.86	2.576 (2)	145

Symmetry code: (i) x + ½, -y + ½, z + ½.

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with O—H = 0.82 Å, C—H = 0.93 Å, and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXL97.

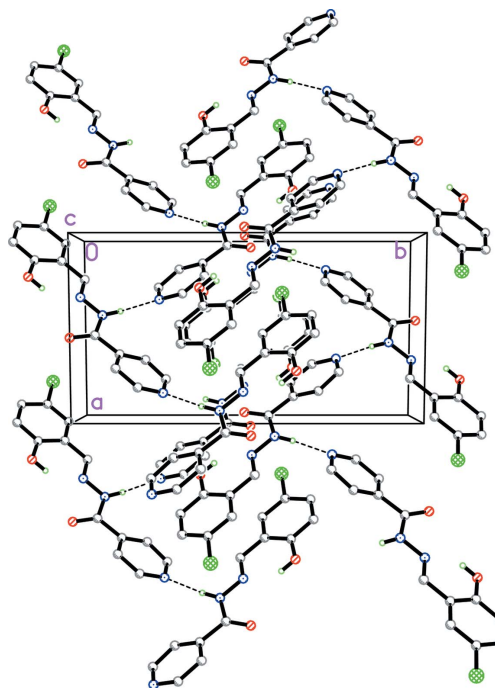


Figure 2

Packing of (I) viewed along the c axis. Dashed lines indicate intermolecular hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Financial support from the Baoji College of Arts and Sciences research funds is gratefully acknowledged.

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.
 Bernardo, K., Leppard, S., Robert, A., Commenges, G., Dahan, F. & Meunier, B. (1996). *Inorg. Chem.* **35**, 387–396.
 Bruker (2002). *SAINT and SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Musie, G. T., Wei, M., Subramaniam, B. & Busch, D. H. (2001). *Inorg. Chem.* **40**, 3336–3341.
 Paul, S., Barik, A. K., Peng, S. M. & Kar, S. K. (2002). *Inorg. Chem.* **41**, 5803–5809.
 Qian, H.-Y., Yin, Z.-G., Jia, J., Liu, S.-M. & Feng, L.-Q. (2006). *Acta Cryst.* **E62**, o3623–o3624.
 Qiu, X.-Y., Fang, X.-N., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* **E62**, o2685–o2686.
 Qiu, X.-Y., Fang, X.-N., Yang, S.-L., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* **E62**, o2687–o2688.
 Qiu, X.-Y., Xu, H.-J., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* **E62**, o2304–o2305.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). *SHELXL97 and SHELXS97*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 Yang, D.-S. (2006a). *Acta Cryst.* **E62**, o1395–o1396.
 Yang, D.-S. (2006b). *Acta Cryst.* **E62**, o1591–o1592.
 Yang, D.-S. (2006c). *Acta Cryst.* **E62**, o2365–o2366.