Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Chloro-2-(2-hydroxybenzylideneamino)-benzonitrile

Kui Cheng,[a] Hai-Liang Zhu,[a]* Zhi-Bin Li[b] and Zheng Yan[a]

[a]Department of Chemistry, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China, and [b]Department of Environment and Urban Construction, Wuhan University of Science and Engineering, Wuhan 430073, People's Republic of China

Correspondence e-mail: hailiang_zhu@163.com

Received 2 May 2006
Accepted 17 May 2006

The molecule of the title compound, $C_{14}H_9ClN_2O$, is essentially planar, suggesting a high degree of conjugation throughout the system. Intermolecular hydrogen bonds link adjacent molecules, forming one-dimensional chains running parallel to the *b* axis.

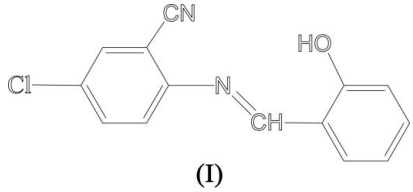
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.073
wR factor = 0.168
Data-to-parameter ratio = 14.1

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

Comment

Recently, we have reported a few Schiff base compounds (Cheng *et al.*, 2005, 2006; Zhu *et al.*, 2005). As an extension of our work on the structural characterization of Schiff bases, the title compound, (I), is reported here.



(I)

In the title compound, all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C1═N1 bond length of 1.275 (4) Å conforms to the value for a double bond. A strong intramolecular O—H···N hydrogen bond (Table 1) results in the formation of a pseudo-six-membered planar ring (C7/C6/C1/O1/H1/N1) (Fig. 1). In the crystal packing, intermolecular C—H···O interactions (Table 1) link the molecules, forming chains running parallel to the *b* axis (Fig. 2).

Experimental

Salicylaldehyde and 2-cyano-4-chloroaniline were available commercially and were used without further purification. A solutiom of salicylaldehyde (2.0 mmol, 244 mg) in methanol (20 ml) was added to a solution of 2-cyano-4-chloroaniline (2.0 mmol, 304 mg) in ethanol (20 ml). The mixture was stirred for 20 min and filtered. After leaving the filtrate to stand in air for 6 d, large yellow prismatic crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 88.7%). Analysis found: C 83.8, H 5.1, N 28.3%; calculated for $C_{17}H_{13}NO$: C 84.1, H 5.0, N 28.0%.

Crystal data

$C_{14}H_9ClN_2O$
M_r = 256.68
Monoclinic, $P2_1/c$
a = 4.7060 (12) Å
b = 14.372 (4) Å
c = 18.225 (5) Å
β = 91.228 (4)°
V = 1232.4 (6) Å^3
Z = 4
D_x = 1.383 Mg m^{-3}
Mo *Kα* radiation
μ = 0.30 mm^{-1}
T = 292 (2) K
Elongated prism, yellow
0.62 × 0.35 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.883, T_{max} = 0.928
9840 measured reflections
2299 independent reflections
1696 reflections with $I > 2\sigma(I)$
R_{int} = 0.117
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.168
S = 1.10
2299 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.9611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.98	2.620 (4)	135
C10—H10···O1^{i}	0.93	2.50	3.321 (4)	147

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

H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances of 0.93 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). The rather high R_{int} value (0.12) may result from the relatively poor quality of the crystal.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

This project was sponsored by the Scientific Research Foundation for returned overseas Chinese scholars.

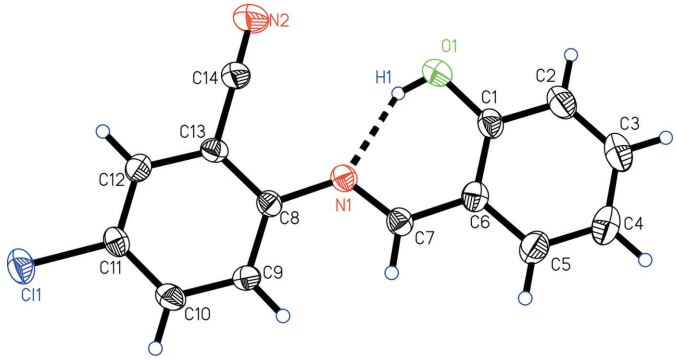


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates a hydrogen bond.

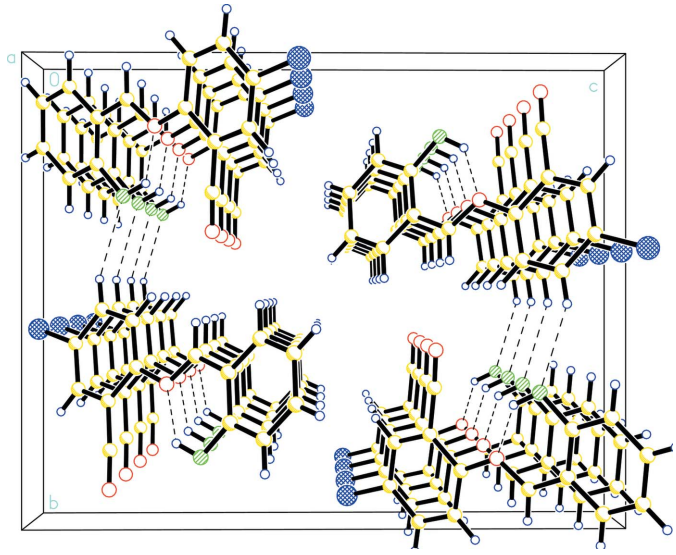


Figure 2
The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are indicated by dashed lines.

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.
Cheng, K., You, Z.-L., Li, Y.-G. & Zhu, H.-L. (2005). *Acta Cryst.* E**61**, o1137–o1138.
Cheng, K., Zhu, H.-L., Liu, J.-J., Gao, M. & Zeng, J.-H. (2006). *Acta Cryst.* E**62**, o1932–o1933.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zhu, H.-L., Cheng, K., You, Z.-L. & Li, Y.-G. (2005). *Acta Cryst.* E**61**, m755–m756.