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2-Hydroxy-6-[(2-hydroxyphenylamino)methylene]-cyclohexa-2,4-dienone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.098
wR factor = 0.296
Data-to-parameter ratio = 17.4

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

The title compound, $C_{13}H_{11}NO_3$, adopts the keto–amine tautomeric form, with the H atom located on N rather than on O. This H atom is involved in a strong intramolecular hydrogen bond. There are two independent molecules in the asymmetric unit. The molecules are linked by intramolecular N—H···O and O—H···O and intermolecular O—H···O hydrogen bonds into a three-dimensional network.

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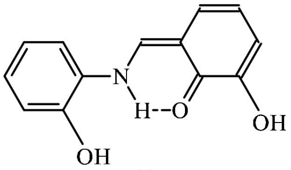
Comment

o-Hydroxy Schiff bases derived from the reaction of *o*-hydroxy aldehydes with aniline have been examined extensively (Stewart & Lingafelter, 1959; Calligaris *et al.*, 1972; Maslen & Waters, 1975). Schiff base compounds display interesting photochromic and thermochromic features and can be classified by them (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1980; Hadjoudis *et al.*, 1987). Photo- and thermochromism arise *via* H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994).



(I)

There are two types of intramolecular hydrogen bonds in Schiff bases, in keto–amine (N—H···O) and enol–imine (N···H—O) tautomeric forms. The present X-ray investigation shows that the title compound, (I), exists in the keto–amine form.

The asymmetric unit of (I) contains two independent molecules, labelled *A* and *B*. Fig. 1 shows the position of these two molecules relative to each other. Selected bond lengths and angles are listed in Table 1. There is good agreement between the bond lengths and angles of molecules *A* and *B*. The C13*A*—O2*A*, C7*A*—N1*A*, C13*B*—O2*B* and C7*B*—N1*B* bond lengths confirm the keto–amine form of (I). These distances agree with the corresponding distances in 3-[(2-oxo-1-naphthylidene)methylamino]benzoic acid [1.290 (2) and 1.319 (3) Å; Pavlović & Sosa, 2000], which also shows the keto–amine form. These bond lengths are completely different in *N*-[3,5-bis(trifluoromethyl)-phenyl]-3-methoxysalicylaldimine [1.352 (3) and 1.280 (4) Å; Karadayı *et al.*, 2003], which exists in the enol–imine form.

Compound (I) displays strong intramolecular N—H···O hydrogen bonds between atoms N1*A* and O2*A* and atoms N1*B* and O2*B* (Table 2). This type of strong intramolecular

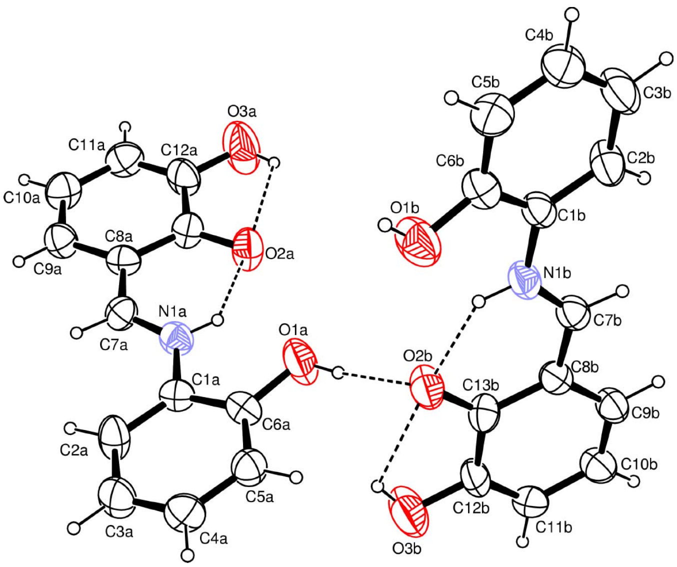


Figure 1
A view of the asymmetric unit of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

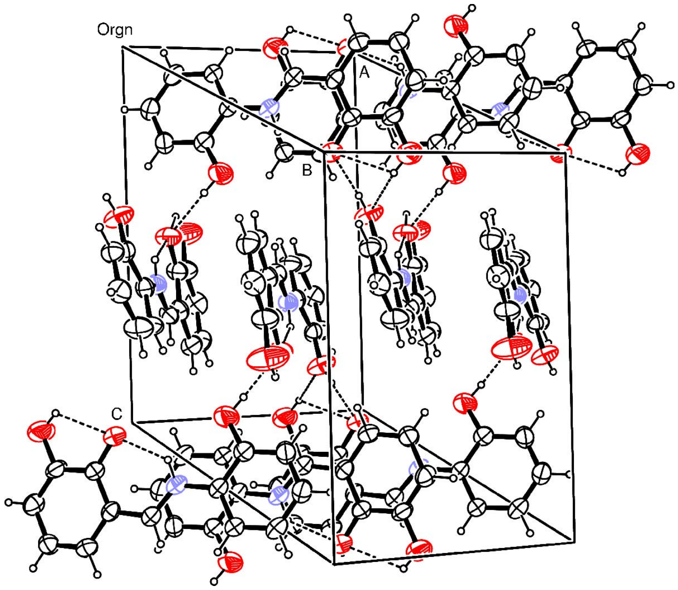


Figure 2
A packing diagram of the title compound. Dashed lines indicate hydrogen bonds.

hydrogen bond is a common feature of *o*-hydroxysalicylidene systems (Filarowski *et al.*, 2003; Yıldız *et al.*, 1998; Odabaşoğlu, Albayrak, Büyükgüngör & Lönnecke, 2003).

Experimental

The title compound was prepared as described by Odabasoğlu, Albayrak, Büyükgüngör & Goesmann (2003), using 2-hydroxyaniline and 3-hydroxysalicylaldehyde as starting materials. Well shaped crystals of (I) were obtained by slow evaporation of an ethanol solution (yield 86%; m.p. 449–450 K).

Crystal data

$C_{13}H_{11}NO_3$
$M_r = 229.23$
Triclinic, $P\overline{1}$
$a = 8.938$ (2) Å
$b = 10.520$ (3) Å
$c = 12.548$ (3) Å
$\alpha = 67.726$ (18)°
$\beta = 89.769$ (18)°
$\gamma = 77.689$ (18)°
$V = 1062.9$ (5) Å^3
$Z = 4$
$D_x = 1.433$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9705 reflections
$\theta = 2.2$–27.0°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Plate, red
0.38 × 0.26 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
ω rotation method
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.965$, $T_{\max} = 0.992$
18 950 measured reflections
5355 independent reflections
1774 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.113$
$\theta_{\max} = 28.5°$
$h = -10 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.098$
$wR(F^2) = 0.296$
$S = 0.89$
5355 reflections
307 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.145P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.88$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected bond lengths (Å).

N1*A*—C7*A*	1.296 (6)	N1*B*—C7*B*	1.294 (6)
O2*A*—C13*A*	1.291 (6)	C13*B*—O2*B*	1.296 (6)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O2*A*	0.86	1.98	2.655 (5)	134
O1*A*—H1*A*1···O2*B*	0.82	1.85	2.664 (5)	174
O3*A*—H33*A*···O2*A*	0.82	2.27	2.710 (6)	114
N1*B*—H1*B*···O2*B*	0.86	1.96	2.637 (5)	135
O3*B*—H33*B*···O2*B*	0.82	2.25	2.694 (6)	115
O1*B*—H1*B*1···O2*A*$^{\rm i}$	0.82	1.84	2.658 (6)	176

Symmetry code: (i) $x - 1, y, z$.

All H atoms were treated using a riding model, with C—H = 0.93 Å, O—H = 0.82 Å and N—H = 0.86 Å, and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), 1.2$U_{\rm eq}$(N) or 1.5 $U_{\rm eq}$(O). Although the data completeness is 0.995, the observed proportion of data is low (0.33) and the *R* and $R_{\rm int}$ values are not low and they must be because of the crystal poor quality and its unstability in room temperature. Attempts to collect data at low temperature failed because the crystal decomposed with time.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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