Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

A redetermination of 1-{4-[(2-hydroxybenzylidene)amino]phenyl}ethanone

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Received 9 March 2004
Accepted 29 March 2004
Online 9 April 2004

The crystal structure of the title compound, $C_{15}H_{13}NO_2$, has been redetermined with better precision and with the location and free refinement of all H atoms [previous report; Rekhlova, Furmanova, Chanturiya & Chikhladze (1991). *Kristallografiya*, **36**, 117–120]. The molecule is present as the phenol–imine tautomeric form with strong intramolecular O—H···N hydrogen bonds.

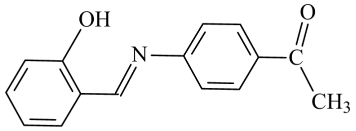
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.100
Data-to-parameter ratio = 11.1

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

Comment

Schiff bases are widely used as ligands in the field of coordination chemistry (Calligaris & Randaccio, 1987). The overall behaviour of these compounds has been defined as a proton transfer reaction between the phenol–imine and keto–amine tautomers. It is known that the phenol–imine tautomer is dominant in salicylaldimine, while the keto–amine form is preferred in the naphthaldimine Schiff bases, depending on the solvent polarities. Moreover, in the solid state, the keto–amine tautomer is present in naphthaldimines (Özek *et al.*, 2004), while the phenol–imine form exists in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998; Yüce *et al.*, 2004).



(I)

We report here a re-determination of the crystal structure of the title compound, (I), which has been determined earlier by Rekhlova *et al.* (1991) with a higher *R* value (0.061) and without location of the H atoms. All bond lengths and angles are normal (Table 1). Compound (I) adopts the phenol–imine tautomeric form with intramolecular O—H···N hydrogen bonding (Fig. 1 and Table 2). The O1···N1 distance of 2.5941 (15) Å is comparable to those observed in (3-methoxyphenyl)salicylaldimine [2.598 (2) Å; Elmalı *et al.*,

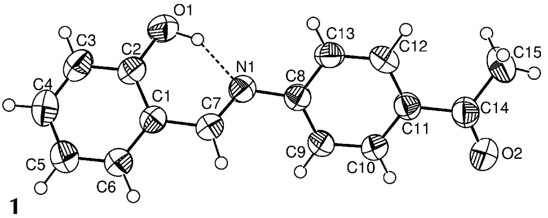


Figure 1
An *ORTEP*-3 (Farrugia, 1997) view of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. The intramolecular hydrogen bond is indicated by a dashed line.

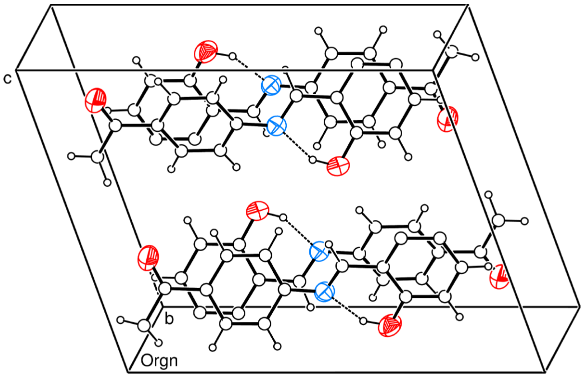


Figure 2
A packing diagram of (I), viewed approximately along the *b* axis.

1999], *N*-(2-hydroxyphenyl)salicylaldimine [2.625 (7) Å; Elerman *et al.*, 1995], 2,2-salicylaldimine [2.611 (6) Å; Xu *et al.*, 1994], 2-{[tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one and its 6-hydroxy and 6-methoxy derivatives [2.556 (2) Å; Odabaşoğlu *et al.*, 2003]. The N1—C7 bond length of 1.2772 (16) Å indicates a high degree of double-bond character comparable with that in (3-methoxyphenyl)salicylaldimine [1.280 (2) Å; Elmalı *et al.*, 1999]

It is known that Schiff bases may exhibit thermochromism or photochromism, depending on the planarity or non-planarity of the molecule, respectively. Therefore, one can expect photochromic properties in (I) caused by non-planarity of the molecule; the dihedral angle between the planes of the two aromatic rings is 35.69 (5)°.

Experimental

The title compound, (I), was prepared as described in the literature (Odabaşoğlu *et al.*, 2003) using 4-acetylaniline and salicylaldehyde as starting materials (yield 82%, m.p. 383–385 K).

Crystal data

$C_{15}H_{13}NO_2$
$M_r = 239.26$
Monoclinic, $P2_1/c$
$a = 14.7692$ (11) Å
$b = 7.4051$ (5) Å
$c = 11.5752$ (14) Å
$\beta = 106.898$ (8)°
$V = 1211.29$ (19) Å^3
$Z = 4$

$D_x = 1.312$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10198 reflections
$\theta = 2.9$–26°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Irregular, orange
0.50 × 0.29 × 0.16 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{min} = 0.961$, $T_{max} = 0.987$
16727 measured reflections

2377 independent reflections
1639 reflections with $I > 2\sigma(I)$
$R_{int} = 0.094$
$\theta_{max} = 26.0°$
$h = -18 \rightarrow 18$
$k = -9 \rightarrow 8$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.100$
$S = 0.97$
2377 reflections
215 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.10$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.4428 (18)	C10—C11	1.3857 (18)
C2—O1	1.3500 (17)	C11—C14	1.484 (2)
C7—N1	1.2772 (16)	C14—O2	1.2138 (19)
C8—N1	1.4138 (17)		
O1—C2—C3	119.12 (13)	C9—C8—N1	123.50 (11)
O1—C2—C1	121.22 (12)	O2—C14—C11	120.79 (13)
N1—C7—C1	121.89 (12)	O2—C14—C15	120.52 (15)
N1—C7—H1	122.5 (8)	C7—N1—C8	121.09 (11)
C13—C8—C9	119.16 (12)		
C6—C1—C2—O1	179.56 (13)	N1—C8—C13—C12	−176.69 (13)
C7—C1—C2—O1	0.0 (2)	C12—C11—C14—O2	174.13 (15)
C7—C1—C2—C3	179.90 (14)	C12—C11—C14—C15	−5.6 (2)
C7—C1—C6—C5	−179.68 (14)	C1—C7—N1—C8	−177.43 (12)
C6—C1—C7—N1	−179.62 (12)	C13—C8—N1—C7	−146.92 (13)
C2—C1—C7—N1	−0.1 (2)	C9—C8—N1—C7	36.54 (19)
N1—C8—C9—C10	176.78 (13)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H10···N1	0.94 (2)	1.73 (2)	2.5941 (15)	150.2 (18)

All the H atoms were found in a difference map and refined freely (C—H = 0.92–1.00 Å).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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