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3-(4-Acetylphenyliminomethyl)-1,2-dihydroxybenzene

Süheyla Yüce,[a]* Arzu Özek,[a] Çiğdem Albayrak,[b] Mustafa Odabaşoğlu[b] and Orhan Büyükgüngör[a]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey, and [b]Department of Chemistry, Ondokuz Mayıs University, TR-55139, Samsun, Turkey

Correspondence e-mail: syuce@omu.edu.tr

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Key indicators

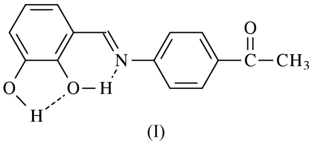
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.086
Data-to-parameter ratio = 10.8

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

The molecule of the title compound, $C_{15}H_{13}NO_3$, is not planar and the dihedral angle between the planes of the two aromatic rings is 53.93 (7)°. The molecule exists in the crystal structure in the phenol–imine tautomeric form and has two 'active' H atoms, which participate in strong intramolecular O—H···N and O—H···O hydrogen bonds. One of the H atoms is also involved in an intermolecular hydrogen bond, which links the molecules into centrosymmetric dimers.

Comment

Schiff bases are widely used as ligands in metal complexes (Calligaris & Randaccio, 1987). The chemical behavior of Schiff bases involving *ortho*-hydroxyphenyl fragments was shown to be determined to a large degree by a proton transfer reaction between phenol–imine and keto–amine tautomers. It is believed that, in DMSO and methanol solutions, the phenol–imine form is dominant in salicylaldimine, while the keto–amine form is preferred for *ortho*-hydroxynaphthaldimine Schiff bases. It was also observed that, in the solid state, the keto–amine form is present in hydroxynaphthaldimine, while the phenol–imine form exists in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998). The title compound, (I), being a derivative of salicylaldehyde with additional hydroxy substitution, exists as the phenol–imine tautomeric form in the crystal structure.



(I)

An *ORTEP*-3 (Farrugia, 1997) plot of the molecule of (I) is shown in Fig. 1. The molecule is not planar; the dihedral angle formed by the planes of the C1–C6 and C8–C13 aromatic rings is 53.93 (7)°. The N1—C7 bond length of 1.271 (2) Å indicates a high degree of double-bond character. This double-bond

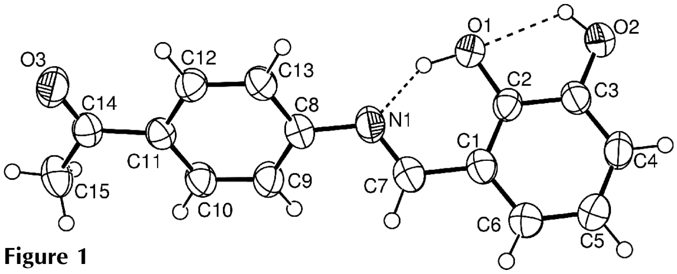


Figure 1
A view of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. Dashed lines indicate intramolecular hydrogen bonds.

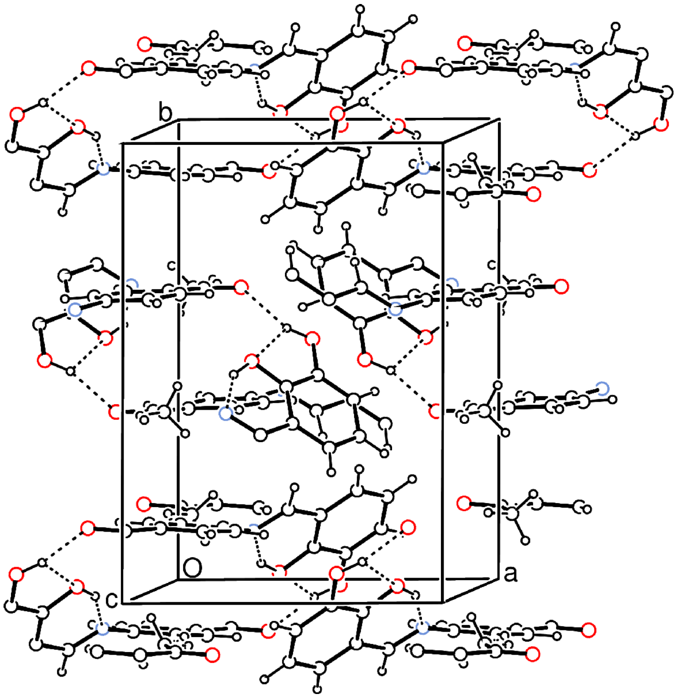


Figure 2
A packing diagram of (I), viewed approximately along the *c* axis. Dashed lines indicate hydrogen bonds.

distance is comparable to that in *N*,*N'*-bis(2-hydroxy-3-methoxyphenylmethylidene)-2,6-pyridinediamine [1.2973 (3) Å; Galic *et al.*, 2000].

Fig. 1 also shows two strong intramolecular hydrogen bonds (O1—H1···N1 and O2—H2···O1), which give rise to two five-membered pseudo-rings. The O1···N1 distance of 2.5737 (15) Å is comparable to those observed for analogous hydrogen bonds in *N*-(2-hydroxyphenyl)salicylaldimine [2.625 (7) Å; Elerman *et al.*, 1995], 2,2-salicylaldimine [2.611 (6) Å; Xu *et al.*, 1994], and 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].

In the structure of (I), there is also an intermolecular O2—H2···O3^{i} [symmetry code (i): $2 - x$, $1 - y$, $1 - z$] hydrogen bond, which links the molecules of (I) into centrosymmetric dimers (Fig. 2 and Table 2).

Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2003), using 4-acetylaniline and 2,3-dihydroxybenzaldehyde as starting materials (yield 79%, m.p. 432–434 K).

Crystal data

$C_{15}H_{13}NO_3$
$M_r = 255.26$
Monoclinic, $P2_1/c$
$a = 10.0014\ (11)$ Å
$b = 14.4188\ (4)$ Å
$c = 8.8212\ (10)$ Å
$\beta = 104.413\ (9)°$
$V = 1232.1\ (2)$ Å^3
$Z = 4$

$D_x = 1.376$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7244 reflections
$\theta = 2.1–26.0°$
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
Irregular shape, red
0.46 × 0.32 × 0.19 mm

Data collection

Stoe IPDS–II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\min} = 0.970$, $T_{\max} = 0.985$
8659 measured reflections

2425 independent reflections
1660 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\max} = 26.0°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.086$
$S = 0.92$
2425 reflections
224 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.3475 (17)	N1—C8	1.4155 (18)
O2—C3	1.3590 (18)	C1—C2	1.3983 (19)
O3—C14	1.2166 (17)	C1—C7	1.460 (2)
N1—C7	1.271 (2)	C11—C14	1.4839 (19)
C7—N1—C8	122.08 (13)	N1—C7—C1	120.84 (14)
C2—C1—C7	119.70 (13)	C13—C8—N1	117.87 (12)
O1—C2—C3	116.29 (12)	C9—C8—N1	122.36 (14)
O1—C2—C1	123.72 (12)	O3—C14—C11	120.33 (12)
O2—C3—C4	119.73 (13)	O3—C14—C15	119.87 (14)
O2—C3—C2	120.19 (13)	C11—C14—C15	119.79 (14)
C15—C14—C11—C10	−0.9 (2)	O1—C2—C1—C7	1.5 (2)
O3—C14—C11—C12	−2.6 (2)	C8—N1—C7—C1	176.34 (13)
C13—C8—N1—C7	135.50 (16)	C6—C1—C7—N1	176.60 (14)
C9—C8—N1—C7	−49.3 (2)	C2—C1—C7—N1	−4.6 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3^{i}	0.90 (2)	2.15 (2)	2.8550 (17)	134.3 (18)
O2—H2···O1	0.90 (2)	2.15 (2)	2.6774 (15)	116.5 (17)
O1—H1···N1	1.00 (2)	1.67 (2)	2.5737 (15)	149.2 (19)

Symmetry code: (i) $2 - x, 1 - y, 1 - z$.

All H atoms were located in a difference map and included in the refinement in an isotropic approximation [O1—H1 = 1.00 (2) Å, O2—H2 = 0.90 (2) Å and C—H = 0.91 (2)–0.988 (16) 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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