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Key indicators

Single-crystal X-ray study
$T = 296$ K
Mean σ(C–C) = 0.003 Å
H-atom completeness 99%
Disorder in solvent or counterion
R factor = 0.052
wR factor = 0.147
Data-to-parameter ratio = 15.3

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

Zwitterionic (E)-2-hydroxy-6-[(o-tolyliminio)-methyl]phenolate 0.07-hydrate

The title compound, $C_{14}H_{13}NO_2 \cdot 0.07H_2O$, crystallizes in a zwitterionic form. The dihedral angle between the aromatic rings is 29.23 (4)°. An N—H···O hydrogen bond generates an $S(6)$ ring motif and intermolecular O—H···O hydrogen bonds generate a centrosymmetric $R_2^2(10)$ dimer.

Comment

We have reported the crystal structures of Schiff base systems formed by organic amines and salicylaldehyde derivatives (Odabaşoğlu *et al.*, 1999, 2003, 2004, 2005, 2006; Yüce *et al.*, 2004a,b,c, 2006; Şahin, Albayrak *et al.*, 2005a,b; Şahin, Büyükgüngör *et al.*, 2005a,b; Özek *et al.*, 2004a,b,c,d, 2005; Albayrak *et al.*, 2005; Koşar *et al.*, 2004, 2005a,b,c; Ersanlı *et al.*, 2003, 2004a,b). The present work is part of a structural study of compounds of Schiff base systems and we report here the structure of the title compound, (I).
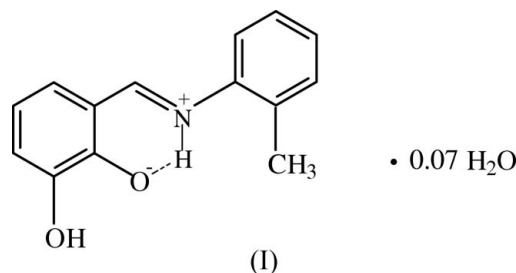
The molecular structure of (I) is shown in Fig. 1. It is well known that Schiff bases show keto–amine and enol–imine tautomerism. However, the title molecule has a zwitterionic form with a strong intramolecular N1—H1···O1 hydrogen bond (Table 1) which generates an $S(6)$ ring motif (Bernstein *et al.*, 1995). The C7═N1 [1.2946 (19) Å] and C2—O1 [1.3160 (19) Å] bond distances are comparable to those [1.2954 (19) and 1.2946 (17) Å] observed in a similar zwitterionic structure (Yüce *et al.*, 2006). The dihedral angle between the two benzene rings is 29.23 (4)°. The C2—C1—C7═N1 and C1—C7═N1—C8 torsion angles are 2.0 (2) and −179.65 (12)°, respectively.

In the crystal structure of (I), the molecules are linked into centrosymmetric $R_2^2(10)$ dimers by O—H···O hydrogen bonds (Fig. 2).

The solvent water O atom, O3, lies on a crystallographic twofold axis with a partial occupation factor. It is located 2.768 (7) Å from atoms O1(x, 1 + y, z) and O1(1 − x, 1 + y, $\frac{1}{2}$ − z). A C6—H6···O3 interaction [H6···O3 = 2.19 Å, C6···O3 = 3.047 (10) Å and C6—H6···O3 = 153°] is also observed.

Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2005), using *o*-toluidine and 2,3-dihydroxybenzaldehyde as starting materials (yield 84%; m.p. 384–385 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{14}H_{13}NO_2 \cdot 0.07H_2O$	$Z = 8$
$M_r = 228.52$	$D_x = 1.314$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 23.9334$ (14) Å	$\mu = 0.09$ mm^{-1}
$b = 7.2265$ (5) Å	$T = 296$ K
$c = 13.9798$ (10) Å	Prism, colourless
$\beta = 107.135$ (5)°	$0.74 \times 0.55 \times 0.31$ mm
$V = 2310.6$ (3) Å^3	

Data collection

Stoe IPDS-2 diffractometer	17777 measured reflections
ω scans	2571 independent reflections
Absorption correction: integration	1917 reflections with $I > 2\sigma(I)$
(X-$RED32$; Stoe & Cie, 2002)	$R_{int} = 0.091$
$T_{min} = 0.945$, $T_{max} = 0.975$	$\theta_{max} = 27.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.12P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.052$	$+ 0.2796P]$
$wR(F^2) = 0.147$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
2571 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
168 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	Extinction correction: $SHELXL97$
	Extinction coefficient: 0.0019 (6)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2—H2$\cdots$O1^i	0.89 (3)	1.95 (3)	2.787 (2)	157 (3)
N1—H1$\cdots$O1	0.918 (10)	1.733 (17)	2.5651 (16)	149 (3)

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

The H atom on the imino N atom was located in a difference map and refined with an N—H distance restraint of 0.90 (1) Å. The hydroxyl H atom was also located in the difference map and refined freely. All other H atoms were placed in calculated positions and refined as riding, with C—H distances constrained to 0.93 (aromatic) or 0.96 Å (methyl) and with $U_{iso}(H) = 1.2U_{eq}$(aromatic C) and $1.5U_{eq}$(methyl C). The occupation factor of the water O atom, O3, was initially refined to 0.068 (3) and later fixed at 0.07. The H atoms attached to O3 were not located in the difference map.

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).
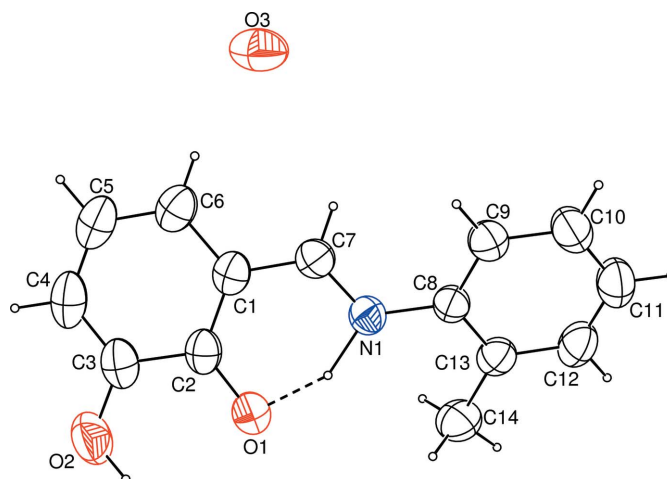
Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme and the hydrogen bond as a dashed line. Displacement ellipsoids are drawn at the 40% probability level.
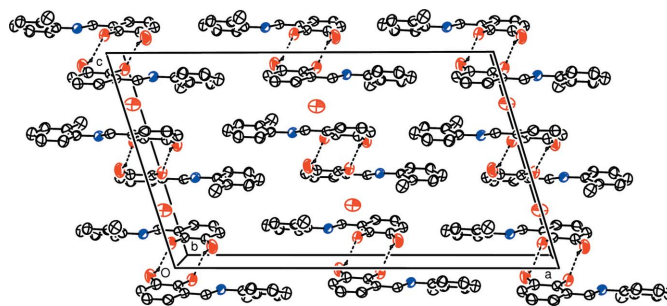

Figure 2
A packing diagram of (I), showing the hydrogen-bonded (dashed lines) dimers. H atoms not participating in hydrogen bonding have been omitted for clarity.

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