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Key indicators

Single-crystal X-ray study

T = 100 K

Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$

R factor = 0.047

wR factor = 0.127

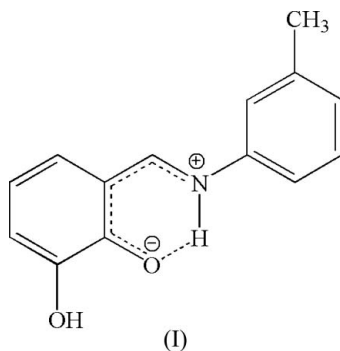
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2-Hydroxy-6-[(*m*-tolyliminio)methyl]phenolate

In the solid state, the title compound, $\text{C}_{14}\text{H}_{13}\text{NO}_2$, crystallizes as a zwitterion. Two molecules comprise the asymmetric unit. The molecules exhibit two types of hydrogen bonds: $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds involving hydroxy and imine groups generate an $S(6)$ ring motif, and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds linking two symmetry-related molecules form a centrosymmetric dimer.

Comment

Hydroxy Schiff bases have been extensively studied due to their biological, photochromic and thermochromic properties (Garnovskii *et al.*, 1993; Hadjoudis *et al.*, 2004). They can be used as potential materials for optical memory and switch devices (Zhao *et al.*, 2007). Proton transfer in these compounds forms the basis for an explanation of the mechanisms of various biological processes where proton transfer is the rate-determining step (Lussier *et al.*, 1987). The title Schiff base, (I), was obtained by the condensation of 2,3-dihydroxybenzaldehyde with 3-methylaniline.



The molecular structure of (I) is similar to that of the recently published structure, 2-[(4-carboxycyclohexyl)methylaminomethyl]-6-hydroxyphenolate (Shuja *et al.*, 2006), which also crystallizes as a zwitterion. The aromatic rings C1–C6 and C8–C13 form dihedral angles of 6.01 (9) and 12.92 (9)° in molecules (I) and (II), respectively. (In the Figures and tables, the first digit of the atom label gives the residue number, *i.e.* molecule 1 or molecule 2). The C8–N1–C7–C6 torsion angles are -177.42 (17) and -174.99 (16)°, respectively. The central C7=N1 bond lengths of 1.301 (2) and 1.305 (2) Å are smaller than the N1–C8 bond lengths of 1.421 (2) and 1.420 (2) Å. The C1–O1 and C6–C7 bond lengths indicate double-bond character.

Molecules 1 and 2 exhibit two types of hydrogen bonds, an intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond and two intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 3 and Table 1). In

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the crystal packing of (I), symmetry-related molecules are linked by O—H···O hydrogen bonds forming centrosymmetric dimers, which stack along the *b* axis direction.

Also observed are a weak intramolecular O—H···O hydrogen bond and a weak intermolecular C—H···O(*x* − 2, 1 + *y*, *z*) hydrogen bond between molecules 1 and 2 (Table 1).

Experimental

An ethanolic solution (20 ml) of 3-methylaniline (2.5 mmol, 0.27 g) was added dropwise with constant stirring to a hot ethanolic (20 ml) solution of 2,3-dihydroxybenzaldehyde (2.5 mmol, 0.34 g) in a round-bottomed flask equipped with a water condenser. The reaction mixture was kept under reflux for 3 h, cooled and kept at room temperature for 72 h. Red crystals of (I) were obtained on slow evaporation of the solvent.

Crystal data

$C_{14}H_{13}NO_2$	$\gamma = 74.2580 (15)^\circ$
$M_r = 227.25$	$V = 1109.52 (17) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 4$
$a = 7.7094 (7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.5939 (9) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 14.8307 (13) \text{ \AA}$	$T = 100 (1) \text{ K}$
$\alpha = 72.2740 (15)^\circ$	$0.39 \times 0.17 \times 0.12 \text{ mm}$
$\beta = 83.0670 (16)^\circ$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7014 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2006)	4253 independent reflections
$T_{\min} = 0.955$, $T_{\max} = 0.989$	2951 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.127$	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
$S = 0.99$	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
4253 reflections	
315 parameters	

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H11···O11	1.00 (2)	1.61 (2)	2.528 (2)	150.8 (18)
O12—H12···O11	0.91 (2)	2.29 (2)	2.719 (2)	108.7 (18)
O12—H12···O11 ⁱ	0.91 (2)	1.94 (2)	2.774 (2)	152 (2)
N2—H21···O21	0.87	1.82	2.550 (2)	140
O22—H22···O21	0.83	2.30	2.7501 (19)	114
O22—H22···O21 ⁱⁱ	0.83	1.97	2.6965 (19)	145
C13—H13···O22 ⁱⁱⁱ	0.95	2.57	3.507 (3)	171

Symmetry codes: (i) $-x - 1, -y + 1, -z + 1$; (ii) $-x + 2, -y, -z$; (iii) $x - 2, y + 1, z$.

N- and O-bound H atoms were located in a difference Fourier map and refined with isotropic displacement parameters. All other H atoms were generated by geometrical considerations and were included in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$, where $x = 1.5$ for methyl and $x = 1.2$ for the other H atoms. The methyl groups were refined as rigid groups, which were allowed to rotate freely. Assigned values of bond distances: methyl C—H = 0.98 \AA and aromatic C—H = 0.95 \AA . The N—H bonds are involved in

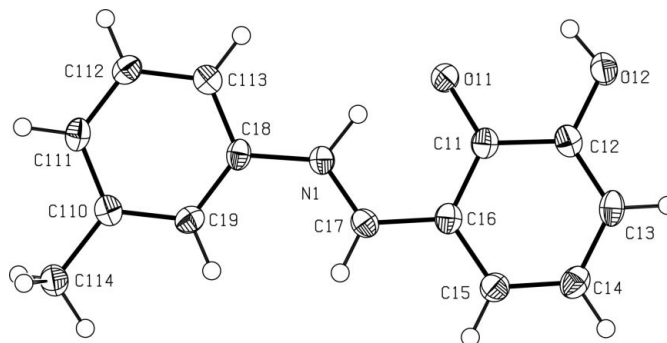


Figure 1

The structure of molecule 1 of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown with an arbitrary radius.

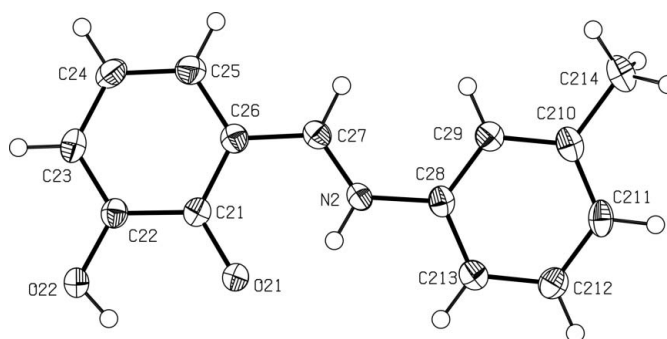


Figure 2

The structure of molecule 2 of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown with an arbitrary radius.

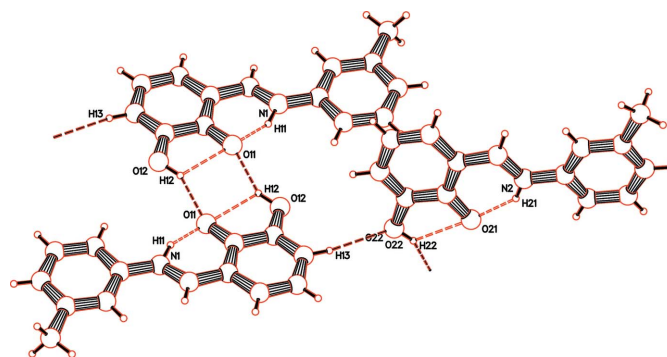


Figure 3

A perspective *PLUTO* (Meetsma, 2007) drawing, showing the dimers formed by O—H···O hydrogen bonds (symmetry code: $-x - 1, -y + 1, -z + 1$) and the aggregates formed by the weak C—H···O bonds (symmetry code: $x - 2, y + 1, z$). Hydrogen bonds are shown as dashed lines.

an intramolecular hydrogen bond; the observed N—H bond distances are elongated compared with commonly observed values of around 0.85–0.90 \AA .

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINTE-Plus* (Bruker, 2006); data reduction: *SAINTE-Plus*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

PLUTO (Meetsma, 2007) and *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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