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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.090  
Data-to-parameter ratio = 13.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(Z)-6-[(2-Methoxyphenylamino)methylene]-4-methylcyclohexa-2,4-dien-1(2H)-one monohydrate**

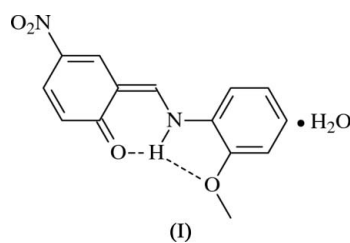
The title compound,  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_4 \cdot \text{H}_2\text{O}$ , is stabilized in the solid state as a keto–amine tautomer, with two strong intramolecular  $\text{N}-\text{H} \cdots \text{O}$ , two intermolecular  $\text{O}-\text{H} \cdots \text{O}$  and three intermolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds. The organic molecule is approximately planar, with a dihedral angle of  $1.90(8)^\circ$  between the two carbocyclic rings. The water molecules lie on a twofold symmetry axis.

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## Comment

Salicylaldehyde Schiff bases derived from the reaction of salicylaldehyde or salicylaldehyde derivatives with aniline derivatives have been examined extensively (Stewart & Lingafelter, 1959; Calligaris *et al.*, 1972; Maslen & Waters, 1975). Schiff base compounds display interesting photochromic and thermochromic features in the solid state and can be classified in terms of these properties (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). Photochromic compounds are of great interest for the control and measurement of radiation intensity, optical computers and display systems (Dürr & Bouas-Laurent, 2003).



There are two possible types of intramolecular hydrogen bonds in salicylaldehyde Schiff bases, as exhibited by the keto–amine ( $\text{N} \cdots \text{H}-\text{O}$ ) and enol–imine ( $\text{N}-\text{H} \cdots \text{O}$ ) tautomeric forms. Salicylaldehyde Schiff bases have been found in the keto form (Odabaşoğlu *et al.*, 2003; Ersanlı *et al.*, 2004; Koşar *et al.*, 2004), in the enol form (Leardini *et al.*, 1998; Karadayı *et al.*, 2003; Odabaşoğlu *et al.*, 2005) and as enol/keto mixtures (Nazır *et al.*, 2000). The present X-ray investigation shows that the title compound, (I), prefers the keto–amine tautomeric form.

The molecular structure of (I) is shown with the atom-numbering scheme in Fig. 1. Selected bond lengths and angles are listed in Table 1. The organic molecule is situated on a general position, while water molecules O5 and O6 lie on a twofold axis. The  $\text{C}8=\text{C}9$ ,  $\text{C}10=\text{O}1$  and  $\text{C}8-\text{N}1$  bond lengths verify the stabilization of the keto–amine tautomeric form.

These distances agree with the corresponding distances in our previous studies (Odabaşoğlu *et al.*, 2003; Ersanlı *et al.*, 2004; Koşar *et al.*, 2004), which also show the keto–amine tautomeric form. The same bond lengths can be compared with the corresponding distances in 2-[[tris(hydroxymethyl)methyl]aminomethylene]cyclohexa-3,5-dien-1(2*H*)-one [C=O = 1.3025 (16) Å and C–N = 1.2952 (18) Å; Odabaşoğlu *et al.*, 2003], which shows the keto–amine tautomeric form. The C13–N2 bond length in (I) is also in good agreement with the corresponding distances found in the literature, for instance, 1.4671 (18) (Zeller & Hunter, 2004) and 1.456 (4) Å (Glide-well *et al.*, 2004), for related compounds containing a nitro group.

Compound (I) displays a strong hydrogen bond (Table 2) involving atoms N1 and O1 (Filarowski *et al.*, 2003; Yıldız *et al.*, 1998), a common feature of *o*-hydroxysalicylidene systems. In (I), the organic molecule forms two N–H···O intramolecular hydrogen bonds and molecules are linked through two O–H···O and three C–H···O intermolecular hydrogen bonds (Fig. 2 and Table 2). Rings *A* (C1–C6), *B* (H1/N1/C8/C9/C10/O1), *C* (C9–C14) and *D* (H1/N1/C1/C2/O2) are almost planar; the dihedral angles between rings *A/B*, *A/C*, *A/D*, *B/C*, *B/D* and *C/D* are 0.27 (8), 1.90 (8), 1.57 (10), 2.16 (08), 1.70 (9) and 2.19 (9)°, respectively (Nardelli, 1995).

## Experimental

Compound (I) was prepared by refluxing a mixture of a solution containing 4-nitrosalicylaldehyde (3.5 mmol) in ethanol (95%, 10 ml) and a solution containing 2-methoxyaniline (3.5 mmol) in ethanol (10 ml). The reaction mixture was refluxed for 1 h and then left to cool. The powder product was recrystallized from ethanol. Single crystals were grown from methanol–water (9:1) (yield 84%; m.p. 465–466 K).

### Crystal data

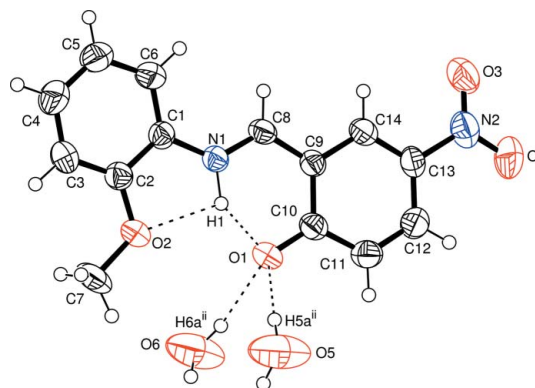
C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O	$D_x = 1.427 \text{ Mg m}^{-3}$
$M_r = 290.27$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4712 reflections
$a = 26.099 (3) \text{ \AA}$	$\theta = 1.4\text{--}26.9^\circ$
$b = 7.0229 (6) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 15.8664 (19) \text{ \AA}$	$T = 296 \text{ K}$
$\beta = 111.644 (9)^\circ$	Rod, brown
$V = 2703.1 (5) \text{ \AA}^3$	$0.41 \times 0.28 \times 0.14 \text{ mm}$
$Z = 8$	

### Data collection

Stoe IPDS-2 diffractometer	1116 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.077$
Absorption correction: integration ( <i>X-RED32</i> ; Stoe & Cie, 2002)	$\theta_{\text{max}} = 26.0^\circ$
$T_{\text{min}} = 0.965$ , $T_{\text{max}} = 0.987$	$h = -32 \rightarrow 32$
8400 measured reflections	$k = -7 \rightarrow 8$
2637 independent reflections	$l = -18 \rightarrow 19$

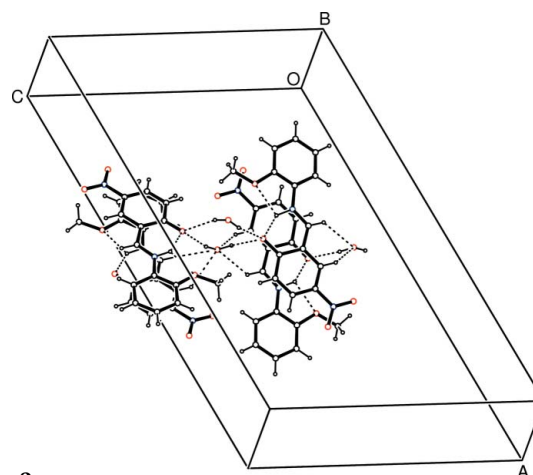
### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$
$wR(F^2) = 0.090$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.83$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2637 reflections	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
201 parameters	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$



**Figure 1**

A view of (I), with the atomic numbering scheme and the hydrogen bonds represented as dashed lines. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code for H atoms of the water molecules: (ii)  $-x, y, -z + \frac{1}{2}$ .]



**Figure 2**

A packing diagram of (I), showing the hydrogen-bonding scheme (dashed lines).

**Table 1**

Selected geometric parameters (Å, °).

C1–C6	1.384 (3)	C8–C9	1.412 (3)
C1–C2	1.391 (3)	C9–C10	1.438 (3)
C1–N1	1.412 (3)	C10–O1	1.279 (3)
C2–O2	1.365 (3)	C13–N2	1.448 (3)
C8–N1	1.297 (3)		
C2–C1–N1	115.6 (2)	C8–N1–C1	129.1 (2)
N1–C8–C9	121.0 (2)		
N1–C1–C2–C3	−178.4 (2)	N1–C8–C9–C10	−0.2 (4)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N1–H1···O1	1.02 (3)	1.67 (3)	2.553 (3)	143 (2)
N1–H1···O2	1.02 (3)	2.17 (2)	2.572 (3)	101.1 (16)
O5–H5A···O1 <sup>i</sup>	0.859 (10)	2.052 (12)	2.895 (3)	167 (3)
O6–H6A···O1 <sup>i</sup>	0.833 (10)	2.111 (13)	2.918 (3)	163 (3)
C3–H3···O4 <sup>ii</sup>	0.93	2.46	3.386 (3)	174
C8–H8···O5 <sup>iii</sup>	0.93	2.83	3.511 (3)	131
C14–H14···O5 <sup>iv</sup>	0.93	2.58	3.306 (3)	135

Symmetry codes: (i)  $-x + 1, y, -z + \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, y - \frac{1}{2}, z$ ; (iii)  $-x + 1, -y + 1, -z + 1$ ; (iv)  $x, -y + 1, z + \frac{1}{2}$ .

Atom H1, bonded to N1 and involved in hydrogen bonding, as well as H atoms bonded to water O atoms were found in a difference Fourier 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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C})$  and  $1.5U_{\text{eq}}(\text{methyl C})$ .

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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