2-(3-Methoxysalicylideneamino)-1*H*-benzimidazole monohydrate

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The molecule of the title compound, $C_{15}H_{13}O_2N_3 \cdot H_2O$, is nearly planar, with an intramolecular N···O hydrogen bond of 2.616 (2) Å. It exists in the phenol–imine form and the dihedral angle between the two aromatic ring systems is 1.04 (5)°. An unsolvated form, crystallized from the same medium, has also been reported [Odabaşoglu, Albayrak & Büyükgüngör (2005). *Acta Cryst.* E**61**, o425–o426].
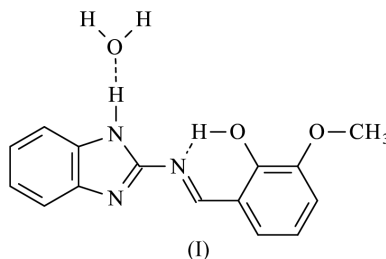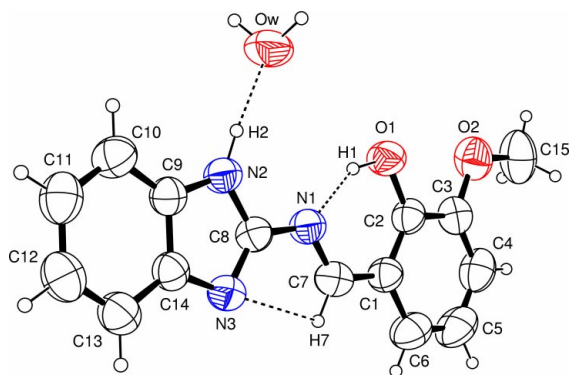
Comment

Schiff bases derived from 2-aminobenzimidazole generally exhibit antiproliferative activity (Nawrocka *et al.*, 2004). Salicylidene-2-aminobenzimidazole Schiff bases have been used as ligands in the field of coordination chemistry (Mohamed & Abd El-Wahab, 2003). Schiff bases show photochromism and thermochromism in the solid state (Hadjoudis *et al.*, 1987). Photochromic compounds are of great interest for the control and measurement of radiation intensity, optical computers and display systems (Dürr & Bouas-Laurent, 2003).

(I)

2-Hydroxy Schiff bases exist in two forms, *viz.* keto–amine (Özek *et al.*, 2004; Ersanlı *et al.*, 2003) and phenol–imine (Ersanlı *et al.*, 2004; Yüce *et al.*, 2004). In the course of our ongoing work on the synthesis and structural characterization studies of Schiff bases, (I) was synthesized and we report here its crystal structure.

The molecular structure with the atom-labelling scheme is shown in Fig. 1, and selected bond lengths and angles are listed in Table 1.

In (I), the dihedral angle between the salicylidene and benzimidazole ring systems is 1.04 (5)° and, excluding the methyl H atoms, the molecule is planar. In (I), the phenol–imine tautomer is favoured over the keto–amine form in the solid state. This is evident from the observed O1—C2 bond distance of 1.357 (2) Å, which is consistent with an O—C single bond; in addition, the C7—N1 distance of 1.287 (2) Å is consistent with a C=N double bond, as in *N*-(2-fluoro-3-methoxy)salicylaldimine [O—C = 1.347 (3) Å and C=N = 1.280 (3) Å; Ünver *et al.*, 2002].

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

There is a strong intramolecular O—H···N hydrogen bond and a weak C—H···N interaction, together with strong N—H···O and O—H···N intermolecular hydrogen bonds (Table 2).

In addition to this monohydrate, the structure of the solvent-free compound has also been determined (Odabaşoğlu et al., 2005).

Experimental

The title compound was prepared by refluxing a mixture of a solution containing o-vanillin (0.5 g, 3.2 mmol) in ethanol (20 ml) and a solution containing 2-aminobenzimidazole (0.43 g, 3.2 mmol) in ethanol (20 ml). The reaction mixture was stirred for 1 h under reflux. The resulting orange precipitate was filtered off and recrystallized from ethanol by slow evaporation. Crystals of (I) suitable for X-ray analysis were obtained from the solution. (Yield 95%, m.p. 487–490 K.)

Crystal data

$C_{15}H_{13}N_3O_2 \cdot H_2O$
$M_r = 285.30$
Monoclinic, $C2/c$
$a = 11.2152 (14)$ Å
$b = 8.7122 (10)$ Å
$c = 29.091 (3)$ Å
$\beta = 95.719 (9)°$
$V = 2828.3 (6)$ Å^3
$Z = 8$

$D_x = 1.340$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9918 reflections
$\theta = 1.4–24.0°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Block, orange
$0.36 \times 0.26 \times 0.11$ mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (X-RED; Stoe & Cie, 2002)
$T_{min} = 0.967$, $T_{max} = 0.990$
9918 measured reflections
2193 independent reflections

1167 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 24.0°$
$h = -12 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -31 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.062$
$S = 0.83$
2193 reflections
207 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: 0.0050 (2)

Table 1
Selected geometric parameters (Å, °).

C2—O1	1.357 (2)	C8—N1	1.393 (2)
C3—O2	1.363 (2)	C9—N2	1.373 (2)
C7—N1	1.287 (2)	C14—N3	1.389 (2)
C8—N3	1.314 (2)	C15—O2	1.437 (2)
C8—N2	1.351 (2)		
N1—C7—C1	122.69 (18)	C7—N1—C8	118.88 (16)
N3—C8—N2	113.90 (16)	C8—N2—C9	106.56 (16)
N3—C8—N1	128.24 (17)	C8—N3—C14	103.86 (15)
N2—C8—N1	117.86 (17)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	1.01 (2)	1.69 (2)	2.616 (2)	150.6 (19)
N2—H2···Ow	0.94 (2)	1.78 (2)	2.717 (2)	175.6 (19)
Ow—H1w···N3^i	0.93 (4)	1.91 (4)	2.813 (2)	162 (3)
Ow—H2w···O1^{ii}	1.04 (4)	2.07 (4)	3.009 (2)	148 (3)
Ow—H2w···O2^{ii}	1.04 (4)	2.51 (4)	3.270 (2)	129 (3)
C7—H7···N3	0.93	2.49	2.829 (2)	102

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

H atoms bonded to N and O were located in a difference map and refined isotropically. Other H atoms were placed in calculated positions (C—H = 0.93–0.96 Å), with U_{iso}(H) values constrained to be $1.5U_{eq}$ of the carrier atom for the methyl-group H atoms and $1.2U_{eq}$ for the remaining H atoms.

Data collection: X-AREA (Stoe & Cie, 2002); cell refinement: X-AREA; data reduction: X-RED (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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