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1-[(3-Hydroxypyridin-2-ylamino)methylene]-naphthalen-2(1H)-one

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The molecule of the title compound, $C_{16}H_{12}N_2O_2$, is nearly planar, and adopts the keto–amine tautomeric form with an intramolecular N—H···O hydrogen bond. The molecules are linked by O—H···O hydrogen bonds into a three-dimensional network.
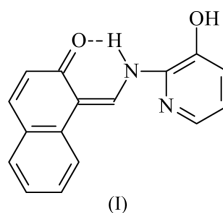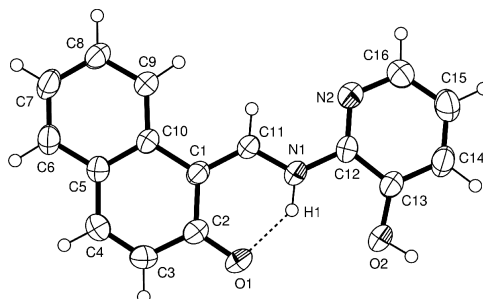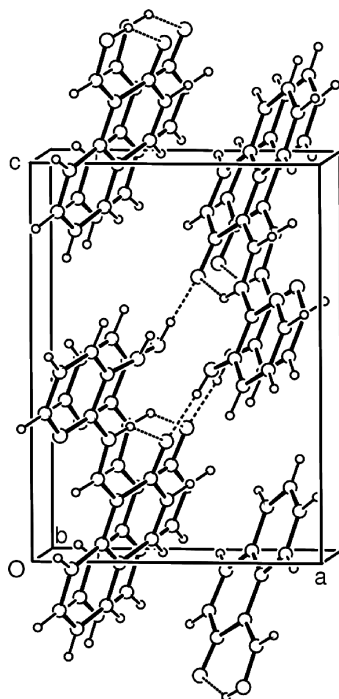
Comment

Most Schiff bases have antibacterial, anticancer, anti-inflammatory and antitoxic properties (Williams, 1972). In addition, Schiff bases have been used widely as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). There are two characteristic properties of Schiff bases, *viz.* photochromism and thermochromism (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1978). These properties result from proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). Schiff bases display two possible tautomeric forms, namely the phenol–imine and keto–amine forms. In the solid state, the keto–amine tautomer has been found in naphthaldimine (Hökelek *et al.*, 2000; Ünver *et al.*, 2001; Odabaşoğlu *et al.*, 2003). However, in the solid state, it has been established that there is keto–amine tautomerism in naphthaldimine, while the phenol–imine form exists in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998).

(I)

In the title compound, (I), the keto–amine tautomer is favoured over the phenol–imine form (Fig. 1 and Table 1), and there is an intramolecular N1—H1···O1 hydrogen bond (Table 2). The rather short C2—O1 and C1—C11 bonds can

Figure 1
An *ORTEP*-3 (Farrugia, 1997) view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids.

hydroxy-1-naphthol as starting materials. Crystals of (I) were obtained from a tetrahydrofuran solution by slow evaporation (yield 85%, m.p. 528–529 K).

Crystal data

$C_{16}H_{12}N_2O_2$	$D_x = 1.381$ Mg m^{-3}
$M_r = 264.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 14275
$a = 8.8268$ (14) Å	reflections
$b = 5.9191$ (6) Å	$\theta = 1.7$–29.3°
$c = 12.1670$ (19) Å	$\mu = 0.09$ mm^{-1}
$\beta = 90.277$ (13)°	$T = 293$ (2) K
$V = 635.68$ (16) Å^3	Plate, orange
$Z = 2$	$0.56 \times 0.25 \times 0.11$ mm

Data collection

Stoe IPDS-2 diffractometer	1876 independent reflections
ω scans	1363 reflections with $I > 2\sigma(I)$
Absorption correction: by	$R_{int} = 0.058$
integration (*X-RED*32;	$\theta_{max} = 29.3°$
Stoe & Cie, 2002)	$h = -12 \rightarrow 12$
$T_{min} = 0.964$, $T_{max} = 0.991$	$k = -7 \rightarrow 8$
12064 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2]$
$wR(F^2) = 0.071$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
1876 reflections	$\Delta\rho_{max} = 0.09$ e Å^{-3}
229 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C11	1.394 (2)	C3—C4	1.343 (3)
C1—C2	1.439 (2)	C4—C5	1.432 (3)
C1—C10	1.462 (2)	C5—C10	1.409 (2)
C2—O1	1.276 (2)	C11—N1	1.3237 (19)
C2—C3	1.433 (3)	C12—N1	1.398 (2)
C11—C1—C2	119.67 (14)	N1—C11—C1	123.50 (16)
C11—C1—C10	120.33 (15)	N2—C12—N1	118.69 (14)
O1—C2—C3	120.34 (16)	N1—C12—C13	116.70 (16)
O1—C2—C1	121.47 (17)	C11—N1—C12	125.96 (16)
C11—C1—C2—O1	4.9 (3)	C1—C11—N1—C12	179.67 (17)
C2—C1—C11—N1	0.9 (3)	N2—C12—N1—C11	0.9 (3)
C10—C1—C11—N1	−178.28 (17)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1	0.91 (2)	1.80 (2)	2.560 (2)	139 (2)
O2—H2$\cdots$O1^i	0.88 (3)	1.74 (3)	2.621 (2)	176 (3)
C15—H15$\cdots$Cg1^{ii}	0.97 (3)	3.09 (3)	3.719 (2)	124 (2)
C4—H4$\cdots$Cg2^{iii}	0.95 (2)	2.68 (2)	3.456 (2)	140 (2)
C3—H3$\cdots$Cg3^{iv}	0.97 (2)	3.05 (2)	3.625 (2)	119 (1)
C9—H9$\cdots$Cg3^{iv}	0.96 (2)	2.91 (2)	3.633 (2)	133 (1)

Symmetry codes: (i) $1-x, y-\frac{1}{2}, 1-z$; (ii) $-x, y-\frac{1}{2}, 1-z$; (iii) $1-x, \frac{1}{2}+y, -z$; (iv) $-x, y-\frac{1}{2}, -z$. Cg1, Cg2 and Cg3 are the centroids of rings A, B and C (atoms C5–C10), respectively.

All H atoms were found in difference density maps and refined freely. The C—H bond lengths are in the range 0.92 (2)–0.99 (2) Å. Friedel-pair reflections were merged before the final refinement, because of the meaningless value of the absolute structure parameter.

Figure 2
An *ORTEP*-3 (Farrugia, 1997) packing diagram of (I), viewed along the *b* axis.

be considered as predominantly C=O and C=C double bonds, respectively. This fact, together with the very short C3—C4 bond, suggests the presence of a significant quinoidal effect. A similar quinoidal effect was observed for 1-[*N*-(*p*-hydroxyphenyl)aminomethylidene]naphthalen-2(1*H*)-one propan-1-ol hemisolvate [C=O = 1.292 (2) and 1.295 (2) Å; Odabaşoğlu *et al.*, 2004] and *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine [C=O = 1.277 (2) Å; Kaitner & Pavlovic, 1996]. The keto–amine form is also dominant in *N*-(α-naphthyl)-2-oxo-1-naphthaldimine [C=O = 1.287 (5) Å; Gavranic *et al.*, 1996].

The study of Schiff bases has led to the proposal that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar. This planarity of the molecule allows the proton to be transferred through the hydrogen bond in the ground state with a small energy requirement (Odabaşoğlu *et al.*, 2004; Hadjoudis *et al.*, 1987). The molecule of (I) is almost planar, with a dihedral angle of 2.24 (8)° between ring *A* (atoms C12–C16/N2) and ring *B* (atoms C1–C5/C10). The N—H$\cdots$O hydrogen-bonded ring is almost planar. The C11—N1 bond length and C11—N1—C12 bond angle are 1.3237 (19) Å and 125.96 (16)°, respectively, compared with values of 1.317 (4)/1.330(4) Å and 124.2 (3)/123.2(3)° in *N*-(2-pyridyl)-2-oxo-1-naphthylidenemethylamine (Nazır *et al.*, 2000). The molecules are linked by intermolecular O—H$\cdots$O hydrogen bonds and C—H$\cdots\pi$ interactions (Table 2), forming a three-dimensional network.

Experimental

The title compound, (I), was prepared as described in the literature (Odabaşoğlu *et al.*, 2003) using 2-amino-3-hydroxypyridine and 2-

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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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