

2-Hydroxy-6-[(1-naphthylamino)methylene]-
cyclohexa-2,4-dien-1-oneArzu Özek,^a Süheyla Yüce,^a
Çiğdem Albayrak,^b
Mustafa Odabaşoğlu^b and
Orhan Büyükgüngör^{a*}^aDepartment of Physics, Ondokuz Mayıs
University, TR-55139 Samsun, Turkey, and^bDepartment of Chemistry, Ondokuz Mayıs
University, TR-55139 Samsun, Turkey

Correspondence e-mail: arzuozek@omu.edu.tr

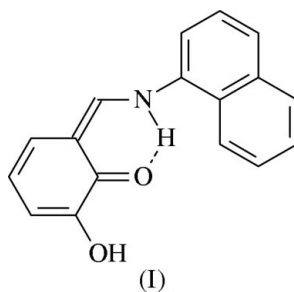
Key indicators

Single-crystal X-ray study
 $T = 100\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.046
 wR factor = 0.111
Data-to-parameter ratio = 10.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The molecule of the title compound, $\text{C}_{17}\text{H}_{13}\text{NO}_2$, is nearly planar and exists in the keto–amine ($\text{N}-\text{H}\cdots\text{O}$) tautomeric form, with a strong intramolecular hydrogen bond of $2.576(2)\text{ \AA}$ between the O and N atoms. The molecules are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds to form dimers, and are further linked by $\text{C}-\text{H}\cdots\pi$ interactions, forming a three-dimensional network.

Comment

Schiff bases are reported to show a variety of biological activities, such as antibacterial (Pandeya *et al.*, 1999; El-masry *et al.*, 2000; Kabeer *et al.*, 2001), anticancer (Phatak *et al.*, 2000; Desai *et al.*, 2001), antifungal (Singh & Dash, 1988; More *et al.*, 2001) and herbicidal properties (Samadhiya & Halve, 2001). Schiff base compounds show photochromism and thermochromism in the solid state by proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987). Schiff bases display two possible tautomeric forms, namely phenol–imine ($\text{O}-\text{H}\cdots\text{N}$) and keto–amine ($\text{N}-\text{H}\cdots\text{O}$) forms. *o*-Hydroxy Schiff bases have previously been observed in the keto form (Ünver, Kabak *et al.*, 2002; Odabaşoğlu, Albayrak, Büyükgüngör & Goesmann, 2003) and in the enol form (Ünver, Yıldız *et al.*, 2002; Karadayı *et al.*, 2003).



In the title compound, (I), the keto–amine tautomer is favoured over the phenol–imine form (Fig. 1). The $\text{C}3-\text{O}1$ and $\text{C}1-\text{N}1$ bond lengths verify the keto–amine form of (I). These distances agree with the corresponding distances in 3-[(2-oxo-1-naphthylidene)methylamino]benzoic acid [$1.290(2)$ and $1.319(3)\text{ \AA}$; Pavlović & Sosa, 2000] and 2-[[tris(hydroxymethyl)methyl]aminomethylene]cyclohexa-3,5-dien-1(2*H*)-one [$1.3025(16)$ and $1.2952(18)\text{ \AA}$; Odabaşoğlu, Albayrak, Büyükgüngör & Lönneche, 2003], which also show the keto–amine tautomeric form. In the crystal structure of *N*-(2-pyridyl)-2-oxo-1-naphthylidenemethylamine, there are two independent molecules which constitute a tautomeric pair, with $\text{C}-\text{O}$ bond distances of $1.263(4)$ and $1.279(4)\text{ \AA}$ in the keto–amine and enol–imine forms, respectively (Nazır *et al.*, 2000).

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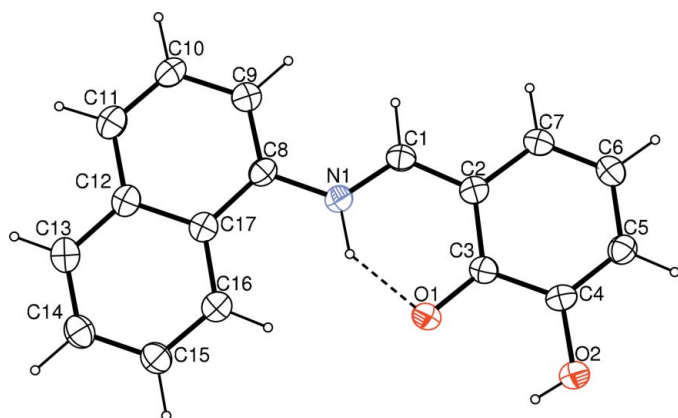


Figure 1

A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964). On the basis of some thermochromic and photochromic Schiff base compounds, it was proposed that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar (Moustakali-Mavridis *et al.*, 1978); the planarity of the molecule makes it possible for the proton to transfer through the hydrogen bond in the ground state with a low energy barrier (Bregman, Leiserowitz & Schmidt, 1964; Bregman, Leiserowitz & Osaki, 1964). The molecule of (I) is almost planar: the angle between the rings of atoms C2–C7 and C8–C12/C17 is 5.87 (8)°.

The intra- and intermolecular hydrogen bonding in (I) is shown in Fig. 2 and geometric details of the hydrogen bonds are given in Table 2. Atom H3 bonded to N1 forms a strong intramolecular hydrogen bond with atom O1, as observed in similar compounds (Odabaşoğlu, Albayrak, Büyükgüngör & Goemann, 2003; Albayrak *et al.*, 2004). The molecules are linked by O–H···O hydrogen bonds to form dimers, and further linked by C–H··· π interactions (Table 2), forming a three-dimensional network.

Experimental

Compound (I) was prepared as described in the literature (Odabaşoğlu, Albayrak, Büyükgüngör & Lönneche, 2003), using 1-aminonaphthalene and 2,3-dihydroxybenzaldehyde as starting materials. Crystals of (I) were obtained from a tetrahydrofuran solution by slow evaporation (yield 88%, m.p. 508–510 K).

Crystal data

$C_{17}H_{13}NO_2$	$D_x = 1.409 \text{ Mg m}^{-3}$
$M_r = 263.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 11212 reflections
$a = 7.3546$ (5) Å	$\theta = 1.7\text{--}26.1^\circ$
$b = 23.7901$ (17) Å	$\mu = 0.09 \text{ mm}^{-1}$
$c = 7.4919$ (5) Å	$T = 100 \text{ K}$
$\beta = 108.738$ (6)°	Plate, red
$V = 1241.35$ (15) Å ³	$0.19 \times 0.13 \times 0.05 \text{ mm}$
$Z = 4$	

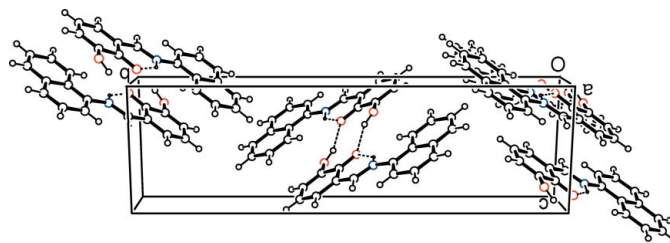


Figure 2

A packing diagram for (I). Dashed lines indicate hydrogen bonds.

Data collection

Stoe IPDS-2 diffractometer	1668 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.063$
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	$\theta_{\text{max}} = 26.1^\circ$
$T_{\text{min}} = 0.987$, $T_{\text{max}} = 0.996$	$h = -8 \rightarrow 9$
11951 measured reflections	$k = -29 \rightarrow 29$
2435 independent reflections	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2]$
$wR(F^2) = 0.111$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2435 reflections	$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
232 parameters	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C1–N1	1.320 (2)	C4–C5	1.367 (3)
C1–C2	1.404 (3)	C4–O2	1.370 (2)
C2–C7	1.427 (3)	C5–C6	1.411 (3)
C2–C3	1.429 (3)	C6–C7	1.357 (3)
C3–O1	1.291 (2)	C8–N1	1.415 (2)
C3–C4	1.429 (3)		
N1–C1–C2	121.77 (18)	O1–C3–C2	122.70 (17)
C1–C2–C7	119.15 (18)	O1–C3–C4	120.45 (17)
C1–C2–C3	120.57 (17)	C1–N1–C8	126.91 (17)
N1–C1–C2–C7	−177.77 (17)	C2–C1–N1–C8	175.65 (16)
N1–C1–C2–C3	0.2 (3)	C9–C8–N1–C1	2.2 (3)
C1–C2–C3–O1	3.1 (3)	C17–C8–N1–C1	−177.96 (17)
N1–C8–C17–C16	−1.0 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

$Cg1$ and $Cg2$ are the centroids of the C8–C17 and C12–C17 rings, respectively.

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N1–H3···O1	1.00 (3)	1.73 (3)	2.576 (2)	140 (2)
O2–H2···O1 ⁱ	0.88 (2)	1.89 (2)	2.670 (2)	148 (2)
C13–H13··· $Cg1$ ⁱⁱ	0.95 (2)	3.12 (2)	4.008 (2)	155 (2)
C13–H13··· $Cg2$ ⁱⁱ	0.95 (2)	3.26 (2)	3.705 (2)	111 (2)
C14–H14··· $Cg2$ ⁱⁱ	1.01 (3)	3.03 (3)	3.604 (2)	117 (2)

Symmetry codes: (i) $-x + 2, -y + 1, -z + 1$; (ii) $x, -y - \frac{1}{2}, z - \frac{3}{2}$.

All H atoms were located in difference Fourier maps and refined isotropically, except for atom H2 bonded to atom O2, which was refined with the O–H bond distance restrained to 0.82 (2) Å, and

with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{iso}}(\text{O})$. The C–H distances are in the range 0.95 (2)–1.02 (3) Å.

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: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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