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1-[(2-Hydroxy-5-methylphenylamino)methylene]naphthalen-2(1*H*)-one

Arzu Özek,[a]* Süheyla Yüce,[a] Çiğdem Albayrak,[b] Mustafa Odabaşoğlu[b] and Orhan Büyükgüngör[a]

[a]Department of Physics, Ondokuz Mayıs University, TR-55139 Samsun, Turkey, and [b]Department of Chemistry, Ondokuz Mayıs University, TR-55139 Samsun, Turkey

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

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Key indicators

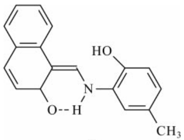
Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.121
Data-to-parameter ratio = 16.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_{18}H_{15}NO_2$, is not completely planar. It adopts a keto–amine tautomeric form with an intramolecular N—H···O and an intermolecular O—H···O hydrogen bond. The molecules are linked by O—H···O hydrogen bonds into a three-dimensional network.

Comment

Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activities (Lozier *et al.*, 1975; Garnovskii *et al.*, 1993). Schiff base compounds show two possible tautomeric forms, namely phenol–imine and keto–amine. In the solid state, the keto–amine tautomer has been found in naphthaldimine (Özek *et al.*, 2004; Odabaşoğlu *et al.*, 2004; Hökelek *et al.*, 2000; Ünver *et al.*, 2002), while the phenol–imine tautomer has been found in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998; Elmalı *et al.*, 1998, 1999; Elmalı & Elerman, 1998; Dey *et al.*, 2001; Yang & Vittal, 2003; Karadayı *et al.*, 2003; Ersanlı, Odabaşoğlu *et al.*, 2004; Ersanlı, Albayrak *et al.*, 2004).



(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 be considered as 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-[(3-hydroxypyridin-2-ylamino)methylene]naphthalen-2(1*H*)-one [C═O =

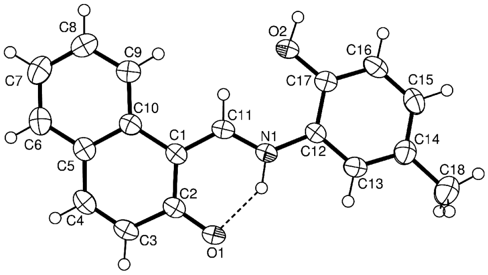


Figure 1
A view of the molecule of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

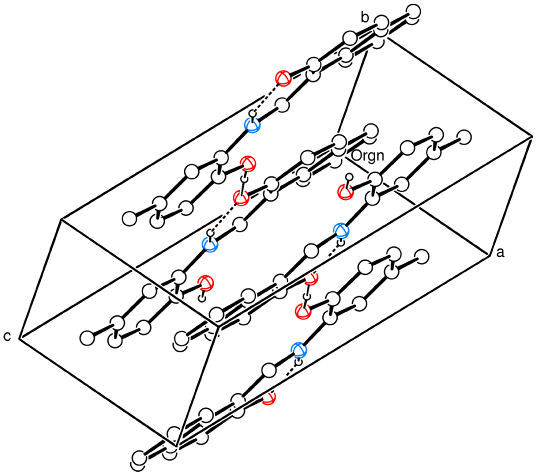


Figure 2
A view of the packing in (I). The dashed lines indicate hydrogen bonds.

1.276 (2) Å; Özek *et al.*, 2004], 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 (Hadjoudis *et al.*, 1987). The title molecule is not exactly planar, with a dihedral angle of 12.37 (9)° between rings *A* (atoms C12–C17) and *B* (atoms C1–C5/C10). The N—H···O hydrogen-bonded ring is almost planar and coupled with the naphthaldimine ring. The C11—N1 bond length and C11—N1—C12 bond angle are 1.306 (2) Å and 129.33 (15)°, respectively, compared with 1.3237 (19) Å and 125.96 (16)° in 1-[(3-hydroxypyridin-2-ylamino)methylene]naphthalen-2(1*H*)-one (Özek *et al.*, 2004). The molecules are linked by intermolecular O—H···O hydrogen bonds (Table 2).

Experimental

The title compound, (I), was prepared as described in the literature (Odabaşoğlu *et al.*, 2003) using 2-amino-4-methylphenol and 2-hydroxy-1-naphthol as starting materials. Crystals of (I) were obtained from an acetone solution by slow evaporation (yield 83%, m.p. 518–520 K).

Crystal data

$C_{18}H_{15}NO_2$
$M_r = 277.31$
Triclinic, $P\bar{1}$
$a = 7.126$ (1) Å
$b = 7.898$ (1) Å
$c = 13.684$ (2) Å
$\alpha = 77.698$ (9)°
$\beta = 85.43$ (1)°
$\gamma = 65.210$ (9)°
$V = 683.1$ (2) Å^3

$Z = 2$
$D_x = 1.348$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4617 reflections
$\theta = 2.9$–27.8°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Plate, orange
0.31 × 0.21 × 0.08 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{min} = 0.978$, $T_{max} = 0.994$
11817 measured reflections

3240 independent reflections
1689 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 27.8°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 9$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.121$
$S = 0.88$
3240 reflections
199 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.008 (2)

Table 1
Selected geometric parameters (Å, °).

C1—C11	1.404 (2)	C3—C4	1.340 (3)
C1—C2	1.429 (2)	C4—C5	1.428 (3)
C1—C10	1.450 (2)	C5—C10	1.414 (2)
C2—O1	1.281 (2)	C11—N1	1.306 (2)
C2—C3	1.438 (2)	C12—N1	1.414 (2)
C11—C1—C2	120.0 (2)	N1—C11—C1	123.8 (2)
C11—C1—C10	119.7 (2)	C13—C12—N1	116.7 (2)
O1—C2—C1	121.7 (2)	C11—N1—C12	129.3 (2)
O1—C2—C3	120.7 (2)		
C11—C1—C2—O1	8.6 (3)	C10—C1—C11—N1	−178.0 (2)
C2—C1—C11—N1	−1.6 (3)	C1—C11—N1—C12	176.4 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.94 (2)	1.78 (2)	2.588 (2)	142 (2)
O2—H2···O1^{i}	0.92 (3)	1.67 (3)	2.581 (2)	170 (3)

Symmetry code: (i) $x, 1 + y, z$.

H atoms attached to C atoms were refined using a riding model, with C—H distances of 0.93 Å for aromatic H atoms and 0.96 Å for methyl H atoms. The U_{iso}(H) values were set at $1.5U_{eq}$ of the carrier atom for the methyl H atom and $1.2U_{eq}$ for the remaining H atoms. H atoms attached to the N and O atoms were located in a difference map and refined freely [N—H = 0.94 (2) Å and O—H = 0.92 (3) Å].

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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