Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-[(4-Nitrophenylamino)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

Received 5 April 2004
Accepted 14 April 2004
Online 24 April 2004

Key indicators

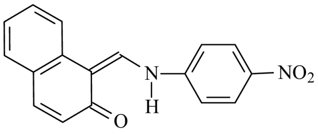
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.145
Data-to-parameter ratio = 14.7

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, $C_{17}H_{12}N_2O_3$, is nearly planar and adopts a keto–amine tautomeric form, with an intramolecular N—H···O hydrogen bond.

Comment

Schiff bases have been used widely as ligands in the field of coordination chemistry (Calligaris *et al.*, 1972). Schiff base compounds show 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 (Özek *et al.*, 2004; Odabaşoğlu *et al.*, 2004; Hökelek *et al.*, 2000; Ünver *et al.*, 2002), while the phenol–imine tautomer is found in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998; Elmalı & Elerman, 1998; Elmalı *et al.*, 1998, 1999; 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 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]-1*H*-naphthalen-2-one [C=O = 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 molecule of (I) is almost planar, with a dihedral angle of 4.63 (1)° between ring *A* (atoms C12–C17) and ring *B* (atoms C1–C5/C10). The N—

DOI: 10.1107/S1600536804008864

H···O hydrogen-bonded ring is almost planar and is coupled with the naphthaldimine ring. The C11—N1 bond length and C11—N1—C12 bond angle are 1.306 (3) Å and 126.35 (19)°, respectively, compared with 1.3237 (19) Å and 125.96 (16)° in 1-[(3-hydroxypyridin-2-ylamino)methylene]-1*H*-naphthalen-2-one (Özek *et al.*, 2004).

Experimental

Compound (I) was prepared as described by Odabaşoğlu *et al.* (2003), using 4-nitroaniline and 2-hydroxy-1-naphthol as starting materials. Crystals of (I) were obtained from an acetone solution by slow evaporation (yield 82%, m.p. 492–494 K).

Crystal data

$C_{17}H_{12}N_2O_3$
$M_r = 292.29$
Monoclinic, $P2_1/c$
$a = 8.0124$ (13) Å
$b = 7.3743$ (8) Å
$c = 22.690$ (4) Å
$\beta = 93.043$ (13)°
$V = 1338.8$ (4) Å^3
$Z = 4$

$D_x = 1.450$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5610 reflections
$\theta = 1.8$–26.9°
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Plate, red
0.60 × 0.30 × 0.06 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
$T_{\min} = 0.954$, $T_{\max} = 0.993$
10 123 measured reflections

2923 independent reflections
1355 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.124$
$\theta_{\max} = 27.1°$
$h = -10 \rightarrow 10$
$k = -8 \rightarrow 9$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.145$
$S = 0.82$
2923 reflections
199 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0772P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C11	1.396 (3)	C4—C5	1.419 (3)
C1—C2	1.430 (3)	C5—C10	1.411 (3)
C1—C10	1.458 (3)	C11—N1	1.306 (3)
C2—O1	1.289 (3)	C12—N1	1.398 (3)
C2—C3	1.431 (3)	C15—N2	1.455 (3)
C3—C4	1.335 (3)		
C11—C1—C2	118.7 (2)	N1—C11—C1	123.8 (2)
C11—C1—C10	121.68 (19)	C13—C12—N1	123.4 (2)
O1—C2—C1	122.4 (2)	C17—C12—N1	117.28 (19)
O1—C2—C3	119.3 (2)	C11—N1—C12	126.35 (19)
C11—C1—C2—O1	2.2 (3)	C10—C1—C11—N1	178.5 (2)
C2—C1—C11—N1	−2.1 (3)	C1—C11—N1—C12	−178.4 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.86	1.85	2.543 (2)	137

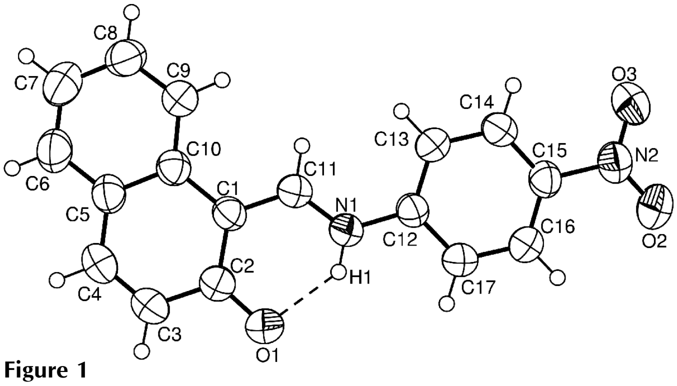


Figure 1
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

All H atoms were refined using a riding model (C—H = 0.93 Å and N—H = 0.86 Å) with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$ (parent atom).

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, 1998).

References

Calligaris, M., Nardin, G. M. J. & Randaccio, C. (1972). *Coord. Chem.* **7**, 385–389.
Dey, D. K., Dey, S. P., Elmalı, A. & Elerman, Y. (2001). *J. Mol. Struct.* **562**, 177–184.
Elmalı, A. & Elerman, Y. (1998). *J. Mol. Struct.* **442**, 31–37.
Elmalı, A., Elerman, Y. & Zeyrek, C. T. (1998). *J. Mol. Struct.* **443**, 123–130.
Elmalı, A., Kabak, M. & Elerman, Y. (1999). *J. Mol. Struct.* **484**, 229–234.
Ersanlı, C. C., Albayrak, Ç., Odabaşoğlu, M. & Erdönmez, A. (2004). *Acta Cryst.* E**60**, o389–o391.
Ersanlı, C. C., Odabaşoğlu, M., Albayrak, Ç. & Erdönmez, A. (2004). *Acta Cryst.* E**60**, o264–o266.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1998). *WinGX*. University of Glasgow, Scotland.
Gavranic, M., Kaitner, B. & Mestrovic, E. (1996). *J. Chem. Crystallogr.* **26**, 23–28.
Hadjoudis, E., Vitterakis, M. & Maviridis, I. M. (1987). *Tetrahedron*, **43**, 1345–1360.
Hökelek, T., Kılıç. Z., Işıklan, M. & Toy, M. (2000). *J. Mol. Struct.* **523**, 61–69.
Kaitner, B. & Pavlovic, G. (1996). *Acta Cryst.* C**52**, 2573–2575.
Karadayı, N., Gözüyeşil, S., Güzel, B. & Büyükgüngör, O. (2003). *Acta Cryst.* E**59**, o161–o163.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2004). *Acta Cryst.* E**60**, o142–o144.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. & Lönneche, P. (2003). *Acta Cryst.* C**59**, o616–o619.
Özek, A., Yüce, S., Albayrak, Ç., Odabaşoğlu, M. & Büyükgüngör, O. (2004). *Acta Cryst.* E**60**, o356–o358.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED*32 (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Ünver, H., Kabak, M., Zengin, D. M. & Durlu, T. N. (2002). *J. Chem. Crystallogr.* **31**, 203–209.
Yang, C.-T. & Vittal, J. (2003). *Inorg. Chim. Acta*, **344**, 65–76.
Yıldız, M., Kılıç. Z. & Hökelek, T. (1998). *J. Mol. Struct.* **441**, 1–10.