Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.133$
$S = 0.986$
1711 reflections
119 parameters
H atoms fixed
$w = 1/[\sigma^2(F_o^2) + (0.0811P)^2 + 4.2404P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.809$ e Å^{-3}
$\Delta\rho_{min} = -0.622$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.0065 (11)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Se1—C9	1.794 (9)	C1—C7	1.498 (8)
Se1—C8	1.978 (7)	C6—C8	1.501 (8)
Se2—C10	1.775 (9)	C9—N1	1.168 (14)
Se2—C7	1.987 (6)	C10—N2	1.172 (12)
C9—Se1—C8	95.9 (3)	C1—C6—C8	124.4 (4)
C10—Se2—C7	98.7 (3)	C1—C7—Se2	114.6 (5)
C2—C1—C7	116.7 (4)	C6—C8—Se1	115.3 (4)
C6—C1—C7	123.3 (4)	N1—C9—Se1	178.4 (7)
C5—C6—C8	115.6 (4)	N2—C10—Se2	176.5 (8)

The relatively high R_{int} value suggests that the ψ-scan absorption correction used in this study may not be an entirely adequate description of the absorption in this system.

Data collection: *CAD*-4-*PC* (Enraf–Nonius, 1993). Cell refinement: *CAD*-4-*PC*. Data reduction: *CAD*-4 *Software* (Enraf–Nonius, 1989). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SNOOPI* (Davies, 1983). Software used to prepare material for publication: *SHELXL*93.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1107). Services for accessing these data are described at the back of the journal.

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1-[*N*-(4-Methyl-2-pyridyl)aminomethylidene]-2(1*H*)-naphthalenone

Yalçin Elerman,[a] Mehmet Kabak,[a] Ayhan Elmali[a] and Ingrid Svoboda[b]

[a]*Department of Physics Engineering, Faculty of Sciences, University of Ankara, 06100 Besevler, Ankara, Turkey, and* [b]*Strukturforschung, FB Materialwissenschaft, Technische Hochschule Darmstadt, Petersenstrasse 20, 64287 Darmstadt, Germany. E-mail: elerman@science.ankara.edu.tr*

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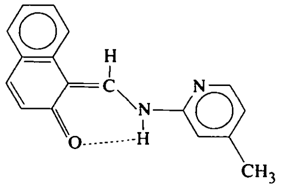
Abstract

The crystal structure of the title compound, $C_{17}H_{14}N_2O$, has been determined and reveals an almost planar structure. Each molecule contains a strong intramolecular $O\cdots N$ hydrogen bond [2.532 (3) Å].

Comment

Schiff bases have been extensively used as ligands in the field of coordination chemistry (Calligaris, Nardin & Randaccio, 1972; Garnovski, Nivorozhkin & Minkin, 1993; Maggio, Pizzino & Romano, 1974; Morassi, Bertini & Sacconi, 1973). The Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen, Schmidt & Flavian, 1964; Moustakali, Mavridis & Hadjoudis, 1978; Hadjoudis *et al.*, 1987). Photochromism is produced by intramolecular proton transfer associated with a change in the π-electron configuration (Barbara, Rentzepis & Brus, 1980; Hadjoudis, 1981; Higelin & Sixl, 1983). Thermochromism is also due to a change in the π-electron configuration induced by a proton transfer and the proton transfer can occur in the ground state (Cohen *et al.*, 1964). Interest in studies on photochromic compounds has been increasing ever since the potential applications of photochromic materials were realised in various areas such as the control and measurement of radiation intensity, optical computers and display systems (Dürr, 1989; Dürr & Bouas-Laurent, 1990).

Our structural investigations of Schiff bases (Elerman, Svoboda & Fuess, 1991; Elerman *et al.*, 1992, 1994, 1995, 1997; Elmali *et al.*, 1995; Kevran, Elmali & Elerman, 1996; Elmali & Elerman, 1997) have led us to examine the title compound, (I).



(I)

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 *et al.*, 1978), and planarity of the molecule makes it possible for the proton to transfer through the hydrogen bond in the ground state with a small energy requirement (Bregman, Leiserowitz & Schmidt, 1964; Bregman, Leiserowitz & Osaki, 1964). The title molecule (Fig. 1) is almost planar; the angle between moieties *A* (O1, C1–C11) and *B* (N1, N2, C12–C17) [both planar with a maximum deviation of −0.063 (2) Å] is 5.08 (9)°. The torsion angles C10—C11—N1—C12 [178.9 (3)°], N2—C12—N1—C11 [−4.4 (4)°], C16—C12—N1—C11 [177.1 (3)°], C9—C10—C11—N1 [−177.7 (3)°] and C1—C10—C11—N1 [−0.1 (4)°] also indicate that the molecule is almost planar.

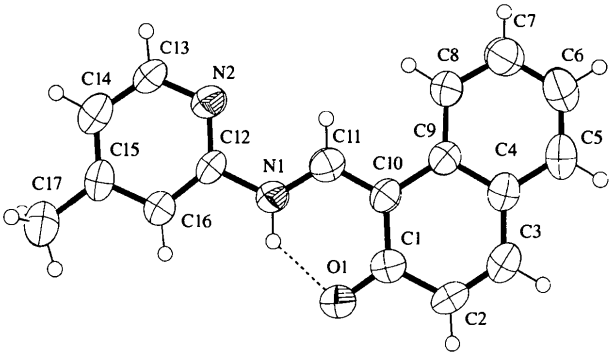


Fig. 1. The molecular structure of the title compound (*PLATON*; Spek, 1996). Displacement ellipsoids are plotted at the 50% probability level.

In (I), a strong intramolecular hydrogen bond occurs between the O1 and N1 atoms [2.532 (3) Å]. The sum of the van der Waals radii of O and N (3.07 Å) is significantly greater than the intramolecular O···N hydrogen-bond length (Bondi, 1964). In the present study, the intramolecular O1···N1 hydrogen-bond length is comparable with that observed for 2-(β-hydroxy-α-naphthylmethylidene)amino-4-ethyl-5-methyl-3-cyanothiophene [2.575 (3) Å; Elerman *et al.*, 1997] and for *N*-(5-bromosalicylidene)-2-aminopyridine [2.581 (6) Å; Moustakali *et al.*, 1978]. The H1N atom was located from a difference Fourier map at the end of the refinement process as a small positive electron density. The N1—H1N and H1N···O1 distances are 0.91 (3) and 1.83 (3) Å, respectively, and the N1—H1N···O angle is 133 (3)°. The C1=O1 bond [1.281 (4) Å] is consistent with C=O double bonding. This, along with the very short C2=C3 bond [1.336 (4) Å], suggests the presence of a significant quinoidal effect. A similar quinoidal effect was observed for *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine (Kaitner & Pavlović, 1996). From the X-ray diffraction experiment, we were only able to detect the existence of the keto tautomer.

Experimental

The title compound was obtained from the reaction of 2-hydroxynaphthalene-1-carbaldehyde (0.01 mol, 1.722 g) with a solution of 2-amino-4-methylpyridine (0.01 mol, 1.081 g) in 50 ml of ethanol. The precipitate which separated from the solution was recrystallized for 5–6 d from 2 g of Schiff base in 25 ml of dioxane solution.

Crystal data

$C_{17}H_{14}N_2O$
$M_r = 262.33$
Orthorhombic
$P2_12_12_1$
$a = 6.574\,(2)$ Å
$b = 13.798\,(2)$ Å
$c = 14.838\,(3)$ Å
$V = 1346.0\,(5)$ Å^3
$Z = 4$
$D_x = 1.295$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71093$ Å
Cell parameters from 25 reflections
$\theta = 2.75$–$11.39°$
$\mu = 0.082$ mm^{-1}
$T = 299\,(2)$ K
Needle
0.45 × 0.14 × 0.04 mm
Yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1884 measured reflections
1764 independent reflections
954 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.020$
$\theta_{\rm max} = 29.66°$
$h = -9 \rightarrow 1$
$k = -1 \rightarrow 16$
$l = -16 \rightarrow 1$
3 standard reflections
frequency: 120 min
intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.180$
$S = 1.101$
1764 reflections
185 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.7121P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = 0.065$
$\Delta\rho_{\rm max} = 0.228$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.257$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.0109 (14)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

C1—O1	1.281 (4)	C9—C10	1.455 (4)
C1—C10	1.422 (4)	C10—C11	1.375 (4)
C1—C2	1.440 (4)	C11—N1	1.322 (4)
C2—C3	1.336 (4)	C12—N2	1.312 (3)
C3—C4	1.425 (4)	C12—C16	1.371 (4)
C4—C5	1.400 (4)	C12—N1	1.415 (3)
C4—C9	1.404 (4)	N2—C13	1.329 (4)
C5—C6	1.359 (5)	C13—C14	1.388 (5)
C6—C7	1.365 (5)	C14—C15	1.354 (4)
C7—C8	1.380 (4)	C15—C16	1.385 (4)
C8—C9	1.408 (4)	C15—C17	1.507 (4)
O1—C1—C10	122.2 (3)	C16—C12—N1	117.2 (2)
O1—C1—C2	118.8 (3)	C12—N2—C13	115.0 (3)
N1—C11—C10	123.4 (3)	N2—C13—C14	123.9 (3)
N2—C12—C16	125.8 (3)	C11—N1—C12	125.3 (2)
N2—C12—N1	117.0 (2)		

The structure was solved by direct phase determination. The parameters of the complete structure could be refined by full-matrix anisotropic least squares. All phenyl rings were refined without any constraints. Values of distances and angles in the rings show no significant differences from those of an ideal benzene ring. All H-atom positions were calculated using a riding model, except for that involved in the molecular N—H···O hydrogen bond, which was found from the difference Fourier maps calculated at the end of the refinement process as a small positive electron density.

Data collection: *SDP* (Frenz, 1985). Cell refinement: *SDP*. Data reduction: *REDU4* (Stoe & Cie, 1988). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLATON96* (Spek, 1996). Software used to prepare material for publication: *SHELXL93*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: KA1241). Services for accessing these data are described at the back of the journal.

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N—H···π(pyrrole) Intermolecular Interactions in 1,4-Bis(di-2-pyrrolylmethyl)benzene

Vanessa Bennis and John F. Gallagher

School of Chemical Sciences, Dublin City University,
Dublin 9, Ireland. E-mail: gallagherjfg@dcu.ie

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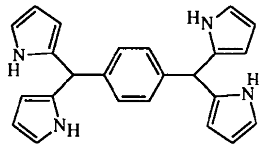
Abstract

The title compound, $C_{24}H_{22}N_4$, lies about an inversion centre which is at the centre of the 1,4-disubstituted benzene ring. Intermolecular N—H···π(pyrrole) interactions form a two-dimensional hydrogen-bonded network with shortest N···(pyrrole centroid) distances of 3.219 (3) and 3.324 (3) Å.

Comment

Dipyrromethane derivatives are useful building blocks in the synthesis of porphyrin model systems with direct approaches to *trans*-substituted porphyrins available by condensation of dipyrromethanes with aldehydes (Lee & Lindsey, 1994). The structural chemistry of these precursors has been underdeveloped, especially in relation to hydrogen-bonding studies. Interactions involving an aromatic π system as a donor or acceptor are well established (Hanton, Hunter & Purvis, 1992). We report herein the structure of 1,4-bis(di-2-pyrrolylmethyl)benzene, (I), where intermolecular N—H···π(pyrrole) interactions arise in a system with pyrrole N—H donors and only heteroaromatic pyrrole systems as acceptors.



(I)

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