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1-(4-((E)-(4-Diethylamino-2-hydroxyphenyl)-methylene]amino}phenyl) ethanone

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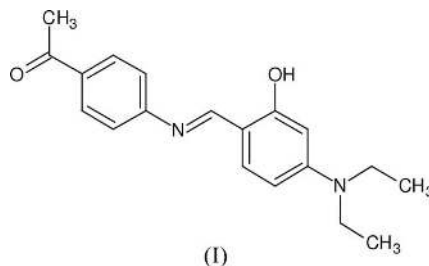
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Michael Bolte^{d*}^aDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^bDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, GermanyCorrespondence e-mail:
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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.040
 wR factor = 0.109
Data-to-parameter ratio = 14.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.1-(4-[[*(E)*-(4-Diethylamino-2-hydroxyphenyl)-methylene]amino]phenyl)ethanoneThe title compound, $\text{C}_{19}\text{H}_{22}\text{N}_2\text{O}_2$, is a Schiff base. Its molecular conformation is stabilized by an $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond. The crystal packing is characterized by $\text{C}-\text{H}\cdots\pi$ and $\pi-\pi$ interactions.Received 19 January 2007
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Comment

Schiff bases are used as substrates in the preparation of a number of industrial and biologically active compounds *via* ring closure, cycloaddition and replacement reactions. Moreover, Schiff bases are also known to have biological activities, such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh & Dash, 1988), antitumour (Hodnett & Dunn, 1970; Desai *et al.*, 2001) and herbicidal (Samadhiya & Halve, 2001) properties. Schiff bases have also been employed as ligands for the complexation of metal ions (Aydogan *et al.*, 2001). On the industrial scale, they have a wide range of applications, *e.g.* as dyes and pigments (Taggi *et al.*, 2002). We present here the crystal structure of the title Schiff base, (I)The molecular structure of compound (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; Allen, 2002; *Mogul* Version 1.1; Bruno *et al.*, 2004). The $\text{C}=\text{N}$ double bond is *trans* configured. The two aromatic rings are almost coplanar: the dihedral angle between them is $9.63(7)^\circ$. The amino N atom shows a trigonal-planar geometry. The sum of the bond angles at N is 359.6° . Thus, the two methylene C atoms are located in the plane of the adjacent benzene ring (Table 1). Methyl atom C18 and carbonyl atom O17 are also in the plane of the adjacent benzene ring (Table 1).The conformation of the molecule is stabilized by an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond (Table 2). The crystal packing shows a $\pi-\pi$ stacking interaction between two centrosymmetrically related molecules [symmetry operator $(1-x, 1-y, 1-z)$], with the centre of the $\text{C}=\text{N}$ double bond located 3.477 Å above the centroid of the C11–C16 benzene ring. Furthermore, two $\text{C}-\text{H}\cdots\pi$ hydrogen bonds can be observed (Fig. 2, Table 2).

Experimental

4-Aminoacetophenone (1.35 g, 0.01 mol) in methanol (25 ml) was mixed with 4-(diethylamino)-2-hydroxybenzaldehyde (1.93 g, 0.01 mol) and the mixture was treated with a 30% aqueous potassium hydroxide solution (4 ml) at 278 K. The reaction mixture was then warmed to room temperature and stirred for 5 h. The solid which precipitated was filtered off and washed with water, dried, and recrystallized from an acetone–toluene (1:1 v/v) mixture (m.p. 395–397 K). Analysis for $C_{19}H_{22}N_2O_2$ (%): found (calculated): C 73.38 (73.52), H 7.05 (7.14), N 8.96 (9.03).

Crystal data

| | |
|---------------------------------|---|
| $C_{19}H_{22}N_2O_2$ | $Z = 4$ |
| $M_r = 310.39$ | $D_x = 1.245 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 16.0234$ (16) Å | $\mu = 0.08 \text{ mm}^{-1}$ |
| $b = 7.6225$ (5) Å | $T = 173$ (2) K |
| $c = 15.0652$ (16) Å | Block, orang–brown |
| $\beta = 115.828$ (7)° | $0.42 \times 0.28 \times 0.19 \text{ mm}$ |
| $V = 1656.2$ (3) Å ³ | |

Data collection

| | |
|--|--|
| Stoe IPDS II two-circle diffractometer | 3092 independent reflections |
| ω scans | 2654 reflections with $I > 2\sigma(I)$ |
| Absorption correction: none | $R_{\text{int}} = 0.049$ |
| 13407 measured reflections | $\theta_{\text{max}} = 25.6^\circ$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.3519P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.109$ | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| $S = 1.03$ | $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$ |
| 3092 reflections | $\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$ |
| 214 parameters | Extinction correction: <i>SHELXL</i> |
| H atoms treated by a mixture of independent and constrained refinement | (Sheldrick, 1997) |
| | Extinction coefficient: 0.021 (2) |

Table 1

Selected torsion angles (°).

| | | | |
|-----------------|------------|-----------------|-----------|
| C15–C14–C17–O17 | −3.32 (18) | C23–C24–N24–C27 | 7.78 (17) |
| C13–C14–C17–C18 | −2.68 (18) | C25–C24–N24–C29 | 0.07 (18) |

Table 2

Geometry of hydrogen bonds and C–H... π contacts (Å, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------|----------|-------------|-------------|---------------|
| O22–H22...N1 | 0.96 (2) | 1.72 (2) | 2.6042 (13) | 151.8 (18) |
| C16–H16...Cg1 ¹ | 0.95 | 2.81 | 3.65 | 148 |
| C25–H25...Cg2 ² | 0.95 | 3.17 | 3.89 | 135 |

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$. Cg1 is the centroid of ring C21–C26 and Cg2 is the centroid of ring C11–C16.

H atoms were found in a difference map, but those bonded to C atoms were refined using a riding model, with C–H distances in the range 0.95–0.99 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The hydroxyl H atom was refined freely.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

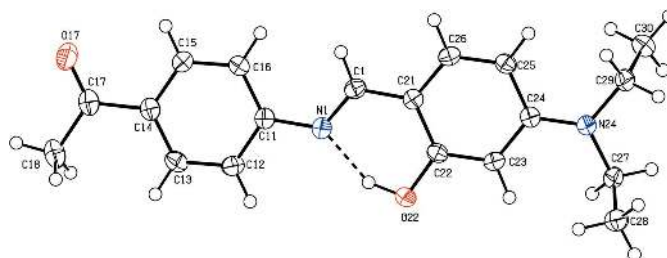


Figure 1

The molecular structure of compound (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

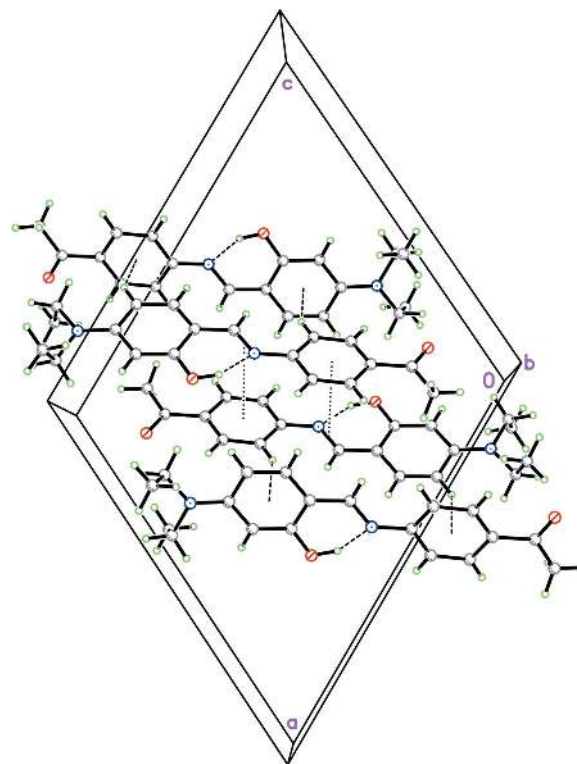


Figure 2

A packing diagram for (I), projected on to the *ac* plane. Hydrogen bonds are shown as dashed lines and π – π interactions as dotted lines.

PLATON (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *PLATON* and *SHELXL97*.

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