Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methoxy-4-(phenyliminomethyl)phenol

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.036
wR factor = 0.093
Data-to-parameter ratio = 7.6

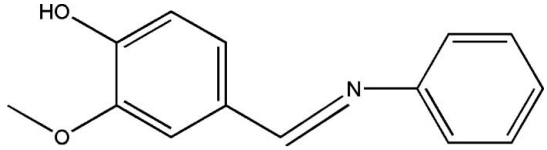
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 July 2005
Accepted 16 August 2005
Online 27 August 2005

The title compound, $C_{14}H_{13}NO_2$, contains two aromatic rings, which are bridged by a C═N unit. The 4-hydroxy-3-methoxyphenyl and phenyl groups are *trans* to each other. The molecular structure is stabilized by an intramolecular O—H···O hydrogen bond. In addition, there is an intermolecular O—H···N hydrogen bond and intermolecular C—H···O close contacts. There are two molecules in the asymmetric unit.

Comment

Much work has been devoted to the physicochemical characterization of substituted aromatic Schiff bases, because these compounds show remarkable photochromic properties. Photochromism arises from intramolecular H-atom transfer, together with a change in the π-electron system. The effect of intermolecular interactions, such as π–π charge transfer or hydrogen bonding, on H-atom transfer processes has been investigated in the solid state (Hadjoudis *et al.*, 1987; Puranik *et al.*, 1992). There are only a few reported crystal structures of Schiff bases derived from vanillin (4-hydroxy-3-methoxybenzaldehyde) (Kaitner & Pavlovic, 1995). We report here the structure of the Schiff base vanillaldimine, (I).



(I)

The crystal structure of (I) (Fig. 1) has two molecules in the asymmetric unit. The molecules contain two aromatic rings, which are bridged by a C═N unit. The 4-hydroxy-3-methoxyphenyl and phenyl moieties are *trans* to each other. The benzene rings are slightly twisted out of the plane of the C═N double bond (Table 1). The bond lengths and angles are within the expected ranges (Allen *et al.*, 1987). The molecular conformation is stabilized by an O—H···O hydrogen bond. The crystal structure is stabilized by an intermolecular O—H···N hydrogen bond and C—H···O close contacts (Table 1).

Experimental

The title compound was prepared by the condensation reaction of vanillin (1.52 g) in 2-propanol (20 ml) and aniline (0.93 g) in 2-propanol (20 ml). The reaction mixture was refluxed and stirred for 2 h. The resulting clear solution was kept in air and after slow evaporation of the solvent over a period of a week, yellow crystals were formed at the bottom of the vessel. The crystals were isolated and washed three times with ethanol and dried in a vacuum desic-

cator using anhydrous $CaCl_2$ (yield 68%). Analysis calculated for $C_{14}H_{13}NO_2$: C 73.99, H 5.77, N 6.16%; found: C 73.66, H 5.88, N 6.31%.

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Orthorhombic, $C222_1$
a = 17.2192 (13) Å
b = 18.0407 (14) Å
c = 15.4424 (12) Å
V = 4797.1 (6) Å^3
Z = 16
D_x = 1.259 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2200 reflections
θ = 2.1–28.6°
μ = 0.09 mm^{-1}
T = 295 (2) K
Block, yellow
0.20 × 0.16 × 0.14 mm

Data collection

Brruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.983, T_{max} = 0.988
13784 measured reflections
2350 independent reflections
2087 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°
$h = -20 \rightarrow 15$
$k = -20 \rightarrow 21$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.093
S = 1.15
2350 reflections
311 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.8026P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C6—N1	1.420 (3)	C20—N2	1.417 (3)
C7—N1	1.272 (3)	C21—N2	1.270 (3)
C7—C8	1.453 (3)	C21—C22	1.455 (4)
C11—O1	1.358 (3)	C25—O3	1.353 (3)
C12—O2	1.359 (3)	C26—O4	1.360 (3)
C14—O2	1.421 (3)	C28—O4	1.419 (3)
N1—C7—C8	124.8 (2)	C7—N1—C6	118.33 (18)
N2—C21—C22	124.44 (19)	C21—N2—C20	119.59 (17)
N1—C7—C8—C13	7.1 (3)	C5—C6—N1—C7	−43.9 (3)
N2—C21—C22—C27	9.5 (3)	C19—C20—N2—C21	−28.0 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O4	0.82	2.23	2.672 (2)	114
O3—H3A···N1^{i}	0.82	2.15	2.886 (2)	150
O1—H1A···O2	0.82	2.22	2.664 (2)	115
O1—H1A···N2^{ii}	0.82	2.14	2.880 (2)	151
C13—H13···O3^{iii}	0.93	2.41	3.301 (3)	159
C27—H27···O1^{iv}	0.93	2.37	3.266 (3)	163

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

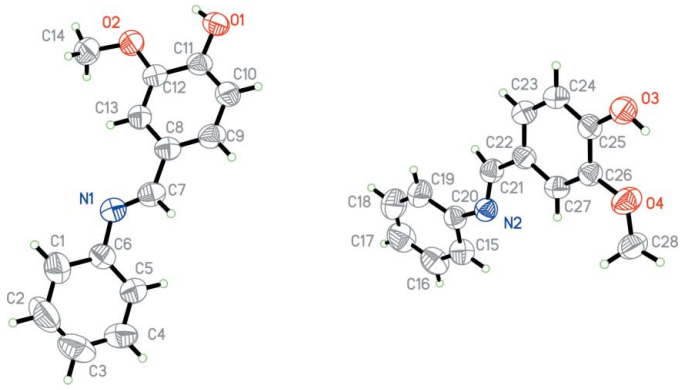


Figure 1
View of the asymmetric unit of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

H atoms were located in a difference map and refined using a riding model, with O—H = 0.82 Å and C—H = 0.93–0.96 Å, with U_{iso}(H) equal to 1.5U_{eq} of the parent atom for the hydroxyl and methyl H atoms and 1.2U_{eq}(C) for the remaining H atoms. The hydroxyl and methyl groups were allowed to rotate but not to tip. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial support from the Bureau of Science & Technology of Wuhan City, Hubei Province, People's Republic of China, through research grant No. 20055003059–28 is gratefully acknowledged.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L. & Orpen, A. G. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Hadjoudis, E., Vittorakis, M. & Mavridis, I. M. (1987). *Tetrahedron*, **43**, 1345–1360.
Kaitner, B. & Pavlovic, G. (1995). *Acta Cryst.* C**51**, 1875–1878.
Puranik, V. G., Tavale, S. S., Kumbhar, A. S., Yerande, R. G., Padhye, S. B. & Butcher, R. J. (1992). *J. Crystallogr. Spectrosc. Res.* **22**, 725–731.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-Ray Instruments Inc., Madison, Wisconsin, USA.