Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-2-Hydroxy-5-methyl-3-[(4-methyl-2-pyridyl)iminomethyl]benzaldehyde

Orhan Büyükgüngör,[a] Mustafa Odabaşoğlu,[b]* B. Narayana,[c] A. M. Vijesh[c] and H. S. Yathirajan[d]

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India

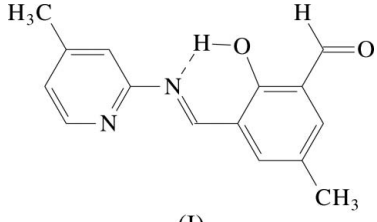
Correspondence e-mail: muodabas@omu.edu.tr

Received 16 March 2007
Accepted 19 March 2007

The title compound, $C_{15}H_{14}N_2O_2$, is stabilized in the solid state as an enol–imine tautomer, with one strong intramolecular O—H···N hydrogen bond and four C—H···O and one C—H···N intermolecular interaction that generate edge-fused $[S(6)R_2^2(8)R_2^2(8)R_5^4(32)]$ motifs. The molecule is approximately planar, with a dihedral angle of 1.72 (3)° between the two aromatic rings.

Comment

The present work is part of a structural study of Schiff bases (Yathirajan *et al.*, 2007; Odabaşoğlu *et al.*, 1999, 2004, 2005*a*,*b*, 2006; Odabaşoğlu, Albayrak, Büyükgüngör & Goesmann, 2003; Odabaşoğlu, Albayrak, Büyükgüngör & Lönnecke, 2003; Odabaşoğlu, Arslan *et al.*, 2007; Odabaşoğlu, Büyükgüngör *et al.* 2007*a*,*b*) and we report here the structure of the title compound, (I) (Fig. 1, Table 1).



(I)

Compound (I) prefers the enol–imine tautomeric form. It displays a strong intramolecular hydrogen bond (Table 2) involving atoms O1 and N1, a common feature of salicylidene systems. In addition, molecules are linked through four C—

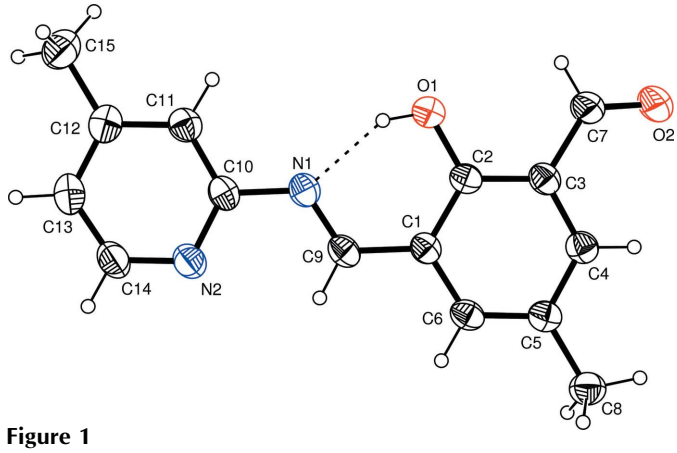


Figure 1
The molecular structure of (I) showing the atomic numbering scheme and with displacement ellipsoids drawn at the 30% probability level. The hydrogen bond is drawn as a dashed line.

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.080
Data-to-parameter ratio = 7.5

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

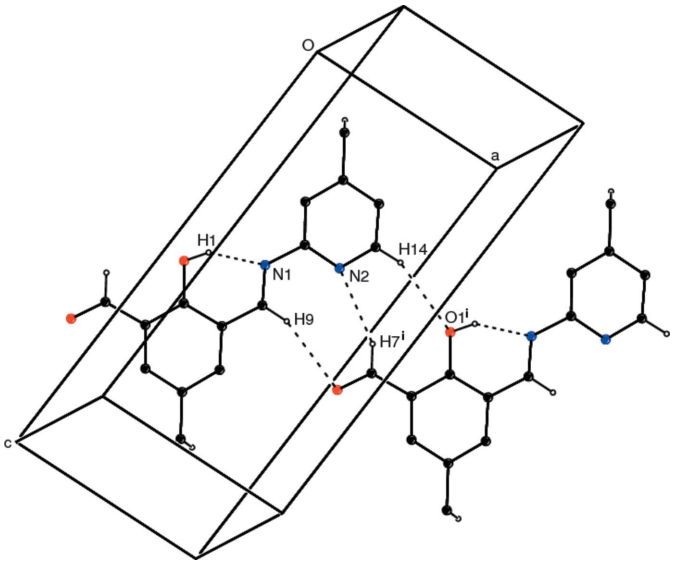


Figure 2
Part of the crystal structure of (I). For the sake of clarity, H atoms not involved in the hydrogen bonding motifs have been omitted; hydrogen bonds are drawn as dashed lines. [Symmetry code: (i) $x+1, y+1, z$.]

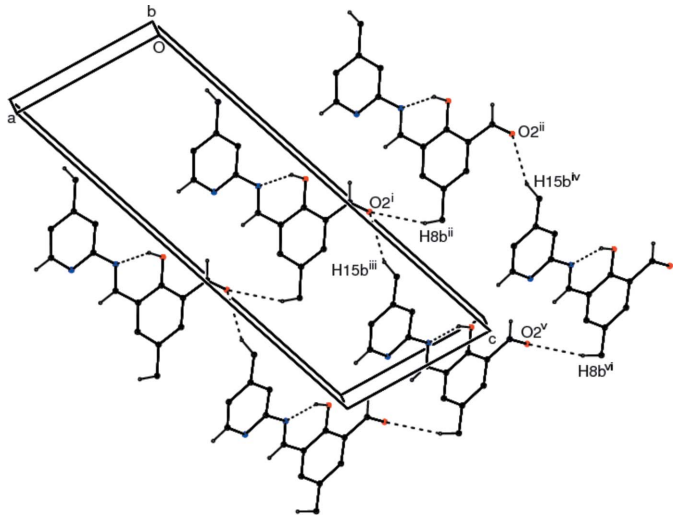


Figure 3
Part of the crystal structure of (I). For the sake of clarity, H atoms not involved in the hydrogen bonding motifs have been omitted; hydrogen bonds are drawn as dashed lines. [Symmetry codes: (i) $x, y+1, z$; (ii) $x-1, y+1, z$; (iii) $x, 1-y, 1-z$; (iv) $x-1, 1-y, 1-z$; (v) $x, 1-y, z+\frac{1}{2}$; (vi) $x-1, 1-y, z+\frac{1}{2}$.]

H···O and one C—H···N weak intermolecular interactions that generate edge-fused $S(6)$ $R_2^2(8)$ $R_2^2(8)$ ring motifs (Fig.2). These motifs are further linked to the $R_5^4(32)$ motifs (Fig. 3) (Etter, 1990) by C8—H8*B*···O2^{i} and C15—H15*B*···O2^{iii} hydrogen bonds (Table 2). The aromatic rings are essentially coplanar with a dihedral angle of 1.72 (3)° between them.

Experimental

A mixture of 5-hydroxy-2-methylisophthalaldehyde (2.58 g, 0.01 mol) and 4-methylpyridin-2-amine (1.1 g, 0.01 mol) in 30 ml of absolute ethanol containing two drops of 4 *M* sulfuric acid was refluxed for about 4 h. On cooling, the solid that separated was filtered off and recrystallized from ethyl alcohol (m.p. 381–385 K). Analysis for $C_{15}H_{14}N_2O_2$ found (calculated): C 70.74 (70.85), H 5.48 (5.55), N 10.93 (11.02)%.

Crystal data

$C_{15}H_{14}N_2O_2$
$M_r = 254.28$
Monoclinic, *Pc*
$a = 7.4936$ (7) Å
$b = 4.5019$ (3) Å
$c = 20.677$ (2) Å
$\beta = 109.273$ (7)°
$V = 658.46$ (10) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 296$ K
0.67 × 0.42 × 0.21 mm

Data collection

Stoe IPDS-II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.954$, $T_{max} = 0.984$
10340 measured reflections
1303 independent reflections
1021 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.081$
$S = 0.95$
1303 reflections
174 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.09$ e Å^{-3}
$\Delta\rho_{min} = -0.09$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.84	2.576 (3)	148
C8—H8*B*···O2^{i}	0.96	2.63	3.474 (4)	147
C9—H9···O2^{ii}	0.93	2.76	3.618 (3)	153
C14—H14···O1^{ii}	0.93	2.77	3.626 (3)	153
C15—H15*B*···O2^{iii}	0.96	2.61	3.516 (4)	158
C7—H7···N2^{iv}	0.93	2.67	3.521 (4)	152

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

In the absence of significant anomalous scattering effects, 1298 Friedel pairs were merged. All carbon-bound H atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic, aldehydic and imino H [U_{iso}(H) = 1.2U_{eq}(C)] and C—H = 0.96 Å for methyl H [U_{iso}(H) = 1.5U_{eq}(C)]. The H atom of the hydroxyl group was refined as riding, with an O—H distance of 0.82 Å and with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS-II diffractometer (purchased under grant F.279 of the University Research Fund).

References

Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2004). *Acta Cryst.* E**60**, o142–o144.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2005*a*). *Acta Cryst.* C**61**, o240–o242.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2005*b*). *Acta Cryst.* E**61**, o425–o426.
Odabaşoğlu, M., Albayrak, Ç. & Büyükgüngör, O. (2006). *Acta Cryst.* E**62**, o1094–o1096.
Odabaşoğlu, M., Albayrak, Ç., Büyükgüngör, O. & Goesmann, H. (2003). *Acta Cryst.* C**59**, o234–o236.
Odabaşoğlu, M., Albayrak, Ç., Büyükgüngör, O. & Lönnecke, P. (2003). *Acta Cryst.* C**59**, o616–o619.
Odabaşoğlu, M., Arslan, F., Ölmez, H. & Büyükgüngör, O. (2007). *Dyes Pigments*, DYPI-2425.
Odabaşoğlu, M., Büyükgüngör, O., Narayana, B., Vijeshi, A. M. & Yathirajan, H. S. (2007*b*). *Acta Cryst.* E**63**, o1916–o1918.
Odabaşoğlu, M., Turgut, G. & Karaer, H. (1999). *Phosphorus Sulfur Silicon*, **152**, 9–25.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.
Yathirajan, H. S., Sarojini, B. K., Narayana, B., Sunil, K. & Bolte, M. (2007). *Acta Cryst.* E**63**, o1398–o1399.