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2-Methoxy-6-[(4-methylpyridin-2-yl)-iminomethyl]phenol

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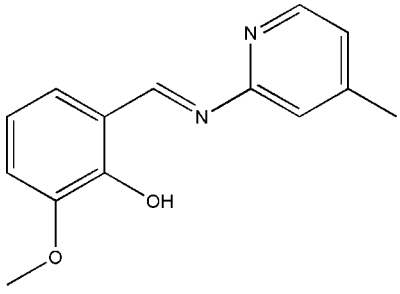
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.060; wR factor = 0.159; data-to-parameter ratio = 15.0.

The title Schiff base compound, $C_{14}H_{14}N_2O_2$, displays an E configuration with respect to the C=N double bond. The dihedral angle between the benzene and pyridine rings is 5.4 (2)°.

Related literature

For related literature, see: Ali *et al.* (2002); Allen *et al.* (1987); Cukurovali *et al.* (2002); Li (2007); Qian *et al.* (2006); Qiu *et al.* (2006); Tarafder *et al.* (2002); Yang (2006); Yang & Guo (2006); Zhao (2006).



Experimental

Crystal data

$C_{14}H_{14}N_2O_2$
M_r = 242.27
Monoclinic, $P2_1/c$
a = 9.997 (2) Å
b = 4.896 (1) Å
c = 24.729 (5) Å
β = 94.24 (3)°
V = 1207.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.23 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.979, T_{max} = 0.982
8333 measured reflections
2498 independent reflections
1384 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.159
S = 1.03
2498 reflections
167 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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	1.86	2.588 (2)	147

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2194).

References

Ali, M. A., Mirza, A. H., Butcher, R. J., Tarafder, M. T. H., Keat, T. B. & Ali, A. M. (2002). *J. Inorg. Biochem.* **92**, 141–148.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Cukurovali, A., Yilmaz, I., Özmen, H. & Ahmedzade, M. (2002). *Transition Met. Chem.* **27**, 171–176.
Li, H.-B. (2007). *Acta Cryst.* E**63**, o972–o973.
Qian, H.-Y., Yin, Z.-G., Jia, J., Liu, S.-M. & Feng, L.-Q. (2006). *Acta Cryst.* E**62**, o3623–o3624.
Qiu, X.-Y., Fang, X.-N., Liu, W.-S. & Zhu, H.-L. (2006). *Acta Cryst.* E**62**, o2685–o2686.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Tarafder, M. T. H., Jin, K. T., Crouse, K. A., Ali, A. M., Yamin, B. M. & Fun, H.-K. (2002). *Polyhedron*, **21**, 2547–2554.
Yang, D.-S. (2006). *Acta Cryst.* E**62**, o3792–o3793.
Yang, D.-S. & Guo, J.-B. (2006). *Acta Cryst.* E**62**, o4414–o4415.
Zhao, L.-F. (2006). *Acta Cryst.* E**62**, o3970–o3971.

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supplementary materials

Acta Cryst. (2007). E**63**, o4246 [**doi:10.1107/S1600536807048350**]

2-Methoxy-6-[(4-methylpyridin-2-yl)iminomethyl]phenol

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Comment

The compounds derived from the condensation reaction of aromatic carbaldehydes with hydrazides exhibit a wide range of biological activities and applications (Tarafder *et al.*, 2002; Cukurovali *et al.*, 2002; Ali *et al.*, 2002). Recently, the author has reported a Schiff base compound (Li, 2007). As a further investigation, the author reports here the crystal structure of the new Schiff base compound, Fig. 1.

All the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable with those observed in similar compounds (Qiu *et al.*, 2006; Yang and Guo, 2006; Yang, 2006). The C8═N1 bond length of 1.285 (3) Å conforms to the value for a double bond, and is comparable with that in other Schiff bases (Qian *et al.*, 2006; Zhao, 2006). The molecule displays an *E* configuration about the C═N double bond. The dihedral angle between the benzene ring and the pyridine ring is 5.4 (2)°.

The molecular structure is stablized by weak πi-πi interactions, stacking along the *b* axis (Fig. 2).

Experimental

3-Methoxysalicylaldehyde (0.1 mmol, 15.2 mg) and 4-methylpyridin-2-ylamine (0.1 mmol, 10.8 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. Crystals of (I) were formed by gradual evaporation of the solvent over a week at room temperature (yield 87.2%).

Refinement

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with O—H = 0.82 Å, C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl},*O*).

Figures

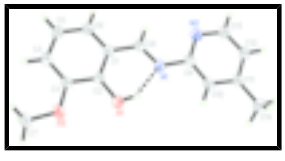

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Intramolecular hydrogen bond is shown as a dashed line.

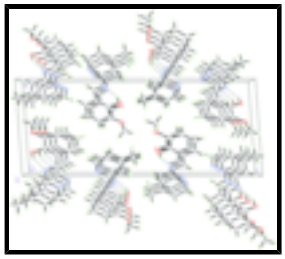

Fig. 2. The crystal packing of (I), viewed along the *b* axis.

2-Methoxy-6-[(4-methylpyridin-2-ylimino)methyl]phenol

Crystal data

$C_{14}H_{14}N_2O_2$	F_{000} = 512
M_r = 242.27	D_x = 1.333 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 713 reflections
a = 9.997 (2) Å	θ = 2.5–24.5º
b = 4.8960 (10) Å	μ = 0.09 mm^{-1}
c = 24.729 (5) Å	T = 298 (2) K
β = 94.24 (3)º	Block, yellow
V = 1207.1 (4) Å^3	0.23 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2498 independent reflections
Radiation source: fine-focus sealed tube	1384 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 298(2) K	θ_{max} = 26.5º
ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.979, T_{max} = 0.982	k = −6→6
8333 measured reflections	l = −30→31

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.159	$(\Delta/\sigma)_{max} < 0.001$
S = 1.03	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
2498 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}

167 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.011 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25493 (18)	0.8248 (4)	0.07335 (7)	0.0551 (6)
H1	0.1972	0.9383	0.0789	0.083*
O2	0.44898 (18)	0.4723 (4)	0.07002 (7)	0.0585 (6)
N1	0.08363 (19)	1.0839 (4)	0.12784 (8)	0.0442 (5)
N2	−0.0684 (2)	1.3400 (4)	0.17759 (8)	0.0516 (6)
C1	0.2269 (2)	0.7364 (5)	0.16759 (10)	0.0407 (6)
C2	0.2902 (2)	0.6903 (5)	0.11964 (10)	0.0403 (6)
C3	0.3939 (2)	0.4971 (5)	0.11899 (10)	0.0438 (6)
C4	0.4341 (2)	0.3547 (5)	0.16547 (11)	0.0491 (7)
H4	0.5037	0.2288	0.1651	0.059*
C5	0.3704 (3)	0.3993 (5)	0.21317 (11)	0.0507 (7)
H5	0.3974	0.3022	0.2444	0.061*
C6	0.2682 (3)	0.5856 (5)	0.21406 (10)	0.0477 (7)
H6	0.2259	0.6124	0.2459	0.057*
C7	0.5342 (3)	0.2432 (5)	0.06291 (11)	0.0584 (8)
H7A	0.6101	0.2514	0.0890	0.088*
H7B	0.5645	0.2463	0.0270	0.088*
H7C	0.4852	0.0775	0.0680	0.088*
C8	0.1211 (2)	0.9378 (5)	0.16942 (10)	0.0425 (6)
H8	0.0793	0.9619	0.2014	0.051*
C9	−0.0183 (2)	1.2843 (5)	0.13012 (10)	0.0412 (6)
C10	−0.0592 (2)	1.4159 (5)	0.08256 (10)	0.0461 (7)
H10	−0.0199	1.3710	0.0508	0.055*
C11	−0.1581 (2)	1.6146 (5)	0.08139 (10)	0.0457 (7)
C12	−0.2092 (2)	1.6755 (5)	0.13031 (11)	0.0499 (7)
H12	−0.2747	1.8093	0.1322	0.060*
C13	−0.1623 (3)	1.5363 (6)	0.17616 (11)	0.0573 (8)
H13	−0.1983	1.5816	0.2086	0.069*

C14	−0.2051 (3)	1.7581 (7)	0.02971 (12)	0.0704 (9)
H14A	−0.2917	1.8374	0.0335	0.106*
H14B	−0.2112	1.6291	0.0004	0.106*
H14C	−0.1425	1.8993	0.0222	0.106*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0617 (13)	0.0558 (13)	0.0489 (11)	0.0195 (9)	0.0112 (9)	0.0103 (9)
O2	0.0626 (12)	0.0599 (13)	0.0553 (12)	0.0237 (9)	0.0197 (9)	0.0067 (10)
N1	0.0431 (12)	0.0400 (13)	0.0496 (13)	0.0046 (10)	0.0053 (10)	−0.0023 (11)
N2	0.0548 (14)	0.0528 (15)	0.0484 (14)	0.0104 (11)	0.0119 (11)	−0.0016 (11)
C1	0.0368 (14)	0.0387 (15)	0.0464 (15)	−0.0021 (11)	0.0034 (11)	−0.0036 (12)
C2	0.0432 (14)	0.0378 (14)	0.0398 (15)	0.0001 (11)	0.0029 (11)	0.0051 (12)
C3	0.0429 (14)	0.0427 (15)	0.0466 (16)	0.0021 (12)	0.0086 (12)	−0.0010 (13)
C4	0.0410 (15)	0.0468 (17)	0.0596 (18)	0.0061 (12)	0.0054 (13)	0.0024 (14)
C5	0.0584 (17)	0.0435 (16)	0.0495 (17)	0.0023 (13)	0.0004 (13)	0.0086 (13)
C6	0.0543 (17)	0.0463 (16)	0.0431 (15)	0.0034 (13)	0.0080 (12)	−0.0010 (13)
C7	0.0523 (16)	0.0560 (19)	0.069 (2)	0.0111 (14)	0.0191 (14)	−0.0042 (15)
C8	0.0429 (15)	0.0392 (15)	0.0460 (15)	−0.0031 (12)	0.0077 (12)	−0.0049 (12)
C9	0.0391 (14)	0.0365 (15)	0.0486 (16)	−0.0014 (11)	0.0072 (12)	−0.0047 (12)
C10	0.0470 (16)	0.0480 (17)	0.0442 (16)	0.0034 (12)	0.0102 (12)	−0.0052 (13)
C11	0.0437 (15)	0.0463 (16)	0.0472 (16)	0.0036 (12)	0.0030 (12)	−0.0024 (13)
C12	0.0458 (15)	0.0444 (16)	0.0601 (18)	0.0102 (12)	0.0082 (13)	−0.0010 (14)
C13	0.0637 (18)	0.0569 (19)	0.0536 (18)	0.0143 (15)	0.0205 (14)	−0.0019 (15)
C14	0.078 (2)	0.075 (2)	0.058 (2)	0.0247 (17)	0.0031 (15)	0.0046 (16)

Geometric parameters (Å, °)

O1—C2	1.345 (3)	C6—H6	0.9300
O1—H1	0.8200	C7—H7A	0.9600
O2—C3	1.372 (3)	C7—H7B	0.9600
O2—C7	1.427 (3)	C7—H7C	0.9600
N1—C8	1.285 (3)	C8—H8	0.9300
N1—C9	1.419 (3)	C9—C10	1.376 (3)
N2—C9	1.338 (3)	C10—C11	1.386 (3)
N2—C13	1.342 (3)	C10—H10	0.9300
C1—C6	1.402 (3)	C11—C12	1.380 (3)
C1—C2	1.403 (3)	C11—C14	1.503 (4)
C1—C8	1.449 (3)	C12—C13	1.375 (3)
C2—C3	1.404 (3)	C12—H12	0.9300
C3—C4	1.379 (3)	C13—H13	0.9300
C4—C5	1.399 (3)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.370 (3)	C14—H14C	0.9600
C5—H5	0.9300		
C2—O1—H1	109.5	H7A—C7—H7C	109.5
C3—O2—C7	117.4 (2)	H7B—C7—H7C	109.5

C8—N1—C9	121.4 (2)	N1—C8—C1	121.6 (2)
C9—N2—C13	115.4 (2)	N1—C8—H8	119.2
C6—C1—C2	118.9 (2)	C1—C8—H8	119.2
C6—C1—C8	120.3 (2)	N2—C9—C10	123.2 (2)
C2—C1—C8	120.8 (2)	N2—C9—N1	119.5 (2)
O1—C2—C1	122.3 (2)	C10—C9—N1	117.3 (2)
O1—C2—C3	117.9 (2)	C9—C10—C11	120.9 (2)
C1—C2—C3	119.9 (2)	C9—C10—H10	119.6
O2—C3—C4	125.4 (2)	C11—C10—H10	119.6
O2—C3—C2	114.5 (2)	C12—C11—C10	116.3 (2)
C4—C3—C2	120.1 (2)	C12—C11—C14	122.1 (2)
C3—C4—C5	120.0 (2)	C10—C11—C14	121.6 (2)
C3—C4—H4	120.0	C13—C12—C11	119.4 (2)
C5—C4—H4	120.0	C13—C12—H12	120.3
C6—C5—C4	120.3 (2)	C11—C12—H12	120.3
C6—C5—H5	119.9	N2—C13—C12	124.9 (2)
C4—C5—H5	119.9	N2—C13—H13	117.6
C5—C6—C1	120.8 (2)	C12—C13—H13	117.6
C5—C6—H6	119.6	C11—C14—H14A	109.5
C1—C6—H6	119.6	C11—C14—H14B	109.5
O2—C7—H7A	109.5	H14A—C14—H14B	109.5
O2—C7—H7B	109.5	C11—C14—H14C	109.5
H7A—C7—H7B	109.5	H14A—C14—H14C	109.5
O2—C7—H7C	109.5	H14B—C14—H14C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.86	2.588 (2)	147

Fig. 1

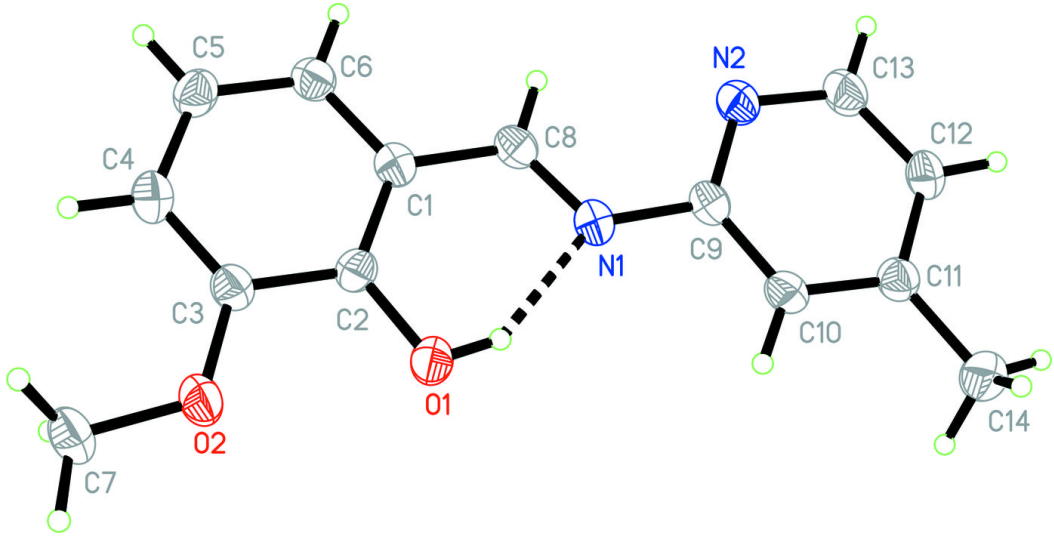

Fig. 2