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2-Methoxy-6-(3-pyridyliminomethyl)phenol

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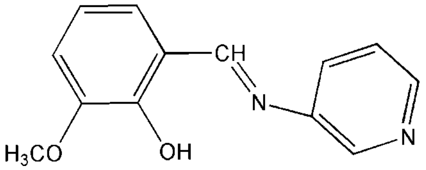
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.084; data-to-parameter ratio = 8.6.

In the title molecule, $C_{13}H_{12}N_2O_2$, the dihedral angle between the benzene ring system and the pyridine ring is 32.0 (1)°. An intramolecular O—H···N hydrogen bond stabilizes the molecular structure. Adjacent aromatic rings indicate the presence of π–π stacking interactions with a distance of 5.610 Å and a perpendicular distance of 2.432 Å.

Related literature

For related literature, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{13}H_{12}N_2O_2$
M_r = 228.25
Orthorhombic, $P2_12_12_1$
a = 5.6101 (19) Å
b = 9.278 (3) Å
c = 21.708 (7) Å
V = 1129.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.978, T_{max} = 0.984
6440 measured reflections
1373 independent reflections
1187 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.084
S = 1.03
1373 reflections
159 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2	0.93 (3)	1.78 (3)	2.611 (2)	147 (3)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: AT2294).

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supplementary materials

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2-Methoxy-6-(3-pyridyliminomethyl)phenol

Z.-L. Jing, R.-N. Li and N. Yang

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*, 2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I).

In the molecular structure of (I) (Fig. 1), the expected geometric parameters are observed. The benzaldehyde ring system (C7—C12) is planar, with an r.m.s. deviation for the fitted atoms of 0.0018 (6) Å, as is the pyridine ring (C1—C5/N2), with an r.m.s. deviation of 0.0069 (5) Å. The dihedral angle between these two planes is 32.0 (1)°. An intramolecular O—H···N hydrogen bond stabilizes the molecular conformation, and the distance of 5.610 Å of the adjacent aromactic rings indicates the presence of π-π stacking interactions, which stabilize the crystal packing, as illustrated in Fig.2.

Experimental

An anhydrous ethanol solution (50 ml) of 2-hydroxy-3-methoxy-benzaldehyde (1.52 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of pyridin-3-ylamine (0.94 g, 10 mmol), and the mixture was stirred at 350 K for 6 h under N_2, whereupon a yellow solution appeared. The solvent was removed and the residue was recrystallized from anhydrous ethanol. The product was isolated and then dried *in vacuo* to give pure compound (I) in 91% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Refinement

The N-bound H atom was located in a difference Fourier map and its positional parameters were refined, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{N})$. C-bound H atoms were included in calculated positions, with C—H = 0.95 (aromatic) or 0.99 Å (methylene), and refined using a riding model, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$.

Figures

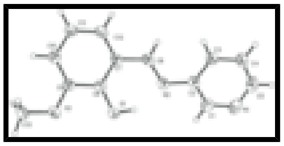

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

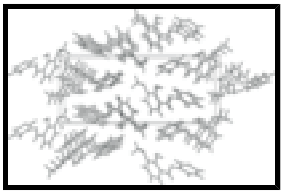

Fig. 2. The crystal packing of (I), shows its layered structure. H atoms have been omitted for clarity.

2-Methoxy-6-(pyridin-3-yliminomethyl)phenol

Crystal data

$C_{13}H_{12}N_2O_2$

$M_r = 228.25$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 5.6101$ (19) Å

$b = 9.278$ (3) Å

$c = 21.708$ (7) Å

$V = 1129.9$ (7) Å^3

$Z = 4$

$F_{000} = 480$

$D_x = 1.342$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 3145 reflections

$\theta = 2.4$–$26.4°$

$\mu = 0.09$ mm^{-1}

$T = 294$ (2) K

Block, yellow

0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 294(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.978$, $T_{max} = 0.984$

6440 measured reflections

1373 independent reflections

1187 reflections with $I > 2\sigma(I)$

$R_{int} = 0.025$

$\theta_{max} = 26.5°$

$\theta_{min} = 1.9°$

$h = -7 \rightarrow 6$

$k = -11 \rightarrow 5$

$l = -26 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.084$

$S = 1.04$

1373 reflections

159 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 0.1574P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = <0.001$

$\Delta\rho_{max} = 0.10$ e Å^{-3}

$\Delta\rho_{min} = -0.16$ e Å^{-3}

Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
N1	−0.2010 (4)	0.4487 (2)	0.29371 (9)	0.0682 (6)
N2	0.3205 (3)	0.39459 (18)	0.19617 (7)	0.0462 (4)
O1	0.5051 (3)	0.54594 (16)	0.10671 (7)	0.0534 (4)
H1A	0.399 (6)	0.522 (3)	0.1380 (13)	0.097 (10)*
O2	0.8401 (3)	0.57453 (15)	0.02324 (6)	0.0560 (4)
C1	−0.0443 (4)	0.4520 (3)	0.24816 (11)	0.0563 (6)
H1	−0.0818	0.5071	0.2137	0.068*
C2	0.1715 (4)	0.3796 (2)	0.24799 (8)	0.0435 (4)
C3	0.2295 (4)	0.3008 (2)	0.30003 (9)	0.0506 (5)
H3	0.3742	0.2523	0.3026	0.061*
C4	0.0693 (5)	0.2959 (3)	0.34784 (10)	0.0593 (6)
H4	0.1036	0.2435	0.3833	0.071*
C5	−0.1414 (5)	0.3690 (3)	0.34257 (11)	0.0657 (7)
H5	−0.2495	0.3629	0.3749	0.079*
C6	0.4585 (4)	0.2907 (2)	0.18057 (8)	0.0471 (5)
H6	0.4471	0.2036	0.2016	0.057*
C7	0.6313 (4)	0.3041 (2)	0.13150 (8)	0.0426 (4)
C8	0.6514 (4)	0.4326 (2)	0.09765 (8)	0.0415 (4)
C9	0.8327 (4)	0.4450 (2)	0.05357 (8)	0.0441 (4)
C10	0.9883 (4)	0.3325 (2)	0.04384 (9)	0.0498 (5)
H10	1.1088	0.3417	0.0147	0.060*
C11	0.9668 (5)	0.2054 (2)	0.07722 (9)	0.0546 (5)
H11	1.0720	0.1297	0.0702	0.066*
C12	0.7905 (4)	0.1918 (2)	0.12035 (9)	0.0518 (5)
H12	0.7767	0.1064	0.1425	0.062*
C13	1.0462 (4)	0.6031 (3)	−0.01286 (10)	0.0625 (6)
H13A	1.1863	0.5897	0.0119	0.094*
H13B	1.0408	0.7007	−0.0275	0.094*
H13C	1.0506	0.5383	−0.0473	0.094*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0526 (11)	0.0777 (13)	0.0742 (12)	0.0044 (12)	0.0053 (11)	−0.0131 (12)
N2	0.0513 (10)	0.0454 (9)	0.0419 (8)	−0.0043 (9)	−0.0010 (8)	0.0020 (7)
O1	0.0621 (9)	0.0419 (7)	0.0563 (8)	0.0063 (8)	0.0091 (8)	0.0068 (7)
O2	0.0678 (9)	0.0453 (8)	0.0548 (8)	0.0007 (9)	0.0127 (8)	0.0113 (6)
C1	0.0570 (14)	0.0585 (13)	0.0534 (11)	0.0038 (12)	−0.0058 (11)	−0.0042 (11)
C2	0.0464 (11)	0.0404 (10)	0.0437 (9)	−0.0073 (10)	−0.0020 (9)	−0.0025 (8)
C3	0.0540 (12)	0.0486 (11)	0.0493 (10)	−0.0023 (11)	0.0022 (10)	0.0026 (9)
C4	0.0738 (16)	0.0558 (12)	0.0484 (11)	−0.0114 (13)	0.0071 (11)	0.0009 (10)
C5	0.0630 (15)	0.0728 (15)	0.0614 (13)	−0.0138 (15)	0.0157 (12)	−0.0117 (13)
C6	0.0581 (12)	0.0405 (10)	0.0429 (10)	−0.0071 (11)	−0.0020 (10)	0.0030 (9)
C7	0.0511 (11)	0.0397 (9)	0.0371 (8)	−0.0026 (10)	−0.0041 (9)	0.0006 (8)
C8	0.0476 (10)	0.0382 (9)	0.0386 (9)	−0.0007 (10)	−0.0046 (8)	−0.0023 (7)
C9	0.0544 (11)	0.0404 (9)	0.0375 (9)	−0.0029 (11)	−0.0027 (9)	0.0016 (8)
C10	0.0526 (12)	0.0529 (12)	0.0440 (10)	0.0005 (11)	0.0006 (10)	−0.0005 (9)
C11	0.0635 (14)	0.0478 (11)	0.0524 (11)	0.0109 (12)	0.0011 (11)	0.0024 (10)
C12	0.0691 (14)	0.0403 (10)	0.0461 (10)	0.0030 (11)	−0.0032 (11)	0.0059 (9)
C13	0.0674 (14)	0.0630 (14)	0.0572 (12)	−0.0082 (13)	0.0092 (12)	0.0157 (11)

Geometric parameters (Å, °)

N1—C1	1.324 (3)	C5—H5	0.9300
N1—C5	1.335 (3)	C6—C7	1.446 (3)
N2—C6	1.282 (3)	C6—H6	0.9300
N2—C2	1.409 (3)	C7—C12	1.394 (3)
O1—C8	1.348 (2)	C7—C8	1.405 (3)
O1—H1A	0.93 (3)	C8—C9	1.401 (3)
O2—C9	1.371 (2)	C9—C10	1.377 (3)
O2—C13	1.422 (3)	C10—C11	1.389 (3)
C1—C2	1.385 (3)	C10—H10	0.9300
C1—H1	0.9300	C11—C12	1.367 (3)
C2—C3	1.384 (3)	C11—H11	0.9300
C3—C4	1.374 (3)	C12—H12	0.9300
C3—H3	0.9300	C13—H13A	0.9600
C4—C5	1.368 (4)	C13—H13B	0.9600
C4—H4	0.9300	C13—H13C	0.9600
C1—N1—C5	116.1 (2)	C12—C7—C6	119.54 (17)
C6—N2—C2	119.67 (17)	C8—C7—C6	120.82 (19)
C8—O1—H1A	107.8 (18)	O1—C8—C9	118.53 (17)
C9—O2—C13	116.95 (18)	O1—C8—C7	122.45 (18)
N1—C1—C2	124.9 (2)	C9—C8—C7	119.01 (18)
N1—C1—H1	117.6	O2—C9—C10	124.84 (18)
C2—C1—H1	117.6	O2—C9—C8	114.96 (17)
C3—C2—C1	117.4 (2)	C10—C9—C8	120.19 (17)
C3—C2—N2	124.35 (19)	C9—C10—C11	120.5 (2)

C1—C2—N2	118.23 (18)	C9—C10—H10	119.7
C4—C3—C2	118.7 (2)	C11—C10—H10	119.7
C4—C3—H3	120.6	C12—C11—C10	119.9 (2)
C2—C3—H3	120.6	C12—C11—H11	120.1
C5—C4—C3	119.0 (2)	C10—C11—H11	120.1
C5—C4—H4	120.5	C11—C12—C7	120.87 (19)
C3—C4—H4	120.5	C11—C12—H12	119.6
N1—C5—C4	123.9 (2)	C7—C12—H12	119.6
N1—C5—H5	118.0	O2—C13—H13A	109.5
C4—C5—H5	118.0	O2—C13—H13B	109.5
N2—C6—C7	122.32 (18)	H13A—C13—H13B	109.5
N2—C6—H6	118.8	O2—C13—H13C	109.5
C7—C6—H6	118.8	H13A—C13—H13C	109.5
C12—C7—C8	119.49 (18)	H13B—C13—H13C	109.5

C5—N1—C1—C2	0.2 (3)	C12—C7—C8—C9	−0.4 (3)
N1—C1—C2—C3	−1.7 (3)	C6—C7—C8—C9	175.32 (17)
N1—C1—C2—N2	−179.5 (2)	C13—O2—C9—C10	−11.2 (3)
C6—N2—C2—C3	32.8 (3)	C13—O2—C9—C8	168.11 (17)
C6—N2—C2—C1	−149.52 (19)	O1—C8—C9—O2	−0.6 (3)
C1—C2—C3—C4	1.6 (3)	C7—C8—C9—O2	−179.39 (17)
N2—C2—C3—C4	179.30 (19)	O1—C8—C9—C10	178.80 (18)
C2—C3—C4—C5	−0.2 (3)	C7—C8—C9—C10	0.0 (3)
C1—N1—C5—C4	1.4 (4)	O2—C9—C10—C11	179.7 (2)
C3—C4—C5—N1	−1.4 (4)	C8—C9—C10—C11	0.4 (3)
C2—N2—C6—C7	−174.12 (17)	C9—C10—C11—C12	−0.3 (3)
N2—C6—C7—C12	174.32 (18)	C10—C11—C12—C7	−0.1 (3)
N2—C6—C7—C8	−1.4 (3)	C8—C7—C12—C11	0.4 (3)
C12—C7—C8—O1	−179.15 (17)	C6—C7—C12—C11	−175.31 (18)
C6—C7—C8—O1	−3.5 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N2	0.93 (3)	1.78 (3)	2.611 (2)	147 (3)

Fig. 1

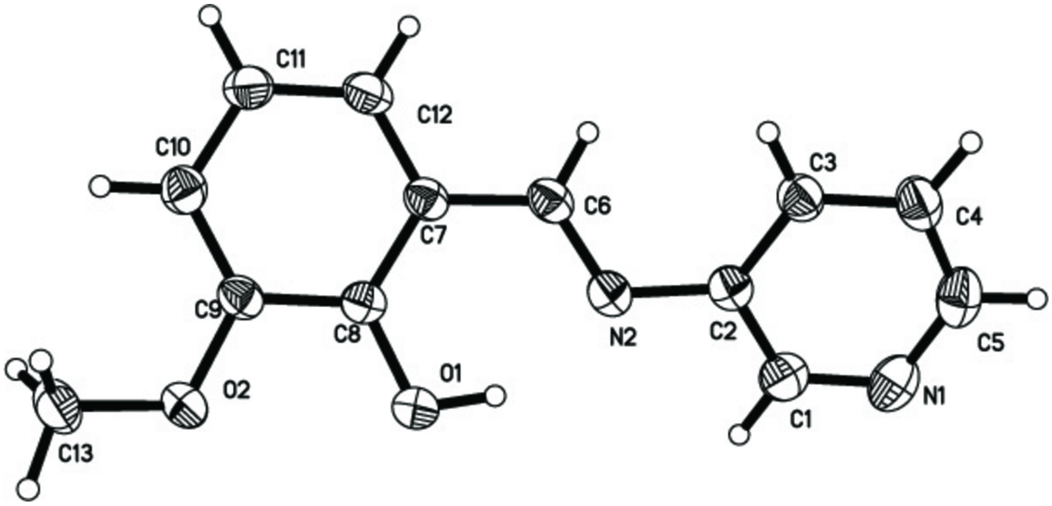

Fig. 2