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(*E*)-2-Methyl-6-{[(5-methylpyridin-2-yl)imino]-methyl}phenol

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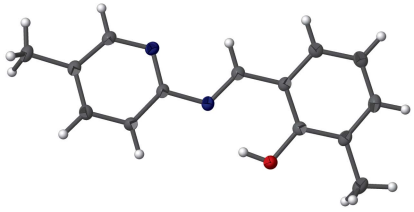
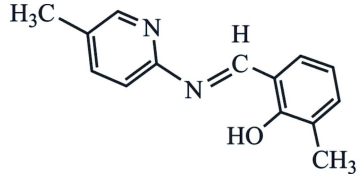
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{14}H_{14}N_2O$, the dihedral angle between the aromatic rings is 5.54 (9)°. The conformation is reinforced by an intramolecular O—H···N hydrogen bond, which closes an *S*(6) ring. The pyridine N atom and methyl group lie to opposite sides of the molecule. In the crystal, the molecules are linked into a zigzag chain propagating in [0$\bar{1}$1] by weak C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

As part of our ongoing studies of phenolic Schiff-base compounds (Adam *et al.* (2015), we now describe the synthesis and structure of the title compound (Fig. 1), which features an intramolecular O—H···N hydrogen bond (Table 1), which helps to establish near-coplanarity of the aromatic rings [dihedral angle = 5.54 (9)°]. In the crystal, the molecules are linked by a C2—H2*A*—O1 hydrogen bond into a zigzag *C*(9) chain propagating in [0$\bar{1}$1] (Table 1, Fig. 2). Adjacent molecules in the chain are related by *c*-glide symmetry.

Synthesis and crystallization

The synthesis scheme is shown in Fig. 3. 2-Hydroxy-3-methylbenzaldehyde (0.681 g, 5 mmol) was dissolved in 20 ml toluene and after adding 0.2 ml acetic acid, the mixture was refluxed for 30 min. Then, 5-methylpyridin-2-amine 0.541 g (5 mmol) solution in 20 ml toluene was added dropwise with stirring to the aldehyde solution. The resulting light-yellow solution was refluxed for 4 h with stirring. The solvent was allowed to evaporate. The crude product was washed with benzene and *n*-hexane. Orange blocks were obtained by slow evaporation of a solution in toluene; m.p.: 363–364 K; yield: 95%.

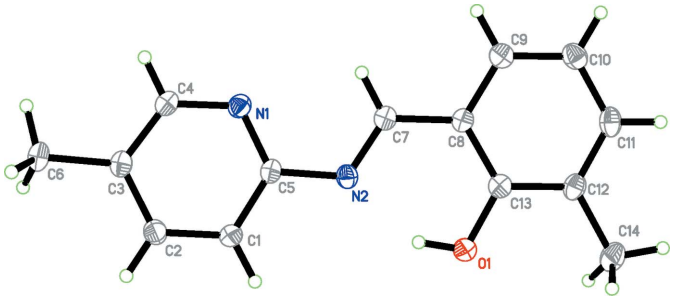


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

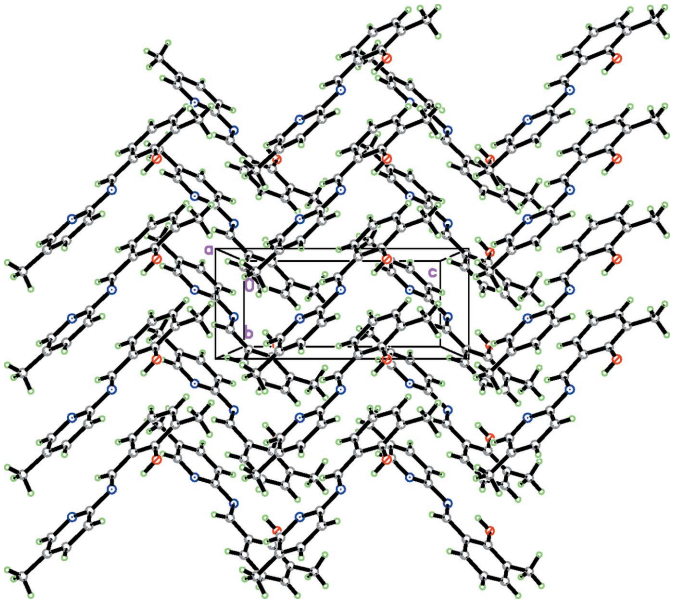


Figure 2
The packing of the title compound viewed along [010].

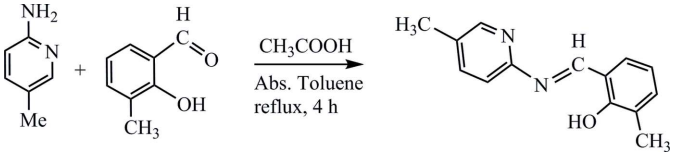


Figure 3
Synthesis of the title compound

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H101···N2	0.87 (3)	1.82 (3)	2.590 (2)	146 (3)
C2—H2A···O1^{i}	0.95	2.52	3.322 (3)	142

Symmetry code: (i) $-x+\frac{3}{2}, y+1, z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{14}N_2O$
M_r	226.27
Crystal system, space group	Orthorhombic, $Pca2_1$
Temperature (K)	100
a, b, c (Å)	23.440 (3), 4.6307 (6), 10.6408 (13)
V (Å^3)	1155.0 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.59 × 0.18 × 0.14
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	–
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9247, 3106, 2792
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.112, 1.09
No. of reflections	3106
No. of parameters	160
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.18

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015).

Funding information

University Sains Malaysia (RU grant 1001/PKIMIA/811269)
The World Academy of Science

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Adam, F., Arafath, M. A., Rosenani, A. H. & Razali, M. R. (2015). *Acta Cryst.* E**71**, o971–o972.
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full crystallographic data

IUCrData (2017). **2**, x162009 [https://doi.org/10.1107/S2414314616020095]

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(*E*)-2-Methyl-6-{[(5-methylpyridin-2-yl)imino]methyl}phenol

Crystal data

$C_{14}H_{14}N_2O$
M_r = 226.27
Orthorhombic, $Pca2_1$
a = 23.440 (3) Å
b = 4.6307 (6) Å
c = 10.6408 (13) Å
V = 1155.0 (3) Å^3
Z = 4
$F(000)$ = 480
D_x = 1.301 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2856 reflections
θ = 2.6–29.1°
μ = 0.08 mm^{-1}
T = 100 K
Block, orange
0.59 × 0.18 × 0.14 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
9247 measured reflections
3106 independent reflections
2792 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 29.1°, θ_{min} = 1.7°
h = −31→31
k = −6→6
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.09
3106 reflections
160 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.0393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.65226 (6)	0.0538 (3)	0.69407 (15)	0.0236 (4)

N1	0.61387 (7)	0.6480 (3)	0.31428 (17)	0.0194 (4)
N2	0.63432 (7)	0.3591 (4)	0.49405 (16)	0.0177 (4)
C1	0.70576 (8)	0.6813 (4)	0.4124 (2)	0.0204 (4)
H1A	0.7307	0.6230	0.4781	0.025*
C2	0.72340 (9)	0.8817 (4)	0.3237 (2)	0.0212 (4)
H2A	0.7608	0.9600	0.3273	0.025*
C3	0.68583 (8)	0.9677 (4)	0.22889 (19)	0.0185 (4)
C4	0.63168 (9)	0.8438 (4)	0.2302 (2)	0.0197 (4)
H4A	0.6055	0.9022	0.1669	0.024*
C5	0.65087 (8)	0.5669 (4)	0.40364 (19)	0.0170 (4)
C6	0.70294 (9)	1.1822 (4)	0.1299 (2)	0.0228 (4)
H6A	0.6696	1.2327	0.0788	0.034*
H6B	0.7324	1.0974	0.0760	0.034*
H6C	0.7180	1.3566	0.1702	0.034*
C7	0.58560 (9)	0.2307 (4)	0.48190 (19)	0.0178 (4)
H7A	0.5619	0.2782	0.4125	0.021*
C8	0.56627 (8)	0.0167 (4)	0.57120 (18)	0.0168 (4)
C9	0.51292 (9)	−0.1140 (4)	0.5548 (2)	0.0205 (4)
H9A	0.4899	−0.0613	0.4849	0.025*
C10	0.49335 (9)	−0.3183 (4)	0.6386 (2)	0.0232 (4)
H10A	0.4570	−0.4051	0.6272	0.028*
C11	0.52755 (9)	−0.3965 (4)	0.7406 (2)	0.0222 (4)
H11A	0.5139	−0.5377	0.7981	0.027*
C12	0.58079 (9)	−0.2740 (4)	0.76055 (19)	0.0205 (4)
C13	0.60016 (8)	−0.0652 (4)	0.67508 (19)	0.0181 (4)
C14	0.61778 (10)	−0.3582 (5)	0.8700 (2)	0.0290 (5)
H14A	0.6269	−0.1862	0.9198	0.043*
H14B	0.6532	−0.4453	0.8388	0.043*
H14C	0.5974	−0.4980	0.9226	0.043*
H101	0.6583 (13)	0.190 (7)	0.639 (3)	0.046 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0218 (7)	0.0269 (8)	0.0221 (8)	−0.0048 (6)	−0.0036 (6)	0.0055 (7)
N1	0.0210 (8)	0.0201 (8)	0.0170 (8)	0.0000 (7)	−0.0007 (7)	0.0006 (7)
N2	0.0182 (8)	0.0172 (8)	0.0178 (8)	0.0001 (6)	0.0024 (6)	0.0005 (7)
C1	0.0190 (10)	0.0206 (9)	0.0217 (11)	−0.0005 (7)	−0.0031 (8)	0.0039 (8)
C2	0.0204 (9)	0.0210 (9)	0.0222 (10)	−0.0015 (8)	0.0014 (8)	0.0014 (9)
C3	0.0233 (10)	0.0163 (9)	0.0159 (9)	0.0013 (7)	0.0029 (7)	−0.0011 (8)
C4	0.0234 (10)	0.0186 (9)	0.0170 (9)	0.0021 (7)	−0.0009 (8)	0.0006 (8)
C5	0.0211 (9)	0.0148 (9)	0.0150 (9)	0.0005 (7)	0.0013 (7)	−0.0003 (7)
C6	0.0288 (11)	0.0200 (10)	0.0196 (10)	0.0007 (8)	0.0037 (8)	0.0039 (8)
C7	0.0197 (9)	0.0168 (8)	0.0169 (10)	0.0018 (7)	0.0016 (7)	−0.0009 (8)
C8	0.0184 (9)	0.0165 (8)	0.0156 (10)	0.0020 (7)	0.0023 (7)	−0.0006 (7)
C9	0.0199 (10)	0.0195 (9)	0.0222 (10)	0.0016 (7)	0.0009 (8)	−0.0015 (8)
C10	0.0190 (9)	0.0224 (10)	0.0281 (11)	−0.0001 (8)	0.0034 (8)	−0.0007 (9)
C11	0.0268 (10)	0.0183 (9)	0.0217 (11)	0.0008 (8)	0.0081 (8)	0.0008 (8)

C12	0.0248 (10)	0.0209 (10)	0.0158 (10)	0.0022 (8)	0.0030 (8)	0.0014 (8)
C13	0.0195 (9)	0.0183 (8)	0.0164 (10)	0.0012 (7)	0.0014 (7)	−0.0025 (8)
C14	0.0349 (12)	0.0318 (12)	0.0202 (11)	−0.0005 (9)	−0.0005 (9)	0.0069 (10)

Geometric parameters (Å, º)

O1—C13	1.355 (2)	C6—H6C	0.9800
O1—H101	0.87 (4)	C7—C8	1.446 (3)
N1—C4	1.341 (3)	C7—H7A	0.9500
N1—C5	1.341 (3)	C8—C9	1.401 (3)
N2—C7	1.294 (3)	C8—C13	1.413 (3)
N2—C5	1.415 (2)	C9—C10	1.379 (3)
C1—C2	1.387 (3)	C9—H9A	0.9500
C1—C5	1.395 (3)	C10—C11	1.397 (3)
C1—H1A	0.9500	C10—H10A	0.9500
C2—C3	1.397 (3)	C11—C12	1.387 (3)
C2—H2A	0.9500	C11—H11A	0.9500
C3—C4	1.393 (3)	C12—C13	1.403 (3)
C3—C6	1.503 (3)	C12—C14	1.503 (3)
C4—H4A	0.9500	C14—H14A	0.9800
C6—H6A	0.9800	C14—H14B	0.9800
C6—H6B	0.9800	C14—H14C	0.9800
C13—O1—H101	110 (2)	C8—C7—H7A	119.1
C4—N1—C5	117.50 (17)	C9—C8—C13	118.92 (17)
C7—N2—C5	119.12 (17)	C9—C8—C7	119.61 (18)
C2—C1—C5	118.93 (19)	C13—C8—C7	121.47 (17)
C2—C1—H1A	120.5	C10—C9—C8	120.8 (2)
C5—C1—H1A	120.5	C10—C9—H9A	119.6
C1—C2—C3	119.62 (18)	C8—C9—H9A	119.6
C1—C2—H2A	120.2	C9—C10—C11	119.32 (19)
C3—C2—H2A	120.2	C9—C10—H10A	120.3
C4—C3—C2	116.74 (18)	C11—C10—H10A	120.3
C4—C3—C6	121.49 (18)	C12—C11—C10	121.93 (19)
C2—C3—C6	121.77 (18)	C12—C11—H11A	119.0
N1—C4—C3	124.66 (19)	C10—C11—H11A	119.0
N1—C4—H4A	117.7	C11—C12—C13	118.30 (19)
C3—C4—H4A	117.7	C11—C12—C14	122.09 (19)
N1—C5—C1	122.52 (18)	C13—C12—C14	119.61 (19)
N1—C5—N2	119.71 (17)	O1—C13—C12	118.38 (18)
C1—C5—N2	117.77 (18)	O1—C13—C8	120.94 (17)
C3—C6—H6A	109.5	C12—C13—C8	120.67 (17)
C3—C6—H6B	109.5	C12—C14—H14A	109.5
H6A—C6—H6B	109.5	C12—C14—H14B	109.5
C3—C6—H6C	109.5	H14A—C14—H14B	109.5
H6A—C6—H6C	109.5	C12—C14—H14C	109.5
H6B—C6—H6C	109.5	H14A—C14—H14C	109.5
N2—C7—C8	121.73 (18)	H14B—C14—H14C	109.5

N2—C7—H7A	119.1		
C5—C1—C2—C3	0.9 (3)	C13—C8—C9—C10	0.4 (3)
C1—C2—C3—C4	0.2 (3)	C7—C8—C9—C10	−179.86 (18)
C1—C2—C3—C6	−179.50 (18)	C8—C9—C10—C11	−0.5 (3)
C5—N1—C4—C3	0.2 (3)	C9—C10—C11—C12	0.2 (3)
C2—C3—C4—N1	−0.8 (3)	C10—C11—C12—C13	0.2 (3)
C6—C3—C4—N1	178.89 (19)	C10—C11—C12—C14	−179.8 (2)
C4—N1—C5—C1	1.0 (3)	C11—C12—C13—O1	−179.71 (18)
C4—N1—C5—N2	−179.48 (17)	C14—C12—C13—O1	0.3 (3)
C2—C1—C5—N1	−1.6 (3)	C11—C12—C13—C8	−0.3 (3)
C2—C1—C5—N2	178.90 (18)	C14—C12—C13—C8	179.73 (18)
C7—N2—C5—N1	6.5 (3)	C9—C8—C13—O1	179.42 (17)
C7—N2—C5—C1	−174.01 (18)	C7—C8—C13—O1	−0.3 (3)
C5—N2—C7—C8	−179.94 (17)	C9—C8—C13—C12	0.0 (3)
N2—C7—C8—C9	179.30 (18)	C7—C8—C13—C12	−179.77 (18)
N2—C7—C8—C13	−0.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H101···N2	0.87 (3)	1.82 (3)	2.590 (2)	146 (3)
C2—H2*A*···O1^{i}	0.95	2.52	3.322 (3)	142

Symmetry code: (i) −*x*+3/2, *y*+1, *z*−1/2.