Crystal structure of 2-((*E*)-(6-methylpyridin-2-ylimino)methyl)-4-methylphenol, C₁₄H₁₄N₂O

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Abstract

C₁₄H₁₄N₂O, monoclinic, *P*2₁/*n* (no. 14), *a* = 16.0418(9) Å, *b* = 4.6119(2) Å, *c* = 17.0111(9) Å, β = 106.585(6)°, *V* = 1206.2 Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0660, *wR*_{ref}(*F*²) = 0.1994, *T* = 293 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.16×0.25×0.42 mm
Wavelength:	Mo <i>K</i> _α radiation (0.71073 Å)
μ :	0.80 cm ^{−1}
Diffractometer, scan mode:	Rigaku R-Axis RAPID, ω
2 θ _{max} :	50°
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} :	5753, 2118
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ (<i>I</i> _{obs}), 1574
<i>N</i> (<i>param</i>) _{refined} :	154
Programs:	SHELX [10]

Source of material

2-Hydroxybenzaldehyde (2.4 g, 20 mmol) and 6-methylpyridin-2-amine (2.2 g, 20 mmol) were dissolved in ethanol respectively. Then these were put together and the mixture was refluxed for 30 minutes. Yellow powder precipitates during the cooling to room temperature. After evaporation, a crude product was recrystallized twice from carbinol to give a pure yellow product. **Elemental Analysis** calcd. for C₁₄H₁₄N₂O: C, 74.31; H, 6.24; N, 12.38; Found: C, 74.27; H, 6.28; N, 12.37.

Discussion

The Schiff base compounds and their derivatives have been playing an important role in the development of coordination chemistry [1,2] because these compounds can accommodate one, two or more metal centers and form homo- and heteronuclear metal complexes with interesting properties [3–6], such as excellent catalytic activities for epoxidation, aziridination, etc. [7], models of reaction centers of metalloenzymes [8], and nonlinear optical materials [9]. Here we designed and synthesized a new Schiff base

named 2-((*E*)-(6-methylpyridin-2-ylimino)methyl)-4-methylphenol. The crystal structure of the title compound is only built up by the C₁₄H₁₄N₂O molecules, in which all bond lengths are in normal ranges. The C7=N2 bond length is 1.281(4) Å whereas the C6–N2 bond length is found to be 1.418(3) Å. The C6, N2 and C7 atoms form a bond angle of 120.5(2)°. The molecular conformation is stabilized by an intramolecular O–H⋯N hydrogen bond (O1–H1D⋯N2).

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(7A)	4e	0.9080	1.0142	0.2277	0.059
H(13A)	4e	0.9627	1.3680	0.3370	0.063
H(10A)	4e	1.2117	1.5135	0.2576	0.079
H(3A)	4e	0.7353	0.1859	−0.0018	0.077
H(5A)	4e	0.9425	0.6757	0.0052	0.073
H(11A)	4e	1.1930	1.7517	0.3696	0.077
H(4A)	4e	0.8385	0.3425	−0.0633	0.082
H(14A)	4e	1.1136	1.8654	0.4625	0.113
H(14B)	4e	1.0581	1.6065	0.4800	0.113
H(14C)	4e	1.0125	1.8631	0.4236	0.113
H(1D)	4e	1.0702	1.0554	0.1411	0.110
H(1A)	4e	0.7213	0.4405	0.1932	0.124
H(1B)	4e	0.7161	0.1346	0.1519	0.124
H(1C)	4e	0.6536	0.3836	0.1078	0.124

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
N(2)	4e	0.9621(1)	0.9117(5)	0.1448(1)	0.048(1)	0.052(1)	0.054(1)	0.003(1)	0.014(1)	0.005(1)
C(7)	4e	0.9562(2)	1.0463(6)	0.2088(2)	0.043(1)	0.050(2)	0.056(2)	0.004(1)	0.016(1)	0.009(1)
C(8)	4e	1.0226(2)	1.2468(6)	0.2526(2)	0.040(1)	0.045(1)	0.052(1)	0.003(1)	0.009(1)	0.013(1)
N(1)	4e	0.8366(1)	0.6280(5)	0.1400(1)	0.046(1)	0.055(1)	0.050(1)	0.002(1)	0.0106(9)	0.001(1)
C(13)	4e	1.0129(2)	1.3973(6)	0.3212(2)	0.048(1)	0.051(2)	0.058(2)	0.000(1)	0.015(1)	0.010(1)
C(6)	4e	0.8967(2)	0.7123(6)	0.1040(2)	0.046(1)	0.049(2)	0.048(1)	0.010(1)	0.009(1)	0.006(1)
C(10)	4e	1.1613(2)	1.4832(7)	0.2731(2)	0.047(2)	0.067(2)	0.083(2)	−0.007(1)	0.020(1)	0.013(2)
C(3)	4e	0.7768(2)	0.3221(7)	0.0242(2)	0.061(2)	0.062(2)	0.061(2)	0.004(2)	0.001(1)	−0.010(2)
C(12)	4e	1.0751(2)	1.5875(6)	0.3660(2)	0.057(2)	0.048(2)	0.056(2)	0.001(1)	0.004(1)	0.011(1)
C(9)	4e	1.0984(2)	1.2953(6)	0.2283(2)	0.050(2)	0.053(2)	0.062(2)	0.002(1)	0.017(1)	0.014(1)
C(5)	4e	0.8998(2)	0.6112(7)	0.0282(2)	0.062(2)	0.067(2)	0.056(2)	0.010(2)	0.022(1)	0.003(2)
C(2)	4e	0.7767(2)	0.4337(6)	0.0997(2)	0.049(2)	0.056(2)	0.055(2)	0.005(1)	0.004(1)	0.002(1)
C(11)	4e	1.1498(2)	1.6261(7)	0.3404(2)	0.054(2)	0.059(2)	0.070(2)	−0.009(1)	0.003(1)	0.011(2)
C(4)	4e	0.8383(2)	0.4134(7)	−0.0122(2)	0.075(2)	0.076(2)	0.052(2)	0.017(2)	0.014(2)	−0.009(2)
C(14)	4e	1.0638(2)	1.7448(7)	0.4397(2)	0.085(2)	0.068(2)	0.067(2)	−0.006(2)	0.011(2)	−0.001(2)
O(1)	4e	1.1118(1)	1.1605(5)	0.1623(1)	0.063(1)	0.086(2)	0.081(1)	−0.007(1)	0.038(1)	−0.000(1)
C(1)	4e	0.7110(2)	0.3397(9)	0.1419(2)	0.065(2)	0.101(3)	0.082(2)	−0.021(2)	0.021(2)	−0.005(2)

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