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Crystal structure of 2-(1*H*-imidazo-[4,5-c]-pyridine-2-yl)-6-methoxy-phenol, $C_{13}H_{11}N_3O_2$

Xinfang Wang*

Department of Chemistry, Dezhou University, Dezhou 253023, Shandong Province, P. R. China

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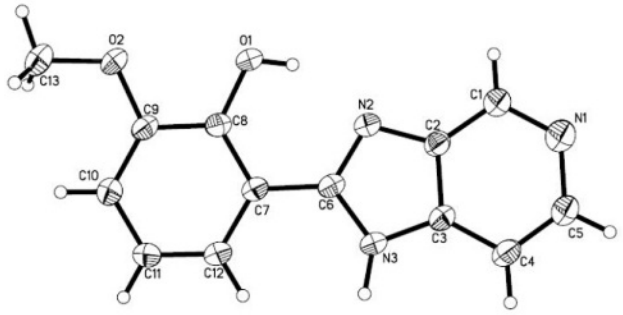

Abstract

$C_{13}H_{11}N_3O_2$, monoclinic, $P2_1/n$ (no. 14), a = 7.6199(9) Å, b = 12.357(2) Å, c = 12.460(1) Å, β = 95.139(2)°, V = 1168.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.0542, $wR_{ref}(F^2)$ = 0.1673, T = 293 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.19×0.31×0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.96 cm^{-1}
Diffractometer, scan mode:	Bruker APEXII CCD, φ and ω
$2\theta_{max}$:	50.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5570, 2024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1578
$N(param)_{refined}$:	163
Programs:	SHELXS-97 [4]

Source of material

The title compound was synthesized by the reaction of 3,4-diaminopyridine and 2-hydroxy-3-methoxybenzaldehyde with the ratio 1:1 in ethanol. After the mixture was refluxed sevral hours, the resulting clear yellow solution was allowed to evaporate slowly in air, and yellow block-like crystals suitable for X-ray diffraction were obtained with a yield 50% about one week later.

Discussion

Due to the excellent coordination ability of the *N*-donor atoms, imidazole and its derivatives have already been introduced into transition metal complexes [1]. Here, we present a new imidazole compound based on 3,4-diaminopyridine and 2-hydroxy-3-methoxybenzaldehyde. The molecluar structure of the title compound is shown in the figure. As can be seen, all the non-hydrogen atoms are located into a good plane with the largest deviation value being 0.0737 Å, indicating that the molecule of the title compound is almost planar. The dihedral angle between the 1*H*-imidazo-[4,5-c]-pyridine plane and the 2-methoxy-phenol plane is 7.9(2)°. All the bond parameters are comparable to the other two benzimidazole compounds [2-3]. Two intra- and intermolecular N···H–O hydrogen bond interactions can be found, and depending on the intermolecular N···H–O hydrogen bond interactions one-dimensional structure are formed.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	0.3096	0.1962	0.5217	0.085
H(3)	4*e*	0.5875	0.2329	0.8570	0.054
H(1A)	4*e*	0.7295	0.0233	0.5146	0.072
H(4)	4*e*	0.9039	0.1266	0.8733	0.063
H(5)	4*e*	1.0775	0.0165	0.7761	0.074
H(10)	4*e*	–0.1323	0.4151	0.7050	0.063
H(11)	4*e*	0.0444	0.3938	0.8664	0.065
H(12)	4*e*	0.3057	0.3040	0.8659	0.056
H(13A)	4*e*	–0.3036	0.3725	0.5524	0.123
H(13B)	4*e*	–0.2764	0.4021	0.4327	0.123
H(13C)	4*e*	–0.1927	0.4747	0.5269	0.123

* e-mail: dzxfwang@yahoo.com.cn

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	4*e*	0.2200(2)	0.2330(2)	0.5122(1)	0.057(1)	0.080(1)	0.0318(9)	0.0212(9)	–0.0082(7)	–0.0061(8)
O(2)	4*e*	–0.0693(2)	0.3384(2)	0.5109(1)	0.057(1)	0.087(1)	0.046(1)	0.025(1)	–0.0180(8)	–0.0082(9)
N(1)	4*e*	0.9186(3)	0.0084(2)	0.6362(2)	0.060(2)	0.090(2)	0.063(2)	0.011(1)	0.001(1)	0.004(1)
N(2)	4*e*	0.4975(2)	0.1554(2)	0.6143(2)	0.045(1)	0.057(1)	0.034(1)	0.0045(9)	–0.0024(8)	–0.0017(8)
N(3)	4*e*	0.5769(2)	0.2019(2)	0.7863(2)	0.044(1)	0.056(1)	0.034(1)	0.0032(9)	–0.0064(8)	–0.0055(8)
C(1)	4*e*	0.7643(3)	0.0434(2)	0.5852(2)	0.051(2)	0.079(2)	0.048(2)	0.012(1)	0.002(1)	0.002(1)
C(2)	4*e*	0.6596(3)	0.1109(2)	0.6430(2)	0.040(1)	0.052(1)	0.038(1)	0.002(1)	–0.0001(9)	0.004(1)
C(3)	4*e*	0.7110(3)	0.1403(2)	0.7508(2)	0.038(1)	0.047(1)	0.041(1)	–0.0025(9)	–0.0029(9)	0.002(1)
C(4)	4*e*	0.8683(3)	0.1065(2)	0.8028(2)	0.046(1)	0.062(2)	0.047(1)	–0.001(1)	–0.009(1)	–0.001(1)
C(5)	4*e*	0.9699(3)	0.0408(2)	0.7438(2)	0.048(2)	0.079(2)	0.055(2)	0.011(1)	–0.003(1)	0.003(1)
C(6)	4*e*	0.4526(3)	0.2081(2)	0.7021(2)	0.040(1)	0.047(1)	0.035(1)	–0.0027(9)	–0.0033(9)	0.0019(9)
C(7)	4*e*	0.2884(3)	0.2661(2)	0.7055(2)	0.041(1)	0.044(1)	0.036(1)	–0.0014(9)	–0.0034(9)	0.0004(9)
C(8)	4*e*	0.1803(3)	0.2754(2)	0.6087(2)	0.045(1)	0.046(1)	0.035(1)	0.001(1)	–0.0011(9)	–0.0009(9)
C(9)	4*e*	0.0232(3)	0.3324(2)	0.6109(2)	0.046(1)	0.053(1)	0.040(1)	0.005(1)	–0.009(1)	0.000(1)
C(10)	4*e*	–0.0269(3)	0.3770(2)	0.7058(2)	0.046(1)	0.059(2)	0.051(1)	0.010(1)	–0.004(1)	–0.006(1)
C(11)	4*e*	0.0794(3)	0.3652(2)	0.8027(2)	0.053(2)	0.066(2)	0.042(1)	0.007(1)	–0.001(1)	–0.013(1)
C(12)	4*e*	0.2338(3)	0.3115(2)	0.8020(2)	0.047(1)	0.055(1)	0.038(1)	0.000(1)	–0.005(1)	–0.004(1)
C(13)	4*e*	–0.2226(4)	0.4020(3)	0.5053(3)	0.071(2)	0.103(2)	0.066(2)	0.036(2)	–0.024(2)	–0.006(2)

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