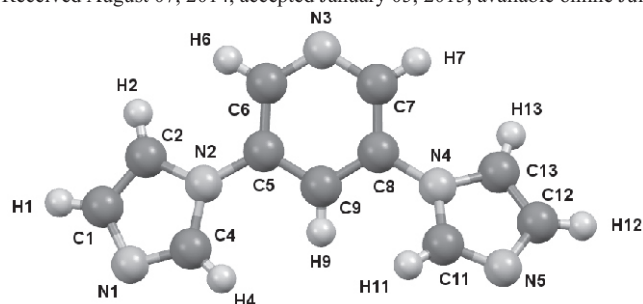


Crystal structure of 3,5-bis(imidazole-1-yl)pyridine, C₁₁H₉N₅

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Abstract

C₁₁H₉N₅, monoclinic, $P2_1/c$ (no. 14), $a = 14.15(1)$ Å, $b = 3.783(3)$ Å, $c = 18.09(2)$ Å, $\beta = 92.28(2)^\circ$, $V = 968.0$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0517$, $wR_{\text{ref}}(F^2) = 0.1504$, $T = 296$ K.

Table 1. Data collection and handling.

Crystal:	colourless blocks, size 0.16×0.18×0.19 mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	0.95 cm ⁻¹
Diffractionmeter, scan mode:	Bruker APEX-II CCD, φ and ω
$2\theta_{\text{max}}$:	52°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	4899, 1901
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1180
$N(\text{param})_{\text{refined}}$:	146
Programs:	SHELX [10]

Source of material

3,5-Bis(imidazole-1-yl)pyridine (*BIP*) has been prepared by a procedure reported in the literature [4]. Single crystals suitable for X-ray diffraction were obtained by crystallization of the title compound from CH₂Cl₂.

Discussion

Organic ligands based on the rigid pyridine and imidazole rings are excellent candidates for the construction of supramolecular architectures, metal–organic frameworks and cocrystals and exhibit diverse coordination modes and desired properties [1–3]. Among them, the newly developed 3,5-bis(imidazole-1-yl)pyridine (*BIP*), has been used as a multidentate coordinated ligand to prepare coordination compounds [4–8]. For example, Luo [4] reported six coordination polymers containing *BIP* molecules, and discussed the influences of the coordination modes, metal ions and counter anions on the crystal structures of these complexes. A view on the title molecular structure and the atom numbering is given in the figure. The asymmetric unit contains one molecule of the title compound, which is constructed by one pyridine and two imidazole moieties. All three rings of *BIP* are exactly not planar, and the angles between the pyridine and imidazole ring planes are 38.30° and 14.12°, respectively, which are larger than those for 2,6-bis(imidazole-1-yl)pyridine [9]. Additionally, the two imidazole rings of *BIP* are not equivalent ex-

pressed by the different bond lengths and angles. The crystal structure of the title compound is stabilized by two weak intermolecular C–H⋯N hydrogen bonds, forming a one-dimensional chain along the a axis. Also, adjacent molecules are connected by the weak π ⋯ π interactions. The centroid-centroid separation between two neighboring pyridine rings is 3.783(4) Å.

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

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.5853	1.3931	0.4803	0.064
H(2)	4e	0.5387	1.2560	0.6043	0.062
H(4)	4e	0.8077	1.0157	0.5832	0.062
H(6)	4e	0.5467	0.9504	0.7128	0.056
H(7)	4e	0.6969	0.6802	0.8878	0.054
H(9)	4e	0.8275	0.9627	0.7059	0.044
H(11)	4e	0.9409	0.5325	0.7582	0.049
H(12)	4e	1.0224	0.7677	0.9594	0.058
H(13)	4e	0.8555	0.9223	0.9468	0.055

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

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(1)	4e	0.7175(1)	1.2168(6)	0.5085(1)	0.055(1)	0.074(2)	0.042(2)	0.004(1)	0.005(1)	0.008(1)
N(3)	4e	0.6087(1)	0.8092(6)	0.8063(1)	0.040(1)	0.071(2)	0.044(1)	−0.002(1)	0.004(1)	0.009(1)
N(5)	4e	1.0156(1)	0.5997(5)	0.8520(1)	0.043(1)	0.057(1)	0.040(1)	0.004(1)	0.003(1)	0.005(1)
C(1)	4e	0.6251(2)	1.2980(7)	0.5173(2)	0.053(2)	0.062(2)	0.045(2)	0.008(1)	−0.003(1)	0.007(1)
C(2)	4e	0.5984(2)	1.2243(7)	0.5857(1)	0.043(1)	0.066(2)	0.047(2)	0.008(1)	−0.000(1)	0.010(1)
N(2)	4e	0.6773(1)	1.0921(5)	0.6226(1)	0.039(1)	0.044(1)	0.035(1)	0.0017(9)	0.0011(9)	0.0024(9)
C(4)	4e	0.7463(2)	1.0939(7)	0.5727(1)	0.045(1)	0.069(2)	0.041(2)	0.006(1)	0.004(1)	0.006(1)
C(5)	4e	0.6851(1)	0.9736(6)	0.6964(1)	0.039(1)	0.037(1)	0.032(1)	0.002(1)	0.002(1)	0.001(1)
C(6)	4e	0.6056(2)	0.9146(7)	0.7362(1)	0.040(1)	0.061(2)	0.040(2)	0.003(1)	0.001(1)	0.005(1)
C(7)	4e	0.6935(2)	0.7557(7)	0.8389(1)	0.045(2)	0.053(2)	0.037(2)	−0.001(1)	0.004(1)	0.005(1)
C(8)	4e	0.7762(2)	0.8078(6)	0.8029(1)	0.033(1)	0.037(1)	0.035(1)	−0.0005(9)	−0.000(1)	−0.003(1)
C(9)	4e	0.7724(2)	0.9217(6)	0.7308(1)	0.036(1)	0.039(1)	0.036(1)	−0.002(1)	0.004(1)	0.001(1)
N(4)	4e	0.8647(1)	0.7458(5)	0.8393(1)	0.036(1)	0.043(1)	0.033(1)	0.0015(8)	0.0022(8)	−0.0010(8)
C(11)	4e	0.9412(2)	0.6100(6)	0.8070(1)	0.040(1)	0.049(1)	0.035(1)	0.004(1)	0.003(1)	0.000(1)
C(12)	4e	0.9846(2)	0.7383(7)	0.9167(1)	0.047(2)	0.062(2)	0.035(2)	0.000(1)	−0.005(1)	0.002(1)
C(13)	4e	0.8924(2)	0.8266(7)	0.9104(1)	0.049(2)	0.058(2)	0.032(1)	0.003(1)	0.002(1)	−0.004(1)

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