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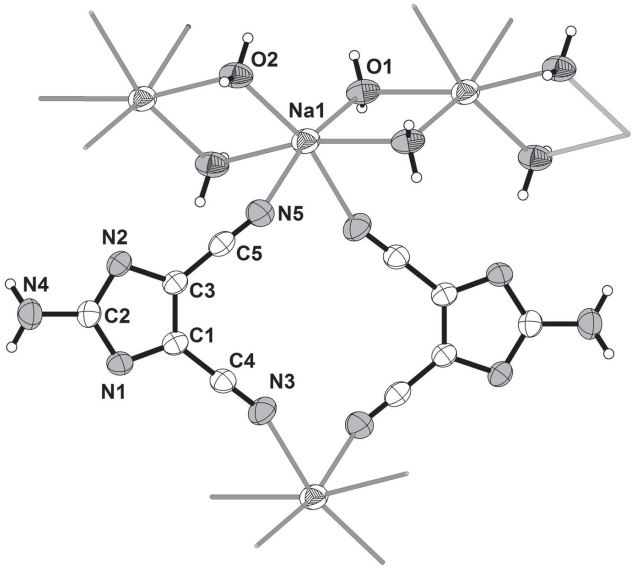
Crystal structure of poly[μ_2-diaqua-(μ_2-2-amino-4,5-dicyano-κ^2N:N'-imidazol-1-ide)sodium(I)], $C_5H_6N_5O_2Na$



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Abstract

$C_5H_6N_5O_2Na$, triclinic, $P\bar{1}$ (no. 2), $a = 7.0140(10)$ Å, $b = 7.4328(13)$ Å, $c = 8.9483(16)$ Å, $\alpha = 103.303(7)°$, $\beta = 103.719(6)°$, $\gamma = 103.634(6)°$, $V = 419.73(12)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0622$, $wR_{ref}(F^2) = 0.1795$, $T = 170(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.10 × 0.08 × 0.05 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.16 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.6°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5029, 1909, 0.055
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1565
$N(param)_{refined}$:	142
Programs:	Bruker [1], SHELX [2–4]

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

Atom	x	y	z	U_{iso}*/U_{eq}
Na1	0.07801(15)	0.28107(15)	0.04930(12)	0.0264(3)
O1	−0.2281(3)	0.0081(3)	−0.0042(2)	0.0278(5)
O2	0.0416(3)	0.4298(3)	−0.1643(2)	0.0303(5)
N1	0.7994(3)	1.1747(3)	0.5303(2)	0.0223(5)
N2	0.5901(3)	1.0520(3)	0.2691(2)	0.0211(5)
N3	0.8449(4)	0.7871(3)	0.6842(3)	0.0291(5)
N4	0.7273(4)	1.3952(3)	0.3837(3)	0.0300(5)
N5	0.4167(4)	0.5437(3)	0.1687(3)	0.0311(5)
C1	0.7394(4)	0.9765(3)	0.4878(3)	0.0200(5)
C2	0.7049(4)	1.2094(3)	0.3954(3)	0.0215(5)
C3	0.6112(4)	0.9004(3)	0.3293(3)	0.0200(5)
C4	0.7994(4)	0.8734(3)	0.5969(3)	0.0219(5)
C5	0.5042(4)	0.7040(4)	0.2393(3)	0.0232(5)
H1A	−0.343(5)	−0.017(5)	−0.086(4)	0.034(8)*
H1B	−0.272(6)	0.019(5)	0.065(5)	0.046(11)*
H2A	0.139(9)	0.488(8)	−0.177(7)	0.10(2)*
H2B	−0.051(6)	0.344(6)	−0.256(5)	0.048(10)*
H4A	0.792(6)	1.491(5)	0.471(5)	0.043(10)*
H4B	0.609(5)	1.407(5)	0.323(4)	0.034(8)*

Source of material

Sodium chloride (0.58 g) and deionized water (10 mL) form an aqueous solution, and 2-amino-4,5-dicyanimidazole (1.33 g) was dissolved in methanol (25 mL). Drop the sodium chloride solution into the methanol solution, which was refluxed for 24 h. The reaction mixture was filtered, and the filtrate was naturally evaporated to obtain transparent crystals.

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Experimental details

The U_{iso} of the H-atoms were constrained to 1.2 times U_{eq} of nitrogen atoms and 1.5 times U_{eq} of oxygen atoms at water.

Comment

Cyanoimidazoles are important intermediates for the preparation of pyrimidine bases and other organic compounds, and also important organic ligands [5–8]. The metal complexes of 2-amino-4,5-dicyanoimidazole have important applications in MOF materials [9, 10].

In the asymmetric unit of title compound (*cf*. the figure), there are one 2-amino-4,5-dicyano-imidazol-1-ide anion, one sodium(I) ion and two water molecules. The dihedral angles between the two cyano, amino and imidazole rings are: 37.29° (C3, C5, N5), 31.40° (C1, C4, N3) and 40.85° (N4, H4A, H4B), respectively. All bond lengths and angles are within normal ranges and in good agreement with those found for the structure of 2-amino-4,5-dicyanoimidazole [11]. In the crystal structure, sodium is sixfold coordinated by two nitrogen atoms groups and four oxygen (see the figure). Each sodium ion can form two parallelograms with two adjacent sodium ions and the four oxygen atoms to create a chain structure. These chains are connected by the organic ligands to a layered structure by the bridging effect of cyano groups and coordinated water molecules. The title structure contains several classical hydrogen bonds.

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