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Crystal structure of *catena*-poly[*diaqua*-bis(μ_2 -5, 5'-(1*H*-imidazole-4,5-diyl)bis(tetrazol-2-ido)- κ^4 N, N':N'',N''')magnesium], C₁₀H₈N₂₀O₂Mg

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Abstract

C₁₀H₈N₂₀O₂Mg, orthorhombic, *Pnma* (no. 62), $a = 12.4217(8)$ Å, $b = 7.3444(6)$ Å, $c = 10.6063(7)$ Å, $V = 967.61(12)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0411$, $wR_{ref}(F^2) = 0.1147$, $T = 293(2)$ K.

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A part of the polymeric title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of magnesium chloride hexahydrate (1 mmol), 4,5-bis(tetrazol-5-yl) imidazole (1 mmol), and *N,N*-dimethylformamide (3.5 mL) were added to deionized water (0.5 mL) in the heat-resistant glass tube. The mixture was

Table 1: Data collection and handling.

Crystal:	Grayish white block
Size:	0.50 × 0.30 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.20 mm ⁻¹
Diffractometer, scan mode:	Bruker Smart Apex, φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	4356, 932, 0.037
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 809
$N(param)_{refined}$:	106
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C1	0.7589(2)	0.750000	0.5525(3)	0.0237(7)
C2	0.8670(2)	0.750000	0.4984(3)	0.0278(7)
C3	1.0435(3)	0.750000	0.5047(3)	0.0430(10)
H3	1.113380	0.750000	0.536629	0.052*
C4	0.9085(2)	0.750000	0.3785(3)	0.0218(6)
C5	0.8637(2)	0.750000	0.2523(3)	0.0210(6)
Mg1	0.60264(7)	0.750000	0.30057(9)	0.0207(3)
N1	0.51977(19)	0.750000	0.1159(2)	0.0277(6)
N2	0.43059(18)	0.750000	0.3447(2)	0.0271(6)
N3	0.3679(2)	0.750000	0.4471(3)	0.0514(10)
N4	0.2672(2)	0.750000	0.4121(3)	0.0551(11)
N5	0.76124(18)	0.750000	0.2156(2)	0.0284(7)
N6	0.66688(18)	0.750000	0.4908(2)	0.0279(6)
N7	0.5916(2)	0.750000	0.5842(3)	0.0496(9)
N8	0.6375(2)	0.750000	0.6942(3)	0.0472(9)
N9	0.7443(2)	0.750000	0.6774(2)	0.0363(8)
N10	0.9552(2)	0.750000	0.5755(3)	0.0470(9)
H10	0.953850	0.750000	0.656890	0.057*
O1	0.60266(13)	0.4682(2)	0.31299(14)	0.0342(5)
H1A	0.597190	0.434819	0.390381	0.051*
H1B	0.664090	0.425710	0.289789	0.051*

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carefully stirred, frozen, and finally sealed with a gas burner. The tube was placed in the oven at 120 °C under the hydrothermal reaction conditions for 7 days to get good quality grayish white block crystals which appeared at the tube wall.

Experimental details

The methyl groups and the NH₃ groups were idealized and refined using rigid groups allowed to rotate about the P–C bond (AFIX 137 option of the SHELXL program [2]).

Comment

Due to the infinite coordination between the tectons of coordination polymers and MOFs (in this case metal ions and tetrazole organic ligand), these compounds own outstanding porosity and a large topological diversity. Thus the metal-organic frameworks have become the most exploited materials [5–7]. Indeed, multinuclear metal-based clusters have been synthesized, wherein tetrazole ligands as the bridge connect metal ions. Accordingly, tetrazoles were coordinated with the metal ions to obtain unimaginable topological structures, which may have interesting applications such as fluorescence, separation, catalysing the organic reactions, gas storage and so on [8–12]. The tetrazole ligand has several coordination points, consequently it is difficult to control to get the desired MOFs.

Single crystal X-ray diffraction reveals that the title complex crystallizes in the orthorhombic space group *Pnma*. The title compound has a polymeric structure and the asymmetric unit consists of one magnesium, one water molecule and one tetrazol-based ligand. The magnesium atom is six-coordinated and connected to two different organic ligands, each in a different bidentate mode along with two water molecules (see the figure). The magnesium atom completed its local coordination environment to a distorted octahedral formed by four nitrogen atoms from two different ligands (Mg1–N1, 2.211(2) Å; Mg1–N2, 2.189(2) Å; Mg1–N5, 2.165(2) Å; Mg1–N6, 2.171(2) Å) and two oxygen atoms of two water molecules (Mg1–O1, 2.059 Å). It is interesting to show that each ligand bridges magnesium atoms to result in the formation of a chain polymer. Meanwhile, all the bond lengths are within a reasonable range [13].

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