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Crystal structure of poly[aqua-(μ_4 -benzene-1,2,4,5-tetracarboxylato- κ^4 O, O', O'', O''')bis(μ_2 -1-(4-(1H-imidazol-1-yl)benzyl)-1H-1,2,4-triazole- κ^2 N:N) dinickel(II)], $\text{NiC}_{17}\text{H}_{14}\text{N}_5\text{O}_5$

Table 1: Data collection and handling.

Crystal:	Block, clear light green
Size:	0.3 × 0.15 × 0.1 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.22 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Quest, φ and ω -scans
θ_{max} , completeness:	27.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6609, 3516, 0.021
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2994
$N(\text{param})_{\text{refined}}$:	254
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

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Abstract

$\text{NiC}_{17}\text{H}_{14}\text{N}_5\text{O}_5$, triclinic, $P\bar{1}$ (no. 2), $a = 7.8199(8)$ Å, $b = 8.6969(8)$ Å, $c = 13.1934(13)$ Å, $\alpha = 93.955(1)^\circ$, $\beta = 99.951(1)^\circ$, $\gamma = 109.946(1)^\circ$, $V = 822.79(14)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0316$, $wR_{\text{ref}}(F^2) = 0.0688$, $T = 150$ K.

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A part of the title crystal 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 materials

$\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$ (0.2 mmol) in H_2O (5 mL) was added into a solution of 1-(imidazo-1-yl)-4-(1,2,4-triazol-1-ylmethyl)benzene (itmb) (0.2 mmol) and 1,2,4,5-benzenetetracarboxylic acid (H_4btec) (0.1 mmol) in H_2O (10 mL) which was adjusted to pH 6.5 with a dilute NaOH solution. The mixture was sealed in a Teflon-lined stainless steel vessel (25 mL) and heated to

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	1.11693(4)	0.42735(3)	0.86241(2)	0.01385(8)
O1	0.8785(2)	0.27386(17)	0.89655(11)	0.0198(3)
O2	0.7743(2)	0.43376(17)	0.99045(11)	0.0189(3)
O3	0.5525(2)	−0.28934(19)	1.18023(11)	0.0213(3)
O4	0.7645(2)	−0.26238(18)	1.08055(12)	0.0218(3)
O5	1.3828(2)	0.56786(19)	0.82992(12)	0.0267(4)
H5A	1.424387	0.489362	0.820411	0.040*
H5B	1.441625	0.619155	0.888133	0.040*
N1	1.0189(3)	0.6108(2)	0.81339(13)	0.0193(4)
N2	0.8882(3)	0.7913(2)	0.78258(13)	0.0205(4)
N3	1.0105(3)	0.8135(3)	0.71804(15)	0.0308(5)
N4	−0.0242(3)	0.6895(2)	0.29079(13)	0.0218(4)
N5	0.1619(3)	0.7691(2)	0.44574(14)	0.0242(4)
C1	1.0853(4)	0.7022(3)	0.73978(18)	0.0282(5)
H1	1.178208	0.686918	0.706717	0.034*
C2	0.8954(3)	0.6710(3)	0.83851(16)	0.0197(5)
H2	0.822787	0.634107	0.888871	0.024*
C3	0.7771(3)	0.8959(3)	0.78666(17)	0.0258(5)
H3A	0.860356	1.012922	0.794486	0.031*
H3B	0.721855	0.880149	0.849006	0.031*
C4	0.6232(3)	0.8617(3)	0.69230(17)	0.0222(5)
C5	0.5190(3)	0.9637(3)	0.68616(17)	0.0231(5)
H5	0.550309	1.053941	0.739383	0.028*
C6	0.3706(3)	0.9362(3)	0.60399(17)	0.0238(5)
H6	0.302925	1.008660	0.600045	0.029*
C7	0.3220(3)	0.8029(3)	0.52795(17)	0.0233(5)
C8	0.4229(4)	0.7002(3)	0.5329(2)	0.0433(8)
H8	0.389004	0.608180	0.480560	0.052*
C9	0.5739(4)	0.7310(3)	0.6141(2)	0.0405(7)

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H9	0.644573	0.661038	0.616053	0.049*
C10	0.1411(3)	0.7086(3)	0.34532(16)	0.0243(5)
H10	0.234147	0.683072	0.317649	0.029*
C11	−0.0007(4)	0.7901(4)	0.45543(18)	0.0346(6)
H11	−0.028768	0.831173	0.516630	0.041*
C12	−0.1134(4)	0.7403(3)	0.35963(18)	0.0323(6)
H12	−0.236369	0.740515	0.342675	0.039*
C13	0.7718(3)	0.2966(2)	0.95147(14)	0.0136(4)
C14	0.6285(3)	0.1415(2)	0.97369(14)	0.0134(4)
C15	0.6881(3)	0.0262(2)	1.02296(15)	0.0146(4)
H15	0.817120	0.043573	1.038152	0.018*
C16	0.5629(3)	−0.1137(2)	1.05035(14)	0.0136(4)
C17	0.6318(3)	−0.2314(2)	1.10908(15)	0.0153(4)

160 °C for 48 h. It was allowed to cool to room temperature at the rate of 5 °C per hour. The green crystals were filtered and washed three times with 5 mL ethanol solvent.

Experimental details

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined as riding on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O})$.

Discussion

Coordination polymers (CPs) and metal-organic frameworks (MOFs) have attracted great attention, because of their diverse topologies and potential applications as functional materials in catalysis, adsorption, magnetism, chemical sensors and so on [4–9]. Because of the diversity of the coordination modes and high-connected nodes, polycarboxylate ligands are used to construct MOFs or CPs [10, 11]. *N*-donor ligands also play an important role in CPs or MOFs. Moreover triazol ligands have been used in the synthesis of metal-organic frameworks [12, 13].

The X-ray structural analysis shows that the title complex crystallizes in a triclinic space group $P\bar{1}$. The asymmetric unit of the title complex consists of one Ni²⁺ ion, one itmb, one coordinated water molecules and one half of btec. Each Ni(II) atom is coordinated by one triazol nitrogen atom and one imidazo nitrogen atom from two different itmb ligands, three oxygen atoms from three different btec and one oxygen atom from one water molecule furnish a [NiN₂O₄] six-coordinate distorted octahedral geometry. The Ni–N bond lengths are 2.0876(17) and 2.0859(18) Å, and the Ni–O distances are in the range of 2.0339(15)–2.1556(16) Å, both of which are in the normal range [14]. The bond angles around the Ni(II) are in the ranges of 84.41(6)–174.72(7)°. The Ni(II) atoms are connected by three btec ligands and one H₂O to form a two-dimensional

network. Each two-dimensional network extends to construct a 3D network through two itmb ligands.

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