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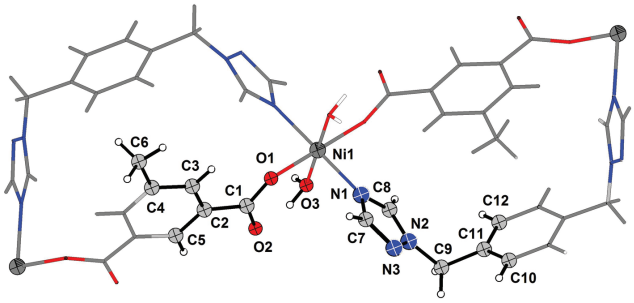
Crystal structure of *catena*-poly[diaqua-(μ_2-5-methylisophthalato-κ^2*O*:*O*′)(μ_2-1,4-bis((1*H*-1,2,4-triazol-1-yl)methyl)benzene-κ^2*N*:*N*′)], $NiC_{21}H_{22}O_6N_6$



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Abstract

$NiC_{21}H_{22}O_6N_6$, orthorhombic, *Pnma*, $a = 18.214(3)$ Å, $b = 20.934(3)$ Å, $c = 5.5296(8)$ Å, $V = 2108.3(5)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0279$, $wR_{ref}(F^2) = 0.798$, $T = 296(2)$ K.

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A part of the title coordination polymer is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

5-methylisophthalic acid (0.02 g, 0.1 mmol), 1,4-bis(triazol-1-ylmethyl)benzene and $NiCl_2$ (0.02 g, 0.1 mmol) were added to H_2O (10 mL) in a teflon-lined stainless steel reactor. The mixture was heated at 393 K for 3 days, and then slowly cooled down to room temperature. Green block crystals of the title compound were obtained.

Experimental details

The hydrogen atoms were placed at calculated positions with the SHELX program [2] (AFIX options: 43 and 147).

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Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.38 × 0.21 × 0.21 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.98 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14935, 2016, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1750
$N(param)_{refined}$:	161
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.0000	0.02170(13)
O1	0.51536(7)	0.42087(6)	0.2310(2)	0.0267(3)
O2	0.58992(9)	0.36555(7)	−0.0104(3)	0.0400(4)
O3	0.55316(7)	0.45801(6)	−0.2950(2)	0.0290(3)
H1W	0.5750	0.4242	−0.2495	0.044*
H2W	0.5355	0.4433	−0.4260	0.044*
N1	0.60169(9)	0.53985(7)	0.0851(3)	0.0286(4)
N2	0.70975(9)	0.58146(8)	0.0296(3)	0.0324(4)
N3	0.70954(12)	0.56076(11)	0.2617(4)	0.0561(6)
C1	0.54553(10)	0.36883(8)	0.1602(3)	0.0238(4)
C2	0.52393(10)	0.30777(8)	0.2858(3)	0.0227(4)
C3	0.47582(11)	0.30713(9)	0.4818(3)	0.0257(4)
H3	0.4596	0.3457	0.5459	0.031*
C4	0.45140(14)	0.2500	0.5843(5)	0.0255(6)
C5	0.54880(14)	0.2500	0.1915(5)	0.0230(5)
H5	0.5823	0.2500	0.0646	0.028*
C6	0.39868(17)	0.2500	0.7936(5)	0.0356(7)
H6A[a]	0.3530	0.2313	0.7439	0.053*
H6B[a]	0.3903	0.2931	0.8459	0.053*
H6C[a]	0.4190	0.2256	0.9244	0.053*
C7	0.64366(13)	0.53611(11)	0.2842(4)	0.0440(6)
H7	0.6273	0.5175	0.4270	0.053*
C8	0.64575(11)	0.56899(10)	−0.0696(4)	0.0353(5)
H8	0.6331	0.5793	−0.2278	0.042*
C9	0.77469(11)	0.61147(10)	−0.0814(5)	0.0417(5)
H9A	0.7786	0.5973	−0.2480	0.050*
H9B	0.8183	0.5971	0.0033	0.050*
C10	0.80520(11)	0.71691(10)	0.1105(4)	0.0346(5)
H10	0.8275	0.6948	0.2366	0.041*
C11	0.77225(10)	0.68356(9)	−0.0763(4)	0.0298(4)
C12	0.73885(12)	0.71693(11)	−0.2611(4)	0.0384(5)
H12	0.7162	0.6949	−0.3865	0.046*

[a]Occupancy: 0.50.

Discussion

The rational design metal-organic coordination polymers (CPs) have received remarkable attention, not only because of their fascinating architectures and topologies but also because of their potential applications as functional materials [3–8]. It is well known that topologies of coordination polymers have a significant impact on their physical and chemical properties [9–13]. Some isophthalic acids have been used in preparation of coordination polymers. For example, Du's group synthesised a series of 1D, 2D and 3D CPs using isophthalic acid and 5-hydroxylisophthalic acid [14]. Guo's group reported zinc(II) CPs based on isophthalic acid, 5-hydroxyisophthalic acid, 5-aminoisophthalic acid, 5-nitroisophthalic acid and 1,3,5-benzenetricarboxylic acid as educt. These compounds present superior CO_2 adsorption, tunable photoluminescence, direct white-light emission [15]. The results show that different substituents lead to different structures and properties. However, the study of CPs based on 5-methylisophthalate has been reported rarely [16, 17]. In order to study the effect of a single methyl group on structural topologies and physicochemical properties we chose 5-methylisophthalic acid along with 1,4-bis(triazol-1-ylmethyl) benzene to elaborate new complexes.

The asymmetric unit possesses one half Ni(II) ions, one half mip (5-methylisophthalic acid) ligand, one half bitb (1,4-bis(triazol-1-ylmethyl)benzene) ligand, and one coordinated water molecule. Ni1 is six-coordinated with a distorted octahedral environment by two carboxylic O atoms from two mip ligands, two N atoms from two bitb ligands and two coordinated water molecules. The bond angles around Ni1 range from 85.36(5) to 180.0°, the Ni1—O bond lengths vary from 2.0910(13) to 2.1103(12) Å, and the Ni1—N bond distances are 2.0852(16). The mip ligand is completely deprotonated. Both carboxylate groups act monodentate to bridge two Ni(II) ions. On the basis of the connection, mip ligands connect Ni1 ions to form a 1D chain. The same is true for the bitb ligand (*cf*. the figure).

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References

1. Bruker: APEX2, SAINT and SADABS. Brucker AXS Inc., Madison, WI, USA (2009).
2. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112–122.
3. Shaffer, D. W.; Xie, Y.; Szalda, D. J.; Concepcion, J. J.: Manipulating the rate-limiting step in water oxidation catalysis by ruthenium bipyridine–dicarboxylate complexes. Inorg. Chem. **55** (2016) 12024–12035.
4. Tian, Y.; Shen, S.; Cong, J.; Yan, L.; Wang, S.; Sun, Y.: Observation of resonant quantum magnetoelectric effect in a multiferroic metal–organic framework. J. Am. Chem. Soc. **138** (2016) 782–785.
5. Wang, B.; Lv, X.-L.; Feng, D.; Xie, L.-H.; Zhang, J.; Li, M.; Xie, Y.; Li, J.-R.; Zhou, H.-C.: Highly stable Zr(IV)-based metal–organic frameworks for the detection and removal of antibiotics and organic explosives in water. J. Am. Chem. Soc. **138** (2016) 6204–6216.
6. Levine, D. J.; Runčevski, T.; Kapelewski, M. T.; Keitz, B. K.; Oktawiec, J.; Reed, D. A.; Mason, J. A.; Jiang, H. Z. H.; Colwell, K. A.; Legendre, C. M.; FitzGerald, S. A.; Long, J. R.: Olsalazine-based metal–organic frameworks as biocompatible platforms for H_2 adsorption and drug delivery. J. Am. Chem. Soc. **138** (2016) 10143–10150.
7. Xu, R.; Wang, Y.; Duan, X.; Lu, K.; Micheroni, D.; Hu, A.; Lin, W.: Nanoscale metal–organic frameworks for ratiometric oxygen sensing in live cells. J. Am. Chem. Soc. **138** (2016) 2158–2161.
8. Lin, G.; Ding, H.; Yuan, D.; Wang, B.; Wang, C.: A pyrene-based, fluorescent three-dimensional covalent organic framework. J. Am. Chem. Soc. **138** (2016) 3302–3305.
9. Ma, L.-F.; Shi, Z.-Z.; Li, F.-F.; Zhang, J.; Wang, L.-Y.: Coordination polymers with free Bronsted acid sites for selective catalysis. New J. Chem. **39** (2015) 810–812.
10. Liu, L.-L.; Yu, C.-X.; Li, Y.-R.; Han, J.-J.; Ma, F.-J.; Ma, L.-F.: Positional isomeric effect on the structural variation of Cd(II) coordination polymers based on flexible linear/V-shaped bipyridyl benzene ligands. CrystEngComm **17** (2015) 653–664.
11. Chang, X. H.; Han, M. L.: A Cu(II) coordination polymer with -tert-butyl isophthalate linker: synthesis, crystal structure, and magnetic properties. Chinese J. Struct. Chem. **34** (2015) 1895–1900.
12. Dong, W.-W.; Li, D.-S.; Zhao, J.; Ma, L.-F.; Wu, Y.-P.; Duan, Y.-P.: Two solvent-dependent manganese(II) supramolecular isomers: solid-state transformation and magnetic properties. CrystEngComm **15** (2013) 5412–5416.
13. Sato, H.; Matsuda, R.; Mir, M. H.; Kitagawa, S.: Photochemical cycloaddition on the pore surface of a porous coordination polymer impacts the sorption behavior. Chem. Commun. **48** (2012) 7919–7921.
14. Li, C.-P.; Yu, Q.; Zhang, Z.-H.; Du, M.: Multifarious ZnII and CdII coordination frameworks constructed by a versatile trans-1-(2-pyridyl)-2-(4-pyridyl)ethylene tecton and various benzene-dicarboxyl ligands. CrystEngComm **12** (2010) 834–844.
15. Luo, F.; Wang, M. S.; Luo, M. B.; Sun, G. M.; Song, Y. M.; Li, P. X.; Guo, G. C.: Functionalizing the pore wall of chiral porous metal-organic frameworks by distinct −H, −OH, $-NH_2$, $-NO_2$, −COOH shutters showing selective adsorption of CO2, tunable photoluminescence, and direct white-light emission. Chem. Commun. **48** (2012) 5989–5991.
16. Abourahma, H.; Bodwell, G. J.; Lu, J.; Moulton, B.; Pottie, I. R.; Walsh, R. B.; Zaworotko, M. J.: Coordination polymers from calixarene-like $[Cu_2(dicarboxylate)_2]_4$ building blocks: structural diversity *via* atropisomerism. Cryst. Growth Des. **3** (2003) 513–519.
17. Dai, J. C.; Wu, X. T.; Fu, Z. Y.; Cui, C. P.; Hu, S. M.; Du, W. X.; Wu, L. M.; Zhang, H. H.; Sun, R. Q.: Synthesis, structure, and fluorescence of the novel Cadmium(II)-trimesate coordination polymers with different coordination architectures. Inorg. Chem. **41** (2002) 1391–1396.