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Crystal structure of *catena*-poly[triaqua-(μ_2 -1,4-di(pyridin-4-yl)benzene- $\kappa^2N:N'$)-(3',5-dicarboxy-[1,1'-biphenyl]-3,4'-dicarboxylato- κO)nickel(II)], $C_{32}H_{26}N_2O_{11}Ni$

$V = 2819.4(3) \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.0571$, $wR_{\text{ref}}(F^2) = 0.1285$, $T = 293(2) \text{ K}$.

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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:	Green block
Size:	$0.43 \times 0.35 \times 0.24 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	0.76 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	25.5° , 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	14931, 5148, 0.062
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3922
$N(\text{param})_{\text{refined}}$:	420
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

A mixture of $Ni(\text{OAc})_2 \cdot 4\text{H}_2\text{O}$ (0.1 mmol, 0.0248 g), 1,4-di(pyridin-4-yl)benzene (0.2 mmol, 0.015 g) and 3,3',4,4'-biphenyl tetracarboxylic acid (H_4btc) (0.1 mmol, 0.0330 g), was dissolved in 10 mL H_2O . The solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 383 K for five days. After cooling to room temperature crystals formed. The green crystals were collected.

Experimental details

Coordinates of hydrogen atoms were positioned according to geometric considerations.

Comment

In the last decades, a large number of mixed ligands metal-organic frameworks (MOFs) have been reported. Mixed ligands-MOFs can be constructed from metal ions and carboxylic acid and nitrogen-containing ligands. In most situations, N-containing ligands are electrically neutral, while carboxylate ligands are negatively charged. Among organic aromatic multicarboxylates like the biphenyl-tetracates can yield predetermined networks and have been widely utilized

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Abstract

$C_{32}H_{26}N_2O_{11}Ni$, monoclinic, $P2_1/c$ (no. 19), $a = 7.6085(5) \text{ \AA}$, $b = 23.5084(14) \text{ \AA}$, $c = 15.8052(9) \text{ \AA}$, $\beta = 94.207(6)^\circ$,

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Ni1	0.82166(6)	0.743933(18)	0.43306(3)	0.02666(17)
N1	0.8342(4)	0.67566(12)	0.51877(17)	0.0261(7)
N2	1.1080(4)	0.30843(12)	0.97874(19)	0.0306(7)
O1	1.0830(4)	0.72959(12)	0.40339(18)	0.0486(8)
H1A	1.1327	0.7398	0.3629	0.073*
H1B	1.1612	0.7108	0.4426	0.073*
O2	0.5560(3)	0.75826(11)	0.44906(18)	0.0440(7)
H2A	0.4820	0.7895	0.4652	0.066*
H2B	0.4862	0.7263	0.4595	0.066*
O3	0.6574(4)	0.73670(11)	0.23195(17)	0.0450(8)
O4	0.7385(4)	0.68465(10)	0.34556(16)	0.0374(7)
O5	0.3512(4)	0.63898(11)	−0.01313(18)	0.0498(8)
H5	0.2919	0.6369	−0.0585	0.075*
O6	0.2957(4)	0.54653(12)	−0.01021(18)	0.0493(8)
O7	0.8218(4)	0.34525(12)	0.16437(17)	0.0456(8)
O8	0.7549(5)	0.28274(13)	0.2576(2)	0.0749(11)
H8	0.688(8)	0.278(3)	0.325(4)	0.11(2)*
O9	0.6674(4)	0.27825(13)	0.3991(2)	0.0635(9)
O10	0.6642(4)	0.33570(13)	0.5067(2)	0.0583(9)
O11	0.8097(3)	0.80557(10)	0.34008(15)	0.0350(6)
H11A	0.9021	0.8205	0.3255	0.053*
H11B	0.7665	0.7892	0.2864	0.053*
C1	0.7739(5)	0.67724(15)	0.5960(2)	0.0273(8)
H1	0.7236	0.7109	0.6133	0.033*
C2	0.7816(5)	0.63232(14)	0.6511(2)	0.0273(8)
H2	0.7359	0.6360	0.7038	0.033*
C3	0.8574(4)	0.58111(14)	0.6289(2)	0.0256(8)
C4	0.9152(5)	0.57915(15)	0.5474(2)	0.0351(10)
H4	0.9633	0.5457	0.5277	0.042*
C5	0.9017(5)	0.62614(15)	0.4958(2)	0.0328(9)
H5A	0.9419	0.6233	0.4418	0.039*
C6	0.8807(4)	0.53286(14)	0.6886(2)	0.0258(8)
C7	0.9127(5)	0.54280(15)	0.7753(2)	0.0307(9)
H7	0.9076	0.5798	0.7956	0.037*
C8	0.9516(5)	0.49941(15)	0.8312(2)	0.0318(9)
H8A	0.9736	0.5077	0.8886	0.038*
C9	0.9587(5)	0.44313(15)	0.8042(2)	0.0273(8)
C10	0.9195(5)	0.43294(15)	0.7182(2)	0.0334(9)
H10	0.9183	0.3957	0.6983	0.040*
C11	0.8823(5)	0.47668(15)	0.6616(2)	0.0345(9)
H11	0.8578	0.4684	0.6044	0.041*
C12	1.0082(5)	0.39656(14)	0.8643(2)	0.0255(8)
C13	1.1129(5)	0.40652(15)	0.9389(2)	0.0341(9)
H13	1.1518	0.4432	0.9521	0.041*
C14	1.1586(5)	0.36242(16)	0.9929(2)	0.0344(9)
H14	1.2287	0.3704	1.0421	0.041*
C15	1.0092(5)	0.29924(16)	0.9070(3)	0.0358(10)
H15	0.9732	0.2621	0.8949	0.043*
C16	0.9570(5)	0.34108(16)	0.8496(2)	0.0343(9)
H16	0.8869	0.3318	0.8009	0.041*
C17	0.5957(5)	0.63822(14)	0.2290(2)	0.0253(8)
C18	0.6210(5)	0.58638(15)	0.2704(2)	0.0295(9)
H18	0.6755	0.5858	0.3251	0.035*
C19	0.5670(4)	0.53538(14)	0.2324(2)	0.0256(8)
C20	0.4842(5)	0.53725(15)	0.1511(2)	0.0285(9)

Table 2 (continued)

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
H20	0.4488	0.5035	0.1242	0.034*
C21	0.4535(5)	0.58883(15)	0.1094(2)	0.0264(8)
C22	0.5099(5)	0.63900(15)	0.1486(2)	0.0283(9)
H22	0.4900	0.6735	0.1207	0.034*
C23	0.5979(5)	0.48148(15)	0.2792(2)	0.0284(8)
C24	0.5803(5)	0.47910(16)	0.3661(2)	0.0343(9)
H24	0.5485	0.5117	0.3947	0.041*
C25	0.6094(5)	0.42937(16)	0.4101(2)	0.0361(10)
H25	0.5963	0.4290	0.4682	0.043*
C26	0.6576(5)	0.37951(16)	0.3710(2)	0.0320(9)
C27	0.6847(5)	0.38116(15)	0.2836(2)	0.0293(9)
C28	0.6531(4)	0.43184(15)	0.2406(2)	0.0298(9)
H28	0.6695	0.4329	0.1829	0.036*
C29	0.6683(5)	0.69107(15)	0.2721(2)	0.0286(9)
C30	0.6670(5)	0.32859(19)	0.4297(3)	0.0447(11)
C31	0.7569(5)	0.33366(17)	0.2317(3)	0.0397(10)
C32	0.3598(5)	0.58786(16)	0.0236(2)	0.0300(9)

[4, 5]. On the other hand, 1,4-di(pyridin-4-yl)benzene serves as bridging ligand [6, 7].

In the title complex, there is one Ni(II) ion, three coordinated water molecules, one H2btc ligand, and one 1,4-di(pyridin-4-yl)benzene ligand in the asymmetric unit. Ni(1) is six-coordinated with a distorted octahedral geometry by four O atoms from one H4btc and three coordinated water molecules, and two N atoms from two 1,4-di(pyridin-4-yl)benzene ligands from the axial positions (see the figure). The Ni—N bond lengths are 2.098(3) Å and 2.102(3) Å, whereas the Ni—O ones are in the range of 2.031(2) to 2.103(3) Å. The bond angles of O—Ni—O are in the range of 86.40(11)°–174.12(11)°.

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