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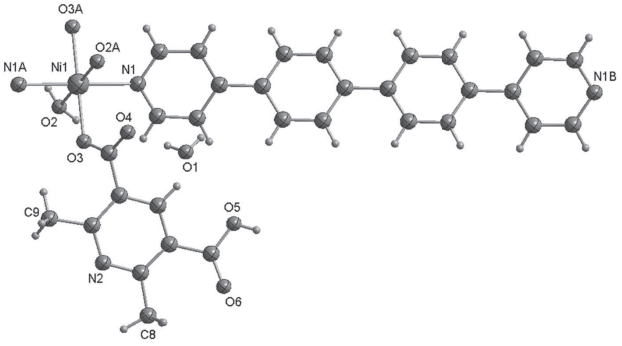
Crystal structure of catena-poly[diaqua-μ_2-4,4′-biphenyl-4,4′-diyldipyridine-κ^2*N*:*N*′-bis(5-carboxy-2,6-dimethylpyridine-3-carboxylato-κ*O*)nickel(II)] dihydrate, $C_{40}H_{40}N_4O_{12}Ni$



DOI 10.1515/ncrs-2015-0066
Received November 6, 2015; accepted January 12, 2016; available online February 12, 2016

Abstract

$C_{40}H_{40}N_4O_{12}Ni$, triclinic, $P\bar{1}$, $a = 7.6612(6)$ Å, $b = 8.0725(7)$ Å, $c = 16.3021(10)$ Å, $\alpha = 89.394(6)°$, $\beta = 77.966(6)°$, $\gamma = 69.868(8)°$, $V = 923.75(12)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0492$, $wR_{ref}(F^2) = 0.1309$, $T = 293(2)$ K.

CCDC no.: 1446735

The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of $Ni(OAc)_2{\cdot}4H_2O$ (0.1 mmol, 0.0248 g), 4,4′-bis(pyrid-4-yl)biphenyl (0.1 mmol, 0.0308 g), 2,6-dimethylpyridine-3,5-dicarboxylic acid (0.1 mmol, 0.0195 g) was dissolved in 10 mL H_2O. Then the solution was heated in a 25 mL Teflon-lined autoclave under autogenous pressure at 403 K for four days. After cooling to room temperature, the green block crystals that formed were collected.

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.28×0.38×0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	5.98 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	50.98°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7301, 3429
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2864
$N(param)_{refined}$:	262
Programs:	SHELX [7]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	2*i*	0.9911	0.4555	0.1553	0.058
H(2W)	2*i*	0.8549	0.4290	0.1971	0.058
H(3W)	2*i*	1.0596	1.2716	−0.0027	0.049
H(4W)	2*i*	1.0636	1.2446	0.0869	0.049
H(5)	2*i*	0.9108	0.5763	0.4480	0.084
H(3)	2*i*	1.0393	0.6568	0.2614	0.038
H(8A)	2*i*	1.7085	0.4441	0.3420	0.076
H(8B)	2*i*	1.5682	0.3503	0.3852	0.076
H(8C)	2*i*	1.5328	0.5462	0.4137	0.076
H(9A)	2*i*	1.6865	0.6570	0.0902	0.070
H(9B)	2*i*	1.5216	0.6735	0.0441	0.070
H(9C)	2*i*	1.6638	0.4864	0.0561	0.070
H(10)	2*i*	0.5702	1.0903	0.0518	0.045
H(11)	2*i*	0.3382	1.0889	0.1629	0.049
H(13)	2*i*	0.7110	1.0194	0.3101	0.042
H(14)	2*i*	0.9305	1.0331	0.1949	0.039
H(16)	2*i*	0.1183	1.1860	0.2848	0.054
H(17)	2*i*	−0.1044	1.1607	0.3971	0.055
H(19)	2*i*	0.3073	0.8639	0.5047	0.061
H(20)	2*i*	0.5305	0.8876	0.3922	0.060

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Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	2*a*	1.0	1.0	0.0	0.0213(3)	0.0339(3)	0.0223(3)	−0.0088(2)	−0.0027(2)	0.0070(2)
O(1)	2*i*	0.9635(3)	0.3747(3)	0.1830(1)	0.036(1)	0.039(1)	0.039(1)	−0.011(1)	−0.006(1)	0.009(1)
O(2)	2*i*	1.0938(3)	1.1959(3)	0.0310(1)	0.034(1)	0.038(1)	0.028(1)	−0.014(1)	−0.008(1)	0.0082(9)
O(3)	2*i*	1.1902(3)	0.8363(3)	0.0662(1)	0.026(1)	0.040(1)	0.029(1)	−0.0110(9)	−0.0047(9)	0.013(1)
O(4)	2*i*	1.0513(4)	0.6355(3)	0.0961(2)	0.046(2)	0.050(1)	0.038(1)	−0.027(1)	−0.018(1)	0.018(1)
O(5)	2*i*	0.9643(4)	0.6075(4)	0.4049(2)	0.033(2)	0.096(2)	0.035(2)	−0.019(1)	−0.004(1)	0.025(1)
O(6)	2*i*	1.2197(4)	0.4753(4)	0.4569(2)	0.043(2)	0.101(2)	0.032(2)	−0.027(2)	−0.011(1)	0.032(2)
N(1)	2*i*	0.7781(4)	1.0544(3)	0.1104(2)	0.024(1)	0.038(2)	0.029(1)	−0.010(1)	−0.002(1)	0.007(1)
N(2)	2*i*	1.5581(4)	0.5387(4)	0.2259(2)	0.028(2)	0.046(2)	0.030(2)	−0.009(1)	−0.006(1)	0.010(1)
C(1)	2*i*	1.4694(4)	0.5986(4)	0.1629(2)	0.025(2)	0.038(2)	0.026(2)	−0.009(1)	−0.002(1)	0.007(1)
C(2)	2*i*	1.2713(4)	0.6462(4)	0.1743(2)	0.027(2)	0.032(2)	0.024(2)	−0.009(1)	−0.005(1)	0.006(1)
C(3)	2*i*	1.1705(5)	0.6283(4)	0.2524(2)	0.027(2)	0.037(2)	0.028(2)	−0.010(1)	−0.003(1)	0.006(1)
C(4)	2*i*	1.2619(5)	0.5684(4)	0.3177(2)	0.031(2)	0.039(2)	0.025(2)	−0.011(1)	−0.005(1)	0.008(1)
C(5)	2*i*	1.4595(5)	0.5253(4)	0.3025(2)	0.033(2)	0.042(2)	0.027(2)	−0.009(1)	−0.008(1)	0.007(1)
C(6)	2*i*	1.1487(5)	0.5461(5)	0.3994(2)	0.035(2)	0.054(2)	0.025(2)	−0.016(2)	−0.005(2)	0.009(2)
C(7)	2*i*	1.1640(4)	0.7097(4)	0.1059(2)	0.023(2)	0.034(2)	0.022(2)	−0.003(1)	−0.000(1)	0.006(1)
C(8)	2*i*	1.5779(5)	0.4607(6)	0.3666(2)	0.032(2)	0.080(3)	0.035(2)	−0.010(2)	−0.012(2)	0.017(2)
C(9)	2*i*	1.5966(5)	0.6044(6)	0.0810(2)	0.030(2)	0.073(3)	0.033(2)	−0.015(2)	−0.003(2)	0.016(2)
C(10)	2*i*	0.5997(5)	1.0746(5)	0.1045(2)	0.030(2)	0.054(2)	0.027(2)	−0.014(2)	−0.006(1)	0.011(2)
C(11)	2*i*	0.4592(5)	1.0736(5)	0.1711(2)	0.023(2)	0.063(2)	0.032(2)	−0.013(2)	−0.003(1)	0.011(2)
C(12)	2*i*	0.4955(5)	1.0498(4)	0.2510(2)	0.028(2)	0.034(2)	0.030(2)	−0.010(1)	−0.001(1)	0.004(1)
C(13)	2*i*	0.6784(5)	1.0340(4)	0.2580(2)	0.029(2)	0.047(2)	0.025(2)	−0.012(1)	−0.001(1)	0.002(1)
C(14)	2*i*	0.8109(5)	1.0397(4)	0.1879(2)	0.025(2)	0.044(2)	0.028(2)	−0.013(1)	−0.002(1)	0.001(1)
C(15)	2*i*	0.3506(5)	1.0380(4)	0.3247(2)	0.027(2)	0.037(2)	0.027(2)	−0.009(1)	0.000(1)	0.004(1)
C(16)	2*i*	0.1585(5)	1.1195(5)	0.3287(2)	0.029(2)	0.066(2)	0.034(2)	−0.011(2)	−0.002(2)	0.021(2)
C(17)	2*i*	0.0240(5)	1.1042(5)	0.3968(2)	0.021(2)	0.069(2)	0.039(2)	−0.007(2)	−0.003(2)	0.022(2)
C(18)	2*i*	0.0729(4)	1.0088(4)	0.4638(2)	0.026(2)	0.039(2)	0.026(2)	−0.008(1)	0.002(1)	0.004(1)
C(19)	2*i*	0.2673(5)	0.9286(6)	0.4603(2)	0.028(2)	0.076(3)	0.037(2)	−0.008(2)	−0.001(2)	0.031(2)
C(20)	2*i*	0.4020(5)	0.9431(6)	0.3924(2)	0.022(2)	0.073(3)	0.043(2)	−0.005(2)	−0.000(2)	0.024(2)

Discussion

In recent years, research on coordination complexes has made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and applications, such as gas storage [1], catalysis [2], magnetism [3] and luminescence [4]. Studies in this field have been focused on the rational design and synthesis of novel frameworks and the relationships between their structures and properties. The observation of coordination complexes constructed from organic ligands and metal ions through a self-assembly route has been explored intensively, and many efforts have been devoted to use of N- and O-donor organic ligands as co-ligands to bridge metal ions to form infinite network structures [5]. However, it is still a great challenge in crystal engineering to obtain designed and predictable frameworks with potential properties assembled by coordination bonds and/or weak supramolecular interactions such as hydrogen bonds, π–π stacking, and host–guest ionic interactions, etc. [6].

The asymmetric unit of the title structure contains one half of a Ni(II) ion, one half of a 4,4′-bis(pyrid-4-yl)biphenyl and one 2,6-dimethyl-pyridine-3,5-dicarboxylate anion as well as one coordinated and one uncoordinated water molecule. The dipyridyl ligand connects nickel atoms to a chain structure (see the figure). The nickel atom is six-coordinated by two oxygen atoms from two 2,6-dimethyl-pyridine-3,5-dicarboxylate ligands, by two nitrogen atom from 4,4′-bis(pyrid-4-yl)biphenyl ligands and two water ligands. The Ni—O bond lengths range from 2.055(2)–2.081(2) Å, the Ni—N bond lengths is 2.132(3) Å. The bond angles of O—Ni—O are in the range of 86.06(8)° to 180°. There are intern molecular hydrogen bonds between coordinated and uncoordinated water molecules (d(O(2)—H(4W)$\cdots$O(1)#4) = 2.696(3) Å). Water molecules are connected with adjacent 4,4′-bis(pyrid-4-yl)biphenyl ligands and 2,6-dimethyl-pyridine-3,5-dicarboxylate anions by further hydrogen bonds (d(O(1)—H(1W)$\cdots$O(4)) = 2.721(3) Å, d(O(1)—H(2W)$\cdots$N(2)#3) = 2.859(4) Å, d(O(2)—H(3W)$\cdots$O(4)#1) = 2.691(3) Å), d(O(5)—H(5)$\cdots$O(6)#5) = 2.608(4) Å). Symmetry

codes: #1 $-x+2$, $-y+2$, $-z$; #3 $x-1$, y, z; #4 x, $y+1$, z; #5 $-x+2$, $-y+1$, $-z+1$.

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