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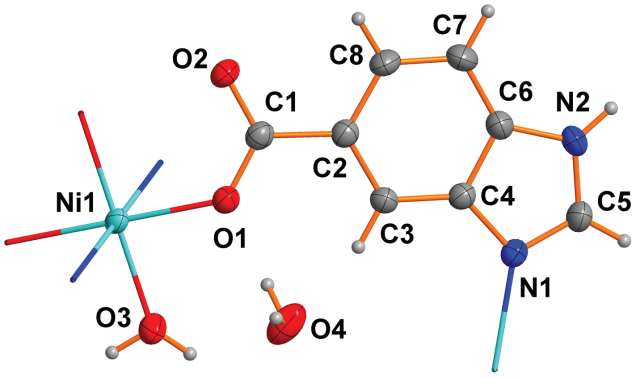
Crystal structure of *catena*-poly[diaqua-bis (μ_2-1*H*-benzo[*d*]imidazole-5-carboxylato-κ^2*N*:*O*) nickel(II)] dihydrate, $C_{16}H_{18}N_4NiO_8$



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Abstract

$C_{16}H_{18}N_4NiO_8$, monoclinic, $C2/c$ (no. 15), $a = 16.1598(8)$ Å, $b = 8.7803(5)$ Å, $c = 14.1809(11)$ Å, $\beta = 118.197(1)°$, $V = 1773.32(19)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0220$, $wR_{ref}(F^2) = 0.0598$, $T = 273(2)$ K.

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A part of the title crystal structure 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

A solution of 1*H*-benzo[*d*]imidazole-5-carboxylic acid (HL, 0.10 mmol) in MeOH (5 mL) was neutralized by NaOH and carefully layered on a solution of $NiBr_2$ (0.10 mmol) in H_2O (5 mL). Diffusion between the two phases over a period of 2 weeks produced lighted yellow block crystals (Yield 46% based on HL).

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.38 × 0.26 × 0.20 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.15 mm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4327, 1568, 0.016
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1474
$N(param)_{refined}$:	133
Programs:	Bruker programs [1], SHELX [2, 3]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0000	1.0000	0.0000	0.02092(11)
O1	0.09367(8)	0.93388(12)	0.16166(8)	0.0272(2)
O2	0.16481(8)	0.72938(13)	0.14089(9)	0.0324(3)
O3	−0.07765(8)	1.13558(13)	0.05024(9)	0.0340(3)
H9	−0.1123	1.1915	−0.0028	0.051*
H10	−0.0999	1.1414	0.0938	0.051*
C1	0.13350(10)	0.80590(17)	0.19249(12)	0.0243(3)
C3	0.10419(10)	0.81796(17)	0.34983(12)	0.0240(3)
H3	0.0768	0.9132	0.3269	0.029*
C2	0.14242(10)	0.74053(17)	0.29469(12)	0.0244(3)
C4	0.10743(10)	0.75090(17)	0.43998(12)	0.0233(3)
C6	0.14652(11)	0.60571(18)	0.47196(12)	0.0269(3)
C7	0.18671(13)	0.52743(19)	0.41909(14)	0.0337(4)
H7	0.2140	0.4322	0.4422	0.040*
C5	0.08998(11)	0.68848(18)	0.57616(12)	0.0291(3)
H5	0.0734	0.6907	0.6306	0.035*
C8	0.18462(12)	0.59641(19)	0.33101(13)	0.0308(4)
H8	0.2117	0.5470	0.2943	0.037*
N1	0.07270(9)	0.80092(15)	0.50807(10)	0.0261(3)
N2	0.13392(10)	0.57039(16)	0.55931(11)	0.0313(3)
H2	0.1511	0.4877	0.5961	0.038*
O4	0.85326(10)	0.16957(16)	0.19135(11)	0.0485(4)
H11	0.8666	0.0973	0.2361	0.073*
H12	0.7999	0.2018	0.1806	0.073*

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Experimental details

All H atoms were placed geometrically and treated as riding on their parent atoms, with C—H 0.96, with $U_{iso}(H) = 1.5U_{eq}(C)$.

Discussion

The understanding of various molecular interactions plays a major role in supramolecular chemistry and crystal engineering. The knowledge of structural motifs generated by such interactions can be utilized in the design of novel materials with desirable physical and chemical properties. Hydrogen bonding and π–π stacking interactions are by far the most well-studied interactions. These interactions are employed to control the conformational and topological features of the molecular assembly in the solid state [e.g. 4, 5]. In the last decade, benzimidazole-5-carboxylic acid (HL) was widely used in the design of therapeutic agents, such as diuretic and natriureitc, antiparasitic, serotonin antagonist, antineoplastic and antiflarial, herbicidal, and antihypertensive compounds. The analysis of various interactions in drugs has attracted considerable interest for their wide-ranging antiviral activity and the possibiligy of forming supramolecular aggregates with transition-metal ions. However, to the best of our knowledge, up to now few of attention has been attached on the coordination behavior of benzimidazole-5-carboxylic acid(HL) [6–8].

As shown in the figure, the Ni ion lies in a slightly distorted environment, consisting of two oxygen donors from two carboxylate groups, two oxygen atoms from two water ligands, and two benzimidazole nitrogen atoms from two ligands. The adjacent Ni ions are linked by the 1*H*-benzo[*d*]imidazole-5-carboxylato ligands to form a 1D chain through. The adjacent 1D chains are linked to a network through hydrogen bonds.

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