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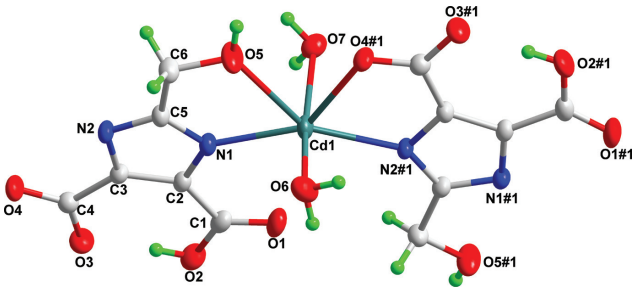
Crystal structure of *catena*-poly[diaqua(μ_2-2-(hydroxymethyl)-1*H*-imidazole-4,5-dicarboxylato) cadmium(II)], $C_6H_8CdN_2O_7$



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Abstract

$C_6H_8CdN_2O_7$, monoclinic, $P2_1/c$ (no. 14), $a = 7.3428(15)$ Å, $b = 11.272(2)$ Å, $c = 12.764(4)$ Å, $\beta = 118.73(2)°$, $V = 926.4(4)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0261$, $wR_{ref}(F^2) = 0.0609$, $T = 293(2)$ K.

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A part of the molecular structure is shown in the figure (#1 = x, 1.5 − y, 0.5 + z). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All chemical reagents were of analytical purity grade and used without further purification. A mixture of $Cd(NO_3)_2 \cdot 4H_2O$ (0.1 mmol), H_4hmIDC (0.1 mmol), methanol (2 mL) and distilled water (2 mL) was sealed in a 25 mL stainless steel container and heated at 393 K for 72 h. After the mixture had been allowed to cool to room temperature at a rate of 5 K h^{-1}, light yellow crystals of $Cd(H_2hmIDC)(H_2O)_2$ were obtained (yield 49%, based on Cd).

Table 1: Data collection and handling.

Crystal:	Yellow prism
Size:	0.21 × 0.20 × 0.18 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.38 mm^{-1}
Diffractometer, scan mode:	Rigaku Saturn, ω
θ_{max}, completeness:	28.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11145, 2218, 0.023
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2179
$N(param)_{refined}$:	146
Programs:	Rigaku [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}
Cd1	0.76875(3)	0.68699(2)	0.60990(2)	0.02556(8)
N1	0.7686(4)	0.7849(2)	0.46006(19)	0.0229(4)
N2	0.7648(4)	0.80884(18)	0.28531(19)	0.0219(4)
O1	0.7577(3)	0.9575(2)	0.61427(17)	0.0374(5)
O2	0.7387(4)	1.10193(18)	0.49297(19)	0.0351(5)
H2	0.7307	1.1083	0.4269	0.042*
O3	0.7292(4)	1.12567(17)	0.29964(19)	0.0335(5)
O4	0.7522(3)	1.01189(17)	0.16483(17)	0.0294(4)
O5	0.7598(4)	0.54989(19)	0.4501(2)	0.0448(6)
H5A	0.7379	0.4788	0.4359	0.054*
O6	1.1297(3)	0.6522(2)	0.7099(2)	0.0383(5)
H1W	1.1674	0.7167	0.7491	0.046*
H2W	1.1516	0.6036	0.7657	0.046*
O7	0.4021(3)	0.67143(17)	0.51172(19)	0.0321(5)
H3W	0.3730	0.7423	0.4861	0.039*
H4W	0.3657	0.6347	0.4465	0.039*
C1	0.7494(4)	0.9896(3)	0.5212(2)	0.0263(5)
C2	0.7543(4)	0.9035(2)	0.4361(2)	0.0218(5)
C3	0.7518(4)	0.9184(2)	0.3279(2)	0.0210(5)
C4	0.7445(4)	1.0247(2)	0.2591(2)	0.0239(5)
C5	0.7736(4)	0.7328(2)	0.3676(2)	0.0225(5)
C6	0.7877(5)	0.6018(2)	0.3587(3)	0.0281(6)
H6A	0.6813	0.5742	0.2813	0.034*
H6B	0.9224	0.5802	0.3677	0.034*

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Experimental details

Hydrogen atoms on carbon atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97 Å. Hydrogen atoms of the nondeprotonated carboxylic acid groups of H_2hmIDC^{2-} and hydroxyl groups (—OH) were refined as riding atoms, with O—H = 0.82 Å. Hydrogen atoms of the water molecules were located in a difference Fourier map and the O—H distance constrained to 0.85 Å.

Comment

N-heterocyclic carboxylic acids have been widely used as ligands since they can offer different donors and diverse coordination modes due to the existence of carboxylate groups as well as potential *N*-donors. So far, complexes with various topologies and potential applications have been synthesized [4–9]. *N*-heterocyclic carboxylic acid, 2-(hydroxymethyl)-1*H*-imidazole-4,5-dicarboxylic acid (H_4hmIDC) is a good linker since it has two potential *N*-donors and five potential *O*-donors and can coordinate to almost all soft and hard metal ions with various coordination modes. Up to now, several complexes based on H_xhmIDC ligand have been reported [6, 7, 10–12].

The asymmetric unit of the title structure consists of one Cd(II) cation, one dianionic H_2hmIDC^{2-} ligand and two coordinating water molecules. Each Cd1 ion is six-coordinated and located in a distorted octahedral CdN_2O_4 coordination environment formed by two N atoms (N1 and N2#1) and two O atoms (O4#1 and O5) from two H_2hmIDC^{2-} anions and by two water molecules (O6 and O7). The Cd—O bond lengths range from 2.357(2) to 2.535(2) Å and the Cd—N bond lengths are 2.207(2) and 2.254(2) Å, respectively; these values are within the normal ranges and close to those reported in other Cd(II) complexes [13–15]. Cd(II) ions are linked by H_2hmIDC^{2-} ligand into one-dimensional chains that run along the *c* axis. The intra-chain Cd(II)—Cd(II) distance is 6.538(2) Å. In addition, there are O—H···O intramolecular hydrogen bonds between carboxyl and carboxylate groups, and five O—H···O intermolecular hydrogen bonds involving hydroxyl groups, carboxyl groups, carboxylate groups and water molecules. Adjacent chains are linked by the hydrogen bonds mentioned above, leading to a three-dimensional network.

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