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Synthesis and crystal structure of *catena*-poly [aqua-bis(nitrato- κ^2 O:O')- (μ_2 -((1 *H*-imidazol-1-yl) methyl)benzene- κ^2 N,N')-H₂O- κ^2 O]cadmium(II), C₁₄H₁₆N₆O₇Cd

<https://doi.org/10.1515/ncrs-2020-0619>

Received December 3, 2020; accepted January 22, 2021;
published online February 11, 2021

Abstract

C₁₄H₁₆N₆O₇Cd, monoclinic, *P*₂/c (no. 14), *a* = 12.7095(3) Å, *b* = 17.4705(4) Å, *c* = 8.5763(3) Å, β = 93.292(10)°, *Z* = 4, *V* = 1901.15(9) Å³, *R*_{gt}(*F*) = 0.0263, *wR*_{ref}(*F*²) = 0.1047, *T* = 296(2) K.

CCDC no.: 2046019

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.18 × 0.14 × 0.12 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	1.20 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ _{max} , completeness:	27.5°, 99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	17257, 4347, 0.028
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 3836
<i>N</i> (<i>param</i>) _{refined} :	255
Programs:	Bruker [1], SHELX [2], Olex2 [3], Diamond [4]

Source of material

All solvents and other reagents were of analytical grade. The method of synthesizing the title complex has been improved [5–8]. A mixture of cadmium nitrate, 1,4-bis(1 *H*-imidazol-1-yl)methylbenzene and water was introduced into a 25 mL Teflon lined reactor autoclave and heated to 115 °C for three days. After cooling to room temperature, colourless block crystals were obtained. **Elemental analysis**—Anal. Calcd. for C₁₄H₁₆N₆O₇Cd: C, 34.13%; H, 3.27%; N, 17.06%. Found: C, 34.19%; H, 3.31%; N, 16.98%.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.9029 (3)	0.85918 (17)	0.5993 (4)	0.0453 (7)
H1A	0.864663	0.902448	0.638863	0.054*
H1B	0.946804	0.837953	0.684911	0.054*
C2	0.8260 (2)	0.79944 (15)	0.5373 (4)	0.0380 (6)
C3	0.6887 (2)	0.68823 (14)	0.4117 (3)	0.0361 (6)
C4	0.7297 (2)	0.82056 (15)	0.4654 (4)	0.0435 (7)
H4	0.710885	0.871952	0.458652	0.052*
C5	0.7850 (2)	0.66764 (14)	0.4814 (4)	0.0429 (7)
H5	0.804352	0.616325	0.486235	0.051*
C6	0.85326 (19)	0.72311 (16)	0.5444 (4)	0.0447 (7)
H6	0.917875	0.708625	0.591684	0.054*
C7	0.6619 (2)	0.76522 (15)	0.4040 (4)	0.0429 (6)
H7	0.597279	0.779698	0.356769	0.051*
C8	0.6107 (3)	0.62868 (14)	0.3551 (4)	0.0416 (7)
H8A	0.566469	0.648854	0.268751	0.050*
H8B	0.647602	0.584172	0.318381	0.050*
C9	0.4474 (2)	0.63175 (13)	0.5052 (4)	0.0344 (6)
H9	0.408295	0.662706	0.435260	0.041*
C10	0.57615 (18)	0.56456 (13)	0.6113 (3)	0.0348 (5)
H10	0.640917	0.540456	0.629791	0.042*
C11	0.49548 (19)	0.56439 (13)	0.7059 (3)	0.0334 (5)
H11	0.494907	0.539529	0.801777	0.040*
C12	1.02184 (19)	0.93879 (14)	0.2643 (4)	0.0394 (6)
H12	1.024478	0.969607	0.176239	0.047*
C13	0.9418 (2)	0.93711 (15)	0.3623 (4)	0.0429 (6)
H13	0.880219	0.965937	0.354111	0.052*
C14	1.0629 (2)	0.85634 (16)	0.4435 (4)	0.0377 (6)
H14	1.098792	0.819168	0.503194	0.045*
Cd1	0.25711 (2)	0.62897 (2)	0.72705 (2)	0.02835 (10)
N1	0.41389 (16)	0.60684 (12)	0.6385 (3)	0.0321 (4)
N2	0.54515 (16)	0.60664 (12)	0.4835 (3)	0.0321 (4)
N3	0.96953 (18)	0.88494 (13)	0.4746 (3)	0.0364 (5)
N4	1.09821 (17)	0.88791 (13)	0.3157 (3)	0.0355 (5)
N5	0.3246 (2)	0.57681 (15)	1.0379 (3)	0.0462 (6)
N6	0.16370 (18)	0.59363 (14)	0.4187 (3)	0.0400 (5)
O1	0.32005 (17)	0.64621 (12)	0.9937 (3)	0.0421 (5)
O2	0.30656 (17)	0.52576 (11)	0.9374 (3)	0.0518 (5)
O3	0.3462 (3)	0.56272 (18)	1.1748 (3)	0.1005 (12)
O4	0.18826 (16)	0.66020 (10)	0.4704 (2)	0.0397 (4)
O5	0.18496 (17)	0.53760 (11)	0.5036 (3)	0.0452 (5)
O6	0.1208 (2)	0.58865 (16)	0.2886 (3)	0.0815 (9)
O7	0.27372 (17)	0.75953 (12)	0.7364 (2)	0.0565 (6)
H7A	0.231101	0.783424	0.812925	0.12 (2)*
H7B	0.293433	0.789077	0.645234	0.072 (12)*

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Coordination polymers (CPs) not only exhibit novel structures and topologies, but also may possess magnetic, optical and catalytic properties, etc. [9–14]. Organic ligands are important for constructing CPs, and flexible ligands have different conformations and can be used to construct CPs with different structures.

In this work, we used ((1 *H*-imidazol-1-yl)methyl)benzene (L_1) as a flexible ligand, assembling with $Cd(NO_3)_2$ to obtain a perfect 1D structure. Li et al. [15] already used the same ligand (L_1) with $Cd(NO_3)_2$ obtaining a 2D structure, and Xu et al. [16] used the ligand (L_1) with $Cd(NO_3)_2$ obtaining a 3D 2-fold interpenetrating structure. It can be seen that L_1 forms different structures at different temperatures and solvents.

The crystal structure shows that the title complex consists of one Cd(II) atom, one L_1 ligand, two nitrate anions and one coordinated water molecule. The Cd(II) atom is seven-coordinated with two nitrogen atoms (N1 and N4) from two L_1 ligands four oxygen atoms (O1, O2, O4 and O5) from two nitrate ions and one oxygen atom (O7) from coordinated water. In the structure, Cd(II) is bridged by L_1 ligands, forming a one-dimensional chain. Bond lengths and angles are all in the expected ranges [15–18].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: The research was financially supported by the Young Teacher Foundation of Lanzhou City University (LZCU-QN2017-17), the Young Teacher Foundation of Lanzhou City University (LZCU-QN2017-23), the Doctoral Research Initiation Fund (LZCU-BS2018-02), the Higher Education Research Project of Gansu Province (2019B-171).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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