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**Synthesis and crystal structure of poly[(μ_2 -nitrato- $\kappa^4 O, O':O', O''$)-nitrato- κO -(μ_2 -1,4-bis((1*H*-imidazol-1-yl)methyl)benzene- $\kappa^2 N:N'$)cadmium(II)],
 $C_{14}H_{14}N_6O_6Cd$**

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Abstract

$C_{14}H_{14}CdN_6O_6$, monoclinic, $P2_1/c$ (no. 14), $a = 11.2983(5)$ Å, $b = 9.2539(4)$ Å, $c = 17.0604(7)$ Å, $\beta = 105.398(1)^\circ$, $Z = 4$, $V = 1719.69(13)$ Å³, $R_{gt}(F) = 0.0321$, $wR_{ref}(F^2) = 0.1060$, $T = 193(2)$ K.

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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 materials

All solvents and other reagents were of analytical grade. The method of synthesizing the title compound has been improved [4]. A mixture of cadmium nitrate, 1,4-bis(1*H*-imidazol-1-yl)methylbenzene and water was introduced into a 25 mL Teflon reactor autoclave and heated to 130 °C for 3 days. After cooling down to room temperature, colourless block crystals suitable for single crystal X-ray crystallographic analysis were obtained. Elemental analysis-*Anal.*

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.19 × 0.18 × 0.13 mm
Wavelength:	Ga K α radiation (1.34139 Å)
μ :	7.09 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω -scans
θ_{max} , completeness:	53.9°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	13166, 3109, 0.062
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2989
$N(param)_{refined}$:	244
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3]

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

Atom	x	y	z	U_{iso}^*/U_{eq}
Cd1	0.52764(2)	0.38396(2)	0.30756(2)	0.03019(14)
O1	0.8422(2)	0.4108(3)	0.22148(15)	0.0548(6)
O2	0.7733(2)	0.2711(3)	0.29949(16)	0.0651(7)
O3	0.66637(16)	0.4534(2)	0.24203(12)	0.0430(4)
O4	0.50244(19)	0.1582(2)	0.23162(12)	0.0381(4)
O5	0.40642(19)	0.3261(2)	0.15234(12)	0.0451(5)
O6	0.3991(2)	0.1034(2)	0.11000(15)	0.0424(6)
N1	0.6817(2)	0.0746(3)	0.49965(14)	0.0337(5)
N2	0.58974(19)	0.2501(2)	0.41944(13)	0.0345(5)
N3	0.7624(2)	0.3769(2)	0.25472(15)	0.0358(6)
N4	0.4345(2)	0.1971(2)	0.16328(13)	0.0311(4)
N5	0.3328(2)	0.4021(2)	0.31408(16)	0.0338(5)
N6	0.16172(19)	0.4862(2)	0.33563(13)	0.0339(5)
C1	1.0928(2)	0.0670(3)	0.55878(16)	0.0366(6)
H1	1.1559	0.1133	0.5990	0.044*
C2	0.9797(3)	0.0383(3)	0.57385(16)	0.0384(6)
H2	0.9663	0.0641	0.6247	0.046*
C3	0.8869(2)	-0.0275(3)	0.51526(15)	0.0333(5)
C4	0.7624(2)	-0.0500(3)	0.52929(16)	0.0375(6)
H4A	0.7249	-0.1385	0.5007	0.045*
H4B	0.7712	-0.0635	0.5881	0.045*
C5	0.6727(3)	0.1464(3)	0.43015(18)	0.0402(6)
H5	0.7201	0.1253	0.3932	0.048*
C6	0.5985(3)	0.1348(3)	0.5354(2)	0.0386(7)
H6	0.5829	0.1062	0.5852	0.046*
C7	0.5428(2)	0.2428(3)	0.48597(15)	0.0391(6)
H7	0.4808	0.3043	0.4956	0.047*
C8	0.2771(2)	0.5164(3)	0.33535(16)	0.0373(6)
H8	0.3147	0.6082	0.3487	0.045*
C9	0.2457(3)	0.2948(3)	0.29974(17)	0.0379(6)
H9	0.2581	0.1991	0.2833	0.046*
C10	0.1405(3)	0.3446(3)	0.31235(18)	0.0401(6)
H10	0.0663	0.2922	0.3063	0.048*
C11	0.0749(3)	0.5872(3)	0.3567(2)	0.0426(6)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H11A	0.0012	0.5956	0.3101	0.051*
H11B	0.1134	0.6839	0.3669	0.051*
C12	0.0361(2)	0.5397(3)	0.43093(17)	0.0357(6)
C13	0.1223(2)	0.4932(3)	0.50065(16)	0.0398(6)
H13	0.2066	0.4889	0.5014	0.048*
C14	0.0863(2)	0.4532(3)	0.56892(17)	0.0394(6)
H14	0.1458	0.4206	0.6160	0.047*

calcd. for C₁₄H₁₄N₆O₆: C, 35.42%; H, 2.97%; N, 17.70%;
Found: C, 35.26%; H, 2.85%; N, 17.59%.

Experimental details

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

Discussion

Flexible ligands have variety of configurations that can be used to construct MOFs with different topologies [5–7]. The imidazole groups have a strong coordination ability, so ((1*H*-imidazol-1-yl)methyl)benzene can be used as a good connector to construct MOFs [8–11]. In this work, we used ((1*H*-imidazol-1-yl)methyl)benzene (L₁) as the ligands, assembling with Cd(NO₃)₂ to obtain a perfect 3D framework.

Before us, Li et al. [12] used the same ligand (L₁) with Cd(NO₃)₂ obtaining a different structure. The structure obtained by Li et al. is a 2D framework, in which the Cd(II) atom is six-coordinated, and the nitrate ions participates in coordination as a counter anion only. The complex we reported is different, forming a three-dimensional (3D) 2-fold interpenetrating structure, in which the Cd(II) atom is seven-coordinated, and the nitrate ions not only acts as a counter anion, but also participates in structural construction as a bridging group.

In detail the title crystal structure shows that the title complex consists of one Cd(II) atom, one L₁ ligand and two nitrate anions. The Cd(II) atom is seven-coordinated with two nitrogen atoms (N2 and N5) from two L₁ ligands and five oxygen atoms (O3, O4, O4[#], O5 and O6) from two nitrate ions.

In the framework, Cd(II) is bridged by nitrate anions, forming a one-dimensional chain. Adjacent one-dimensional chains are connected by L₁ to form a two-dimensional network structure. The two-dimensional network layer is further connected by L₁ to form a three-dimensional framework. Due to the large pores in the three-dimensional structure, the adjacent three-dimensional structures form one stable double-penetrating three-dimensional framework [13].

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