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Crystal structure of poly[(μ_2 -1,3-bis(imidazol-1-ylmethyl)benzene- $\kappa^2 N:N'$)(nitrate- $\kappa^1 O$) cadmium(II)] – water (2/1), $C_{28}H_{32}CdN_{10}O_7$

Abstract

$C_{28}H_{32}CdN_{10}O_7$, triclinic, $P\bar{1}$ (no. 2), $a = 8.2649(5)$ Å, $b = 9.7841(6)$ Å, $c = 10.0808(6)$ Å, $\alpha = 94.069(7)^\circ$, $\beta = 104.912(7)^\circ$, $\gamma = 97.695(7)^\circ$, $V = 775.89(9)$ Å³, $Z = 1$, $R_{gt}(F) = 0.0432$, $wR_{ref}(F^2) = 0.1140$, $T = 293(2)$ K.

CCDC no.: 1908062

A part of the title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.41 \times 0.23 \times 0.12$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.77 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	27.5° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	12375, 3552, 0.023
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3382
$N(\text{param})_{\text{refined}}$:	242
Programs:	Olex2 [1], SHELX [2], CrysAlis ^{PRO} [3]

Source of material

A mixture of 1,3-bis(imidazol-1-ylmethyl)benzene (3.0 mg), $Cd(NO_3)_2 \cdot 4 H_2O$ (4.5 mg), and 5 mL mixed solution of EtOH/ H_2O ($v/v = 1/4$) was added to a hard glass tube, pumped to a near-vacuum, heated at 135°C for 48 h, and cooled to 25°C with a decreasing rate of 3°C/h . Colorless block crystals were obtained with the yield of ca. 42% (based on 1,3-bis(imidazol-1-ylmethyl)benzene).

Experimental details

H atoms were positioned geometrically and refined using a riding model. There is a disorder of the nitrate ligand (Table 2).

Comment

Coordination polymers have gained great interests due to their structural and applications in some fields such as

<https://doi.org/10.1515/ncrs-2019-0126>

Received February 20, 2019; accepted April 5, 2019; available online April 27, 2019

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

Atom	x	y	z	U _{iso} ^a /U _{eq}
Cd1	0.000000	0.000000	0.000000	0.04795(13)
O1 ^a	−0.2772(8)	0.0498(8)	0.2279(6)	0.132(2)
O1 ^b	−0.3226(16)	0.1908(14)	0.0151(11)	0.108(5)
H4C	−0.400643	0.182846	−0.102156	0.130*
H4D	−0.562983	0.107196	−0.196696	0.130*
O2 ^a	−0.2504(6)	0.0745(6)	0.0318(5)	0.1002(15)
O2 ^b	−0.360(4)	0.154(3)	0.211(2)	0.135(7)
O3 ^a	−0.3672(6)	0.2199(5)	0.1317(5)	0.0897(14)
O3 ^b	−0.241(3)	0.0196(15)	0.098(2)	0.096(4)
O4 ^c	−0.4762(14)	0.1718(11)	−0.1816(9)	0.138(3)
N1	0.3707(4)	0.1259(3)	0.4058(3)	0.0538(6)
N3	0.1566(4)	0.0438(3)	0.2270(3)	0.0565(6)
N4	0.0856(4)	0.2240(3)	−0.0479(3)	0.0536(6)
N6	0.0511(4)	0.4201(3)	−0.1366(3)	0.0507(6)
N7	−0.2960(5)	0.1220(4)	0.1235(4)	0.0850(11)
C1	−0.0108(5)	0.3821(3)	−0.4344(3)	0.0567(8)
H1	−0.017826	0.301944	−0.390476	0.068*
C14	−0.0254(4)	0.2989(3)	−0.1127(3)	0.0532(7)
H14	−0.142154	0.270627	−0.138585	0.064*
C2	0.1108(5)	0.0191(3)	0.3445(4)	0.0562(7)
H2	0.005654	−0.026257	0.347579	0.067*
C3	−0.0005(5)	0.6264(3)	−0.4312(3)	0.0557(7)
H3	−0.000513	0.712281	−0.385265	0.067*
C4	−0.0311(5)	0.5209(4)	−0.2192(3)	0.0614(8)
H4A	0.017762	0.613801	−0.174699	0.074*
H4B	−0.150796	0.506956	−0.223130	0.074*
C5	0.2387(5)	0.3023(4)	−0.0314(4)	0.0652(9)
H5	0.342062	0.276167	0.011061	0.078*
C6	0.2208(5)	0.4237(4)	−0.0852(4)	0.0653(9)
H6	0.306675	0.494913	−0.086801	0.078*
C7	0.3155(5)	0.1074(4)	0.2699(4)	0.0619(8)
H7	0.380678	0.135750	0.211182	0.074*
C8	0.2395(5)	0.0697(4)	0.4549(3)	0.0597(8)
H8	0.239989	0.067265	0.547091	0.072*
C9	0.5332(5)	0.2088(4)	0.4847(4)	0.0649(9)
H9A	0.620592	0.193329	0.439533	0.078*
H9B	0.565688	0.179883	0.576666	0.078*
C10	0.5186(4)	0.3608(3)	0.4949(4)	0.0540(7)
C11	0.4718(5)	0.4228(4)	0.6033(4)	0.0635(8)
H11	0.453137	0.371399	0.673567	0.076*
C12	0.5476(5)	0.4380(4)	0.3921(4)	0.0630(8)
H12	0.580364	0.396922	0.319125	0.076*
C13	−0.0119(4)	0.5087(3)	−0.3641(3)	0.0480(6)

^aOccupancy: 0.818(7), ^bOccupancy: 0.182(7), ^cOccupancy: 0.5.

fluorescent probes and magnetism [4]. The suitable organic ligands were used in the preparing coordination polymer which had become an important way. Herein, we selected

1,3-bis(imidazol-1-ylmethyl)benzene to synthesize a Cd(II) coordination polymer.

The primary structural unit contains one half of a Cd²⁺ cation, one 1,3-bis(imidazol-1-ylmethyl)benzene ligands, one NO₃[−] anions and one half occupied isolated water molecule. In the structure, the Cd²⁺ cation is six-coordinated by four nitrogen atoms from four different 1,3-bis(imidazol-1-ylmethyl)benzene ligands and two oxygen atoms from two NO₃[−] anions. By means of such connection modes, a 2D framework is formed. In the framework, each Cd²⁺ cation is surrounded by four 1,3-bis(imidazol-1-ylmethyl)benzene ligands and two NO₃[−] anions. The features of the structure are similar with the known compounds [Cd(NO₃)₂(C₁₄H₁₄N₄)₂]_n [5], [C₂₈H₂₈MnN₁₄]_n [6] and [C₃₃H₃₂MnN₁₄O]_n [6]. The bond lengths of Cd–N and Cd–O are all in their normal ranges and they can be compared with previously reported Cd(II)-coordination polymers [7, 8].

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