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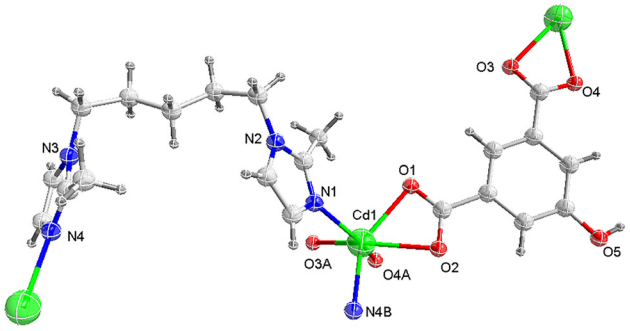
Crystal structure of poly[(μ_2-5-hydroxy-isophthalato-$\kappa^4O,O':O'',O'''$)-(μ_2-1,5-bis(imidazol-2-methyl)pentane-$\kappa^2N:N'$)cadmium(II)], $C_{21}H_{24}CdN_4O_5$



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Abstract

$C_{21}H_{24}CdN_4O_5$, monoclinic, $P2_1/n$ (no. 14), a = 9.5381(7) Å, b = 20.9393(14) Å, c = 11.4813(8) Å, β = 104.3660(10)°, V = 2221.4(3) Å^3, Z = 4, $R_{gt}(F)$ = 0.0319, $wR_{ref}(F^2)$ = 0.0873, T = 296(2) K.

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The molecular 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:	Colorless block
Size:	0.18 × 0.15 × 0.10 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	1.02 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.7°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	11,945, 4216, 0.018
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 3800
$N(param)_{refined}$:	283
Programs:	Bruker [1], SHELX [2–4]

1 Source of materials

All chemicals were purchased from commercial sources and used as received. A mixture of cadmium nitrate hexahydrate (30.8 mg, 0.1 mmol), 5-hydroxyisophthalic acid (Hip) (17.0 mg, 0.1 mmol), 1,5-bis(imidazol-2-methyl) pentane (bimp) (12.0 mg, 0.05 mmol), and NaOH (8.0 mg, 0.2 mmol) was added to 10 mL H_2O, stirred to form a clear solution. The mixture was heated at 413 K for 72 h. Many pale yellow crystals were filtered, washed with distilled water, and dried in air. Yield: 21.5 % (based on 5-hydroxyisophthalic acid).

2 Experimental details

The structure was solved by Direct Methods with the SHELXS-2018 program. All H-atoms were positioned with idealized geometry and refined isotropically (U_{iso}(H) = 1.2 or 1.5 U_{eq}(C)) using a riding model.

3 Comment

As we know, the rational design coordination polymers (CPs) have received remarkable attention, owing to their fascinating structural versatility and their tremendous functional properties in gas storage, chemical separations and so on [5–7]. Some isophthalic acids have been used in preparation of coordination polymers [8–10]. However, the study of cadmium CPs based on 1,5-bis(imidazol-2-methyl)pentane has been reported rarely [11, 12]. In this paper, we have prepared

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	−0.11897 (2)	0.12145 (2)	0.61038 (2)	0.03137 (9)
C1	−0.0100 (4)	0.21422 (18)	0.0577 (3)	0.0415 (8)
H1	−0.003013	0.229609	−0.016656	0.050*
C2	0.0835 (3)	0.23700 (16)	0.1633 (3)	0.0347 (7)
C3	0.0711 (3)	0.21491 (15)	0.2747 (3)	0.0335 (7)
H3	0.132864	0.230297	0.344877	0.040*
C4	−0.0333 (3)	0.16997 (15)	0.2807 (3)	0.0337 (7)
C5	−0.1242 (4)	0.14634 (17)	0.1752 (3)	0.0391 (7)
H5A	−0.192776	0.115412	0.179411	0.047*
C6	−0.1134 (4)	0.16851 (19)	0.0642 (3)	0.0442 (8)
C7	0.1959 (4)	0.28609 (16)	0.1550 (3)	0.0365 (7)
C8	−0.0541 (3)	0.14863 (15)	0.4011 (3)	0.0340 (7)
C9	0.1892 (4)	0.13870 (16)	0.7967 (3)	0.0383 (7)
C10	0.2581 (5)	0.04582 (19)	0.8773 (4)	0.0641 (12)
H10	0.311832	0.013325	0.922698	0.077*
C11	0.1247 (5)	0.04064 (19)	0.8038 (4)	0.0660 (13)
H11	0.070177	0.003346	0.789718	0.079*
C12	0.1930 (5)	0.20729 (19)	0.7672 (4)	0.0662 (13)
H12A	0.259404	0.213921	0.717702	0.099*
H12B	0.224044	0.231507	0.840048	0.099*
H12C	0.098059	0.220995	0.724658	0.099*
C13	0.4383 (4)	0.1360 (2)	0.9341 (4)	0.0528 (10)
H13A	0.461494	0.169875	0.884240	0.063*
H13B	0.512902	0.103649	0.942782	0.063*
C14	0.4417 (5)	0.1629 (2)	1.0559 (4)	0.0554 (10)
H14A	0.358361	0.190521	1.049257	0.067*
H14B	0.527821	0.188952	1.082327	0.067*
C15	0.4409 (5)	0.1126 (2)	1.1502 (4)	0.0591 (11)
H15A	0.346012	0.092742	1.133125	0.071*
H15B	0.510652	0.079697	1.144830	0.071*
C16	0.4760 (6)	0.1382 (2)	1.2761 (4)	0.0660 (13)
H16A	0.395195	0.163939	1.285997	0.079*
H16B	0.559394	0.166149	1.286711	0.079*
C17	0.5077 (4)	0.0883 (2)	1.3733 (4)	0.0553 (11)
H17A	0.580649	0.059447	1.357855	0.066*
H17B	0.548437	0.109180	1.449601	0.066*
C18	0.2860 (5)	0.0743 (2)	1.4475 (5)	0.0655 (12)
H18	0.287010	0.114470	1.482422	0.079*
C19	0.1927 (5)	0.0281 (2)	1.4478 (4)	0.0596 (11)
H19	0.115433	0.030221	1.483583	0.072*
C20	0.3402 (4)	−0.00728 (18)	1.3512 (3)	0.0459 (9)
C21	0.4154 (6)	−0.0493 (2)	1.2818 (5)	0.0707 (13)
H21A	0.409091	−0.092862	1.306092	0.106*
H21B	0.515314	−0.037010	1.296997	0.106*
H21C	0.370528	−0.045182	1.197551	0.106*
N1	0.0816 (3)	0.09907 (14)	0.7530 (3)	0.0424 (7)
N2	0.2993 (3)	0.10784 (14)	0.8724 (3)	0.0430 (7)
N3	0.3841 (3)	0.05112 (16)	1.3841 (3)	0.0497 (8)
N4	0.2274 (3)	−0.02482 (15)	1.3860 (3)	0.0495 (8)
O1	−0.1367 (3)	0.10259 (12)	0.4038 (2)	0.0451 (6)
O2	0.0101 (3)	0.17799 (13)	0.4920 (2)	0.0495 (6)
O3	0.2858 (3)	0.30411 (12)	0.2453 (2)	0.0460 (6)
O4	0.1942 (3)	0.30771 (13)	0.0522 (2)	0.0518 (7)
O5	−0.2082 (3)	0.14441 (18)	−0.0347 (2)	0.0674 (9)
H5	−0.199680	0.163797	−0.094635	0.101*

a new coordination polymer using 5-hydroxylisophthalic acid and 1,5-bis(imidazol-2-methyl)pentane constructing $[Cd(Hip)(bimp)]_n$. The Ortep diagram is presented in the Figure. The asymmetric unit consists of one Cd(II) ion, one Hip anion, and one bimp co-ligand. Each Cd(II) atom is coordinated with four oxygen atoms from two Hip^{2-} ligands, two nitrogen atoms from two bimp ligands, which form a distorted octahedral CdO_4N_2 coordination geometry. The Cd–O and Cd–N lengths are 2.287(3)–2.520(2) Å and 2.238(3)–2.278(3) Å, respectively. In the title compound, the Hip^{2-} ligand serves as a μ_2-bridge linking two adjacent Cd^{2+} ions in the bis-chelating mode to give rise to a one-dimensional chain, while such one-dimensional chains are further double-bridged by bimp ligands into a two-dimensional layer structure.

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

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