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Synthesis and crystal structure of poly[(μ_3 -2-(2-carboxylatophenyl)-1H-benzo[d]imidazole-5-carboxylato- κ O,O':O';:O'', O''')-(μ_2 -1-(4-(1Himidazol-1-yl)phenyl)-1H-imidazole- κ^2 N:N') cadmium(II)], $C_{27}H_{18}CdN_6O_4$

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Abstract

$C_{27}H_{18}CdN_6O_4$, triclinic, $P\bar{1}$ (no. 2), $a = 10.2994(8)$ Å, $b = 10.7795(7)$ Å, $c = 11.0038(7)$ Å, $\alpha = 89.778(5)^\circ$, $\beta = 78.046(6)^\circ$, $\gamma = 83.049(6)^\circ$, $Z = 2$, $V = 1186.11(14)$ Å³, $R_{gt}(F) = 0.0402$, $wR_{ref}(F^2) = 0.0809$, $T = 293$ K.

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

Source of material

All solvents and other reagents were of analytical grade. The method of synthesizing the title complex has been improved [8–12]. A mixture of cadmium nitrate, 2-(2-carboxyphenyl)-

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.15 × 0.05 × 0.03 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.97 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	26.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	7660, 4667, 0.034
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 3885
$N(param)_{refined}$:	347
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], Superflip [3–5], SHELX [6], Diamond [7]

1H-benzo[d]imidazole-5-carboxylic acid, 1-(4-(1H-imidazol-1-yl)phenyl)-1H-imidazole, and water was introduced into a 25 mL Teflon reactor autoclave and heated to 145 °C for three days. After cooling down to room temperature, colorless block crystals were obtained. Elemental analysis-**Anal. Calcd.** for $C_{27}H_{18}CdN_6O_4$: C, 53.79%; H, 3.01%; N, 13.94%. Found: C, 53.80%; H, 3.02%; N, 13.96%.

Experimental details

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

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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_{iso}^*/U_{eq}
Cd1	0.07870 (3)	0.08646 (2)	1.11764 (2)	0.02983 (10)
O1	0.0880 (3)	0.2410 (2)	0.9673 (2)	0.0399 (7)
O2	0.0627 (3)	0.0642 (2)	0.8808 (3)	0.0452 (7)
O3	−0.1243 (3)	0.9317 (2)	0.6747 (2)	0.0453 (7)
O4	−0.2198 (3)	0.7908 (2)	0.7931 (2)	0.0356 (6)
N1	−0.1693 (3)	0.4621 (3)	0.5266 (3)	0.0341 (7)
N2	−0.1408 (3)	0.5637 (3)	0.6943 (3)	0.0286 (7)
H2	−0.153 (4)	0.624 (3)	0.748 (3)	0.040 (12)*
N3	0.2619 (3)	−0.0586 (2)	1.0534 (3)	0.0346 (8)
N4	0.4189 (3)	−0.2162 (2)	1.0534 (3)	0.0319 (7)
N5	0.7133 (3)	−0.6384 (2)	1.2120 (3)	0.0343 (8)
N6	0.8790 (3)	−0.7905 (2)	1.2025 (3)	0.0370 (8)
C1	0.0573 (4)	0.1818 (3)	0.8807 (4)	0.0327 (9)
C2	0.0084 (3)	0.2535 (3)	0.7789 (3)	0.0289 (8)
C3	−0.0069 (4)	0.1912 (3)	0.6727 (3)	0.0340 (9)
H3	0.0217	0.1059	0.6629	0.041*
C4	−0.0630 (4)	0.2516 (3)	0.5820 (3)	0.0355 (9)
H4	−0.0726	0.2086	0.5119	0.043*
C5	−0.1048 (4)	0.3796 (3)	0.5987 (3)	0.0295 (8)
C6	−0.0869 (3)	0.4415 (3)	0.7042 (3)	0.0273 (8)
C7	−0.0302 (4)	0.3819 (3)	0.7955 (3)	0.0313 (8)
H7	−0.0183	0.4252	0.8645	0.038*
C8	−0.1878 (4)	0.5703 (3)	0.5875 (3)	0.0293 (8)
C9	−0.2560 (4)	0.6854 (3)	0.5425 (3)	0.0325 (9)
C10	−0.2557 (4)	0.8082 (3)	0.5850 (3)	0.0309 (8)
C11	−0.3143 (4)	0.9067 (3)	0.5242 (4)	0.0437 (11)
H11	−0.3129	0.9883	0.5505	0.052*
C12	−0.3740 (5)	0.8866 (4)	0.4266 (4)	0.0550 (13)
H12	−0.4135	0.9539	0.3884	0.066*
C13	−0.3751 (5)	0.7668 (4)	0.3857 (4)	0.0583 (13)
H13	−0.4158	0.7526	0.3199	0.070*
C14	−0.3158 (4)	0.6673 (4)	0.4423 (4)	0.0444 (11)
H14	−0.3156	0.5865	0.4129	0.053*
C15	−0.1957 (4)	0.8449 (3)	0.6913 (3)	0.0316 (9)
C16	0.3500 (4)	−0.0651 (3)	0.9421 (4)	0.0406 (10)
H16	0.3432	−0.0118	0.8764	0.049*
C17	0.3056 (4)	−0.1513 (3)	1.1187 (3)	0.0356 (9)
H17	0.2642	−0.1695	1.1990	0.043*
C18	0.4484 (4)	−0.1598 (3)	0.9407 (4)	0.0409 (10)
H18	0.5217	−0.1824	0.8763	0.049*
C19	0.4932 (4)	−0.3246 (3)	1.0944 (3)	0.0293 (8)
C20	0.6305 (4)	−0.3391 (3)	1.0611 (3)	0.0347 (9)
H20	0.6746	−0.2806	1.0116	0.042*
C21	0.7026 (4)	−0.4423 (3)	1.1024 (3)	0.0360 (9)
H21	0.7956	−0.4523	1.0816	0.043*
C22	0.6369 (4)	−0.5299 (3)	1.1739 (3)	0.0310 (9)
C23	0.5005 (4)	−0.5141 (3)	1.2070 (4)	0.0453 (11)
H23	0.4564	−0.5724	1.2568	0.054*
C24	0.4275 (4)	−0.4110 (3)	1.1665 (4)	0.0457 (11)
H24	0.3345	−0.4008	1.1881	0.055*
C25	0.8340 (4)	−0.6901 (3)	1.1485 (4)	0.0403 (10)
H25	0.8798	−0.6585	1.0754	0.048*
C26	0.7818 (4)	−0.8046 (3)	1.3043 (4)	0.0425 (10)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
H26	0.7857	−0.8690	1.3605	0.051*
C27	0.6787 (4)	−0.7123 (3)	1.3127 (4)	0.0445 (11)
H27	0.6007	−0.7012	1.3738	0.053*

Comment

Coordination polymers (CPs) not only exhibit large specific surface area, high porosity, low density, and pore size adjustable but also possess a wide range of applications in the fields of catalysis, energy storage, and separation [13–19]. Benzimidazole carboxyl ligands, as rigid ligands, are relatively fixed during the coordination process, and the structure of their constructions are predictable. Secondly, the presence of nitrogen atoms enriches the diversity of the structure of complexes [20, 21].

In this work, we used 2-(2-carboxyphenyl)-1*H*-benzo[d]imidazole-5-carboxylic acid (H_2L) as a rigid ligand, assembling with $Cd(NO_3)_2$ and 1-(4-(1*H*-imidazol-1-yl)phenyl)-1*H*-imidazole to obtain a 2D framework. The crystal structure shows that the title complex consists of one Cd(II) atom, one L^{2-} ligand, and one 1-(4-(1*H*-imidazol-1-yl)phenyl)-1*H*-imidazole auxiliary ligand.

The Cd(II) is seven-coordinated by two N atoms (N3 and N6) from two 1-(4-(1*H*-imidazol-1-yl)phenyl)-1*H*-imidazole auxiliary ligands and five O atoms (O1, O2, O3, and O4) from three different L^{2-} ligands. In the structure, the Cd(II) are bridged by L^{2-} ligands, forming a 1D chain. The chains are bridged by 1-(4-(1*H*-imidazol-1-yl)phenyl)-1*H*-imidazole auxiliary ligands, forming a 2D network structure.

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