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The crystal structure of poly[($\mu_3$-1,3-phenylenedioxydiacetate-$κ^5O,O,O',O'',O'''$)-bis(4'-(4-(1H-imidazol-1-yl)phenyl)-4,2':6',4'''-terpyridine-$κN$) cadmium(II)], C$_{58}$H$_{42}$CdN$_{10}$O$_6$

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Abstract

C$_{58}$H$_{42}$CdN$_{10}$O$_6$, triclinic, $P\overline{1}$ (no. 2), $a = 9.689(3)$ Å, $b = 10.930(3)$ Å, $c = 23.321(6)$ Å, $α = 80.838(5)$°, $β = 84.261(5)$°, $γ = 79.189(5)$°, $V = 2388.7(12)$ Å$^3$, $Z = 2$, $R_{gt}(F) = 0.0592$, $wR_{ref}(F^2) = 0.1561$, $T = 293$ K.

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

1 Source of material

The reagents were purchased from commercial sources and used without further purification. A mixture of Cd(NO$_3$)$_2$·4H$_2$O (0.031 g, 0.10 mmol), H$_2$pda (0.023 g, 0.10 mmol), and
Table 2: (continued)

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>Uiso*/Ueq</th>
</tr>
</thead>
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<tr>
<td>O1</td>
<td>0.3332 (4)</td>
<td>0.2938 (3)</td>
<td>0.4565 (15)</td>
<td>0.04025 (16)</td>
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<tr>
<td>O2</td>
<td>0.1483 (4)</td>
<td>0.3587 (3)</td>
<td>0.4054 (16)</td>
<td>0.0452 (9)</td>
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<tr>
<td>O3</td>
<td>0.3471 (4)</td>
<td>0.0484 (4)</td>
<td>0.4326 (2)</td>
<td>0.0655 (12)</td>
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<tr>
<td>O4</td>
<td>0.7630 (4)</td>
<td>−0.1911 (4)</td>
<td>0.35530 (17)</td>
<td>0.0556 (11)</td>
</tr>
<tr>
<td>O5</td>
<td>1.0198 (5)</td>
<td>−0.3222 (4)</td>
<td>0.37793 (19)</td>
<td>0.0686 (13)</td>
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<tr>
<td>O6</td>
<td>0.9457 (4)</td>
<td>−0.4045 (4)</td>
<td>0.46343 (17)</td>
<td>0.0497 (10)</td>
</tr>
</tbody>
</table>

4264-imphtpy (0.038 g, 0.10 mmol) was dispersed in mixed DMF (4 mL) and CH3CN (4 mL) solutions in a 16 mL Teflon-lined stainless steel autoclave, which was heated for 3 d at 393 K under autogenous pressure and slowly cooled to room temperature. Pale yellow block crystals were obtained.

2 Experimental details

The structure was solved with the SHELXT-2018 program. All H-atoms from C atoms were positioned with idealized geometry and refined isotropically (Uiso(H) = 1.2Ueq(C)) using a riding model with C–H = 0.93 and 0.97 Å.

3 Comment

In the past decades, a mixed strategy with N-heterocycle rings N-donor ligand and polycarboxylate O-donor ligand has been widely accepted for the diverse structures and wide applications of metal-organic frameworks (MOFs) [5–7]. As a rigid planar ligand, the tridentate ligand 4′-(4-imidazol-1-yl) phenyl)-4.2′-6′,4″-terpyridine (imphtpy) [8, 9] has been adopted for possessing both pyridine and imidazole functional groups, which is rarely used in the realm of MOFs relative to 4′-(4-pyridyl)-4.2′-6′,4″-terpyridine (pytpy) [10, 11]. A Cd(II) coordination complex was obtained successfully along with 1,3-phenylenedioxydiacetate(pda2−) [12–14] and its structure has been determined.

The ORTEP diagram is presented in the left part of the figure. The asymmetric unit contains one Cd(II) ion, two impyth ligands, and one completely deprotonated pda2− anion. As shown in ORTEP Figure, Cd1 is seven coordinated by two imidazole nitrogen atoms (Cd1–N5, 2.302(4) Å, Cd1–N5, 2.261(5) Å) from two individual impyth ligands and five oxygen atoms which are derived from one chelating carboxylate (O1#1 and O2#1, #1, symmetry code: #1, 1−x, −y, 1−z), and two monodentate bridging carboxylate (O6 and O6#2, symmetry code: #2, 2−x, −1−y, 1−z) of three different pda2− anions (Cd1–O, 2.283(3)–2.595(3) Å) to furnish a distorted octahedral geometry. Cd(II) to O/N distances and bond angles are within the normal range [15] except a distance of 2.667 Å between Cd1 and O5 indicating the existence of a weak interaction between them.

Every two neighbouring Cd(II) ions are linked by O6 atoms to form dimers, which are further connected by residue of two pda2− anions to generate one dimensional (1D) chain with impyth as a monodentate ligand through its terminal imidazole nitrogen atom. As there are no classic hydrogen bonds in this complex, the 3D structure is obtained through π–π interactions with Cg–Cg (the aromatic rings center was defined as Cg) distances of 3.902 Å and 3.733 Å between pyridine rings among adjacent chains demonstrated in the right part of the figure along with van der Waals forces.

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

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

References


