Poly[diaqua(μ₄-3-fluorophthalato-κ⁴O:O':O':O")cadmium(II)]
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Poly[diaqua($\mu_4$-3-fluorophthalato-$\kappa^4O$:O':O'')-cadmium(II)]

The crystal structure of the title compound, [Cd(C$_6$H$_4$FO$_2$)$_2$]$_n$, consists of polymeric sheets formed by the bridging of octahedrally coordinated Cd$^{II}$ by carboxylate O atoms of the 3-fluorophthalate (3-fpt$^{2-}$) ligand. The layers exhibit hydrogen bonding between each of two coordinated water molecules and two O atoms of the ligand. Adjacent sheets are connected through $\pi$–$\pi$ interactions.

Comment

Poly-carboxylates represent a versatile class of ligands for the construction of metal-organic coordination polymers (Ye et al., 2005). Their versatility stems from the variety of bridging modes of the carboxylate group (Mehrotra & Bohra, 1983). Many of these solids exhibit properties such as gas absorption, catalytic activity, and luminescence (Rowell et al., 2004; Wasuke et al., 2005; Kim et al., 2004). With this in mind, the title compound, (I), was prepared as a part of our ongoing efforts to construct new coordination polymers employing poly-carboxylate ligands.

The asymmetric unit consists of one Cd$^{II}$ ion, a 3-fluorophthalate (3-fpt$^{2-}$) dianion, and two coordinated water molecules. The Cd$^{II}$ ion exhibits an all-oxygen coordination in a distorted octahedral environment (Fig. 1). The axial sites are defined by a water O atom and a 3-fpt$^{2-}$ O atom, while the equatorial sites are defined by a water O atom and three carboxylate O atoms from three equivalent 3-fpt$^{2-}$ ligands.

The Cd–O bond distances are normal (Table 1), with an average value of 2.3031 (18) Å. All other distances and angles are comparable with those in a similar Cd$^{II}$-phthalate coordination polymer (Vaz et al., 1996).

In (I) there are O–H····O hydrogen bonds involving three H atoms of the two water molecules and two O acceptor atoms of the 3-fpt$^{2-}$ ligand (Table 2). The remaining water H atom along with the other two 3-fpt$^{2-}$ O atoms are not involved in hydrogen bonding.
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Experimental

All chemicals and solvents were purchased from commercial sources and used without further purification. 3-Fluorophthalic acid (3 mmol) was added to 100 ml of water and subsequently brought to pH 6.5 by the addition of 3 M NaOH with constant stirring. To this solution was added 10 ml of a 0.10 M solution of Cd(NO₃)₂·4H₂O. Single crystals of (I) were obtained in two weeks after slow evaporation of this solution.

Crystal data

\[ [\text{Cd}(\text{C}_8\text{H}_7\text{FO}_4)(\text{H}_2\text{O})_2] \]

\[ M = 330.54 \]

Triclinic, \( P\overline{1} \)

\[ a = 6.9460 (5) \text{ Å} \]

\[ b = 7.2330 (5) \text{ Å} \]

\[ c = 10.8199 (8) \text{ Å} \]

\[ \alpha = 103.217 (1) ^\circ \]

\[ \beta = 93.351 (1) ^\circ \]

\[ \gamma = 115.066 (1) ^\circ \]

\[ V = 471.86 (6) \text{ Å}^3 \]

\[ Z = 2 \]

\[ D_{\text{calc}} = 2.326 \text{ Mg m}^{-3} \]

Mo Kα radiation

\[ \mu = 2.34 \text{ mm}^{-1} \]

Irregular cleavage fragment, colorless

\[ \beta = 0.36 \times 0.22 \times 0.16 \text{ mm} \]

Data collection

Bruker SMART APEX CCD diffractometer

4570 measured reflections

1927 independent reflections

1893 reflections with \( I > 2\sigma(I) \)

\[ R_{\text{int}} = 0.012 \]

\[ \theta_{\text{max}} = 26.4^\circ \]

Refinement

Refinement on \( F^2 \)

\[ R(F^2) = 0.017 \]

\[ wR(F^2) = 0.042 \]

\[ S = 1.11 \]

1927 reflections

161 parameters

H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance (Å)</th>
<th>Bond Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cd1–O2^1</td>
<td>2.3226 (15)</td>
<td></td>
</tr>
<tr>
<td>Cd1–O3^2</td>
<td>2.3951 (15)</td>
<td></td>
</tr>
<tr>
<td>Cd1–O3^3</td>
<td>2.2518 (16)</td>
<td></td>
</tr>
<tr>
<td>O2^2–Cd1–O2^3</td>
<td>75.64 (6)</td>
<td></td>
</tr>
<tr>
<td>O2^2–Cd1–O6</td>
<td>167.55 (6)</td>
<td></td>
</tr>
<tr>
<td>O3–Cd1–O2^3</td>
<td>109.30 (6)</td>
<td></td>
</tr>
<tr>
<td>O3–Cd1–O5</td>
<td>161.87 (6)</td>
<td></td>
</tr>
<tr>
<td>O3–Cd1–O6</td>
<td>85.61 (6)</td>
<td></td>
</tr>
<tr>
<td>O4^4–Cd1–O2^2</td>
<td>81.61 (6)</td>
<td></td>
</tr>
<tr>
<td>O4^4–Cd1–O2^2</td>
<td>82.27 (6)</td>
<td></td>
</tr>
</tbody>
</table>

Symmetry codes: (i) \(-x+1, -y+1, -z+1\); (ii) \(-x+1, -y+2, -z+1\); (iii) \(x, y, z\).

Table 2

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D–H···A</th>
<th>D–H (Å)</th>
<th>H···A (Å)</th>
<th>D···A (Å)</th>
<th>D–H···A (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O5–H5A···O4^6</td>
<td>0.765 (18)</td>
<td>2.076 (19)</td>
<td>2.840 (2)</td>
<td>175 (3)</td>
</tr>
<tr>
<td>O5–H5B···O1</td>
<td>0.758 (19)</td>
<td>1.994 (19)</td>
<td>2.749 (2)</td>
<td>175 (4)</td>
</tr>
<tr>
<td>O6–H6B···O1^1</td>
<td>0.764 (19)</td>
<td>2.040 (19)</td>
<td>2.804 (2)</td>
<td>179 (5)</td>
</tr>
</tbody>
</table>

Symmetry codes: (iv) \(x, -y+1, z\); (v) \(x, y+1, z\).
H atoms bonded to C atoms were placed in geometrically idealized positions and included as riding atoms \([C—H = 0.95 \text{ Å} \text{ and } U_{iso}(H) = 1.2U_{eq}(C)]\). The water H atoms were located in difference maps and refined with the six O—H distances restrained to be equal with an effective s.u. of 0.015 Å.

Data collection: SMART-NT (Bruker, 2003); cell refinement: SAINT-Plus-NT (Bruker, 2003); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL and DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXTL (Sheldrick, 2000).

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References