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Diana Rishmawi
Francis Marion University

Katie Lewis
Francis Marion University

Mark D. Smith
University of South Carolina - Columbia, mdsmith3@mailbox.sc.edu

LeRoy Peterson Jr.
Francis Marion University

Hans-Conrad zur Loye
University of South Carolina - Columbia, zurloye@mailbox.sc.edu

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Poly[*diaqua*(μ_4 -3-fluorophthalato- $\kappa^4 O:O:O':O'$)cadmium(II)]

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Poly[diaqua(μ_4 -3-fluorophthalato- κ^4 O:O:O':O'')-cadmium(II)]

Diana Rishmawi,^a Katie Lewis,^a
Mark D. Smith,^b LeRoy Peterson
Jr^a and Hans-Conrad zur Loye^{b*}

^aChemistry Department, Francis Marion University, Florence, South Carolina 29501, USA, and ^bDepartment of Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina 29208, USA

Correspondence e-mail: lpeterson@fmarion.edu

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Key indicators

Single-crystal X-ray study

$T = 294$ K

Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å

R factor = 0.017

wR factor = 0.042

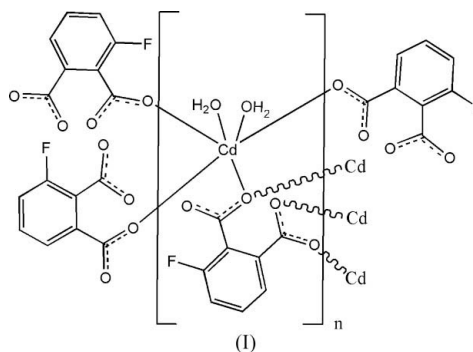
Data-to-parameter ratio = 12.0

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The crystal structure of the title compound, $[\text{Cd}(\text{C}_8\text{H}_3\text{FO}_4)(\text{H}_2\text{O})_2]_n$, 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 π - π interactions.

Comment

Polycarboxylates 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 polycarboxylate 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 $\text{O}-\text{H}\cdots\text{O}$ 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.

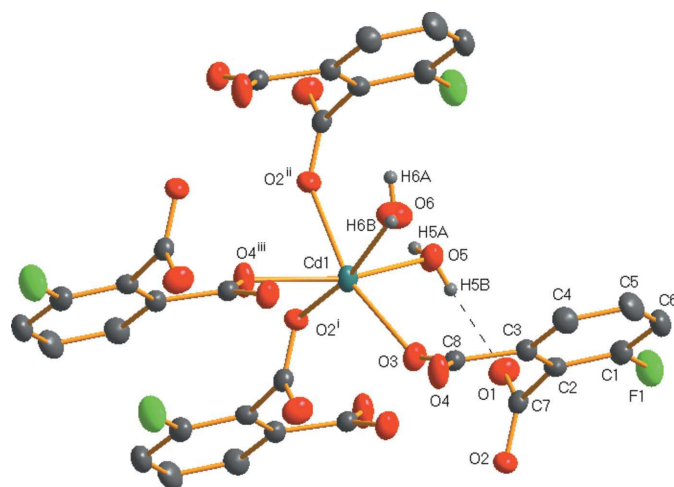


Figure 1
The coordination environment of the Cd^{II} atom in (I), showing the atom-labeling scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Hydrogen bonds are represented by dashed lines. [Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x - 1, y, z$; (iii) $-x + 1, -y + 2, -z + 1$.]

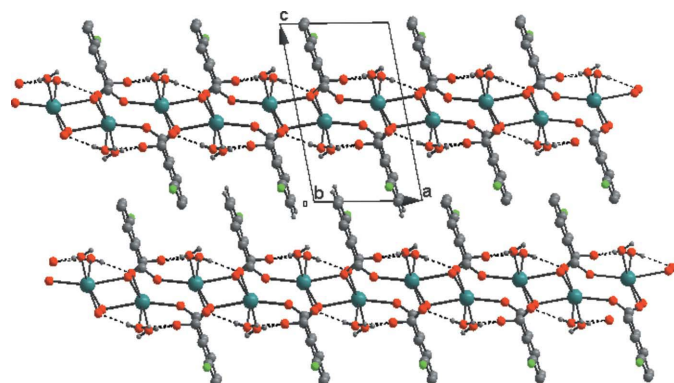


Figure 2
View of the crystal packing in (I). All H atoms, except for those of water, have been omitted for clarity. Hydrogen bonds are represented by dashed lines.

As is typical for metal phthalate-type complexes, the two carboxylate groups in (I) are not coplanar with the aromatic ring (Vaz *et al.*, 1996). One of the carboxylate groups makes a dihedral angle of 72.7 (1)°, while the other is twisted at an angle of 31.5 (1)°.

The 3-ft²⁻ ligand acts in a μ_4 -bridging fashion that links four symmetrically related Cd^{II} centers. The result is the formation of a 14-membered ring, an eight-membered ring, and a four-membered ring with Cd...Cd distances of 5.6292 (4), 4.2213 (3), and 3.7270 (3) Å, respectively. The center of each ring corresponds to a crystallographic inversion center.

The aforementioned bridging of Cd^{II} centers in (I) results in the formation of thick polymeric sheets that are stacked along the *c* axis, with the benzene rings of the 3-ft²⁻ ligands projecting outward from each side (Fig. 2). Adjacent sheets are connected through π - π interactions involving the protruding aromatic rings of 3-ft²⁻ from successive layers, with a centroid-centroid distance of 3.67 (2) Å between rings.

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

[Cd(C₈H₃FO₄)(H₂O)₂]
M_r = 330.54
Triclinic, *P*1̄
a = 6.9460 (5) Å
b = 7.2330 (5) Å
c = 10.8199 (8) Å
 α = 103.217 (1)°
 β = 93.351 (1)°
 γ = 115.066 (1)°

V = 471.86 (6) Å³
Z = 2
D_x = 2.326 Mg m⁻³
Mo *K*α radiation
 μ = 2.34 mm⁻¹
T = 294 (2) K
Irregular cleavage fragment,
colorless
0.36 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEX CCD
diffractometer
 ω scans
Absorption correction: multi-scan
(SADABS; Bruker, 2003)
T_{min} = 0.882, *T_{max}* = 1.000
(expected range = 0.607–0.688)

4370 measured reflections
1927 independent reflections
1893 reflections with *I* > 2σ(*I*)
R_{int} = 0.012
 θ_{\max} = 26.4°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*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

$w = 1/[\sigma^2(F_o^2) + (0.0169P)^2 + 0.4118P]$
where $P = (F_o^2 + 2F_c^2)/3$
(Δ/σ)_{max} = 0.001
 $\Delta\rho_{\max}$ = 0.51 e Å⁻³
 $\Delta\rho_{\min}$ = -0.40 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cd1—O2 ⁱ	2.3226 (15)	Cd1—O4 ⁱⁱⁱ	2.2312 (16)
Cd1—O2 ⁱⁱ	2.3951 (15)	Cd1—O5	2.2866 (17)
Cd1—O3	2.2518 (16)	Cd1—O6	2.3308 (19)
O2 ⁱ —Cd1—O2 ⁱⁱ	75.64 (6)	O4 ⁱⁱⁱ —Cd1—O3	115.46 (6)
O2 ⁱ —Cd1—O6	167.55 (6)	O4 ⁱⁱⁱ —Cd1—O5	157.03 (6)
O3—Cd1—O2 ⁱ	109.30 (6)	O4 ⁱⁱⁱ —Cd1—O6	98.11 (7)
O3—Cd1—O2 ⁱⁱ	161.87 (6)	O5—Cd1—O2 ⁱ	82.75 (6)
O3—Cd1—O5	85.61 (6)	O5—Cd1—O2 ⁱⁱ	77.62 (6)
O3—Cd1—O6	82.16 (7)	O5—Cd1—O6	93.58 (7)
O4 ⁱⁱⁱ —Cd1—O2 ⁱ	81.61 (6)	O6—Cd1—O2 ⁱⁱ	91.96 (6)
O4 ⁱⁱⁱ —Cd1—O2 ⁱⁱ	82.27 (6)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O4 ^{iv}	0.765 (18)	2.076 (19)	2.840 (2)	175 (3)
O5—H5B...O1	0.758 (19)	1.994 (19)	2.749 (2)	175 (4)
O6—H6B...O1 ^v	0.764 (19)	2.040 (19)	2.804 (2)	179 (5)

Symmetry codes: (iv) $x - 1, y - 1, z$; (v) $x, y + 1, z$.

H atoms bonded to C atoms were placed in geometrically idealized positions and included as riding atoms [$C-H = 0.95 \text{ \AA}$ 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 \AA .

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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