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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
H-atom completeness 91%
Disorder in main residue
 R factor = 0.033
 wR factor = 0.102
Data-to-parameter ratio = 16.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Bis(μ -4-formylbenzoato)- $\kappa^3\text{O},\text{O}':\text{O}';\kappa^3\text{O}:\text{O},\text{O}'$ -
bis[(4-formylbenzoato- $\kappa^2\text{O},\text{O}'$)(imidazole- κN)-
cadmium(II)] dihydrate**

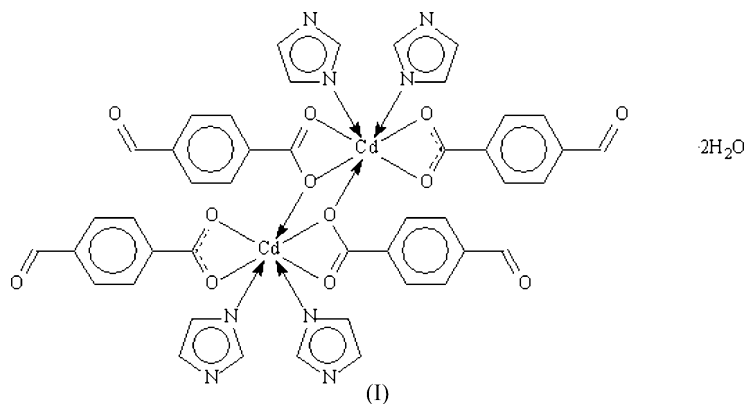
In the molecule of the title compound, $[\text{Cd}_2(\text{C}_8\text{H}_5\text{O}_3)_4(\text{C}_3\text{H}_4\text{N}_2)_4]\cdot 2\text{H}_2\text{O}$, two carboxylate groups chelate to the Cd^{II} atom. In addition, one carboxylate group also functions as a bridging ligand, forming a centrosymmetric dinuclear complex. The Cd^{II} atom is in a seven-coordinate pentagonal-bipyramidal coordination environment, in which the N atoms of the donor ligand occupy the axial sites.

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Comment

Imidazole adducts of water-coordinated copper(II) bis(4-formylbenzoate) (Deng *et al.*, 2006a) and nickel(II) bis(4-formylbenzoate) (Deng *et al.*, 2006b) contain transition metals in an all-*trans* octahedral geometry. The title cadmium bis(4-formylbenzoate) analog, (I), exists as a dinuclear compound, with two monomeric units being bridged through two carboxylate groups about an inversion center. Both carboxylate groups chelate to the metal atom. The coordination geometry of the Cd^{II} atom is *trans*-pentagonal bipyramidal, with the N atoms of the donor ligands occupying the axial sites. The compound crystallizes as a dihydrate (Fig. 1).



In the crystal structure, intermolecular hydrogen bonds (Table 2) link adjacent molecules into a layer structure, with disordered water molecules occupying cavities within each layer.

Experimental

Cadmium diacetate dihydrate (0.133 g, 0.5 mmol) was added to an aqueous solution (10 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) and imidazole (0.068 g, 1 mmol). The pH value of the clear solution was approximately 5. The filtered solution was allowed to evaporate at room temperature, and colorless prismatic crystals were isolated after several days. Elemental analysis calculated for $\text{C}_{44}\text{H}_{40}\text{Cd}_2\text{N}_8\text{O}_{14}$: C 46.78, H 3.57, N 9.92%; found: C 46.88, H 3.58, N 9.85%.

Crystal data

[Cd₂(C₈H₅O₃)₄(C₃H₄N₂)₄].2H₂O
M_r = 1129.64
 Monoclinic, *P*2₁/*c*
a = 12.354 (4) Å
b = 13.241 (5) Å
c = 14.769 (4) Å
 β = 98.784 (13)°
V = 2387.7 (14) Å³

Z = 2
D_x = 1.571 Mg m⁻³
 Mo *K*α radiation
 μ = 0.96 mm⁻¹
T = 293 (2) K
 Prism, colorless
 0.36 × 0.28 × 0.18 mm

Data collection

Rigaku RAXIS-RAPID IP
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
T_{min} = 0.558, *T_{max}* = 0.846

22942 measured reflections
 5455 independent reflections
 4434 reflections with *I* > 2σ(*I*)
R_{int} = 0.025
 θ_{max} = 27.5°

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.102$
 $S = 1.04$
 5455 reflections
 322 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.072P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.80 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.45 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—O1	2.367 (3)	Cd1—O5	2.434 (2)
Cd1—O2	2.573 (2)	Cd1—N1	2.241 (2)
Cd1—O4	2.494 (2)	Cd1—N3	2.242 (2)
Cd1—O4 ⁱ	2.441 (2)		
O1—Cd1—O2	52.40 (8)	O4—Cd1—O4 ⁱ	76.54 (7)
O1—Cd1—O4	169.98 (7)	O4—Cd1—O5	52.62 (7)
O1—Cd1—O4 ⁱ	93.44 (7)	O4—Cd1—N1	90.90 (8)
O1—Cd1—O5	137.40 (7)	O4—Cd1—N3	92.05 (8)
O1—Cd1—N1	88.75 (9)	O4 ⁱ —Cd1—O5	129.16 (7)
O1—Cd1—N3	87.31 (9)	O4 ⁱ —Cd1—N1	87.50 (8)
O2—Cd1—O4	137.62 (7)	O4 ⁱ —Cd1—N3	87.40 (9)
O2—Cd1—O4 ⁱ	145.83 (7)	O5—Cd1—N1	92.28 (8)
O2—Cd1—O5	85.00 (8)	O5—Cd1—N3	94.24 (9)
O2—Cd1—N1	90.49 (9)	N1—Cd1—N3	173.36 (9)
O2—Cd1—N3	91.34 (9)		

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

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>
N2—H2 <i>n</i> ...O5 ⁱⁱ	0.86	2.31	3.049 (4)	144
N4—H4 <i>n</i> ...O1 <i>w</i>	0.86	1.92	2.746 (7)	162
N4—H4 <i>n</i> ...O1 <i>w</i> '	0.86	1.92	2.753 (6)	161

Symmetry code: (ii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.

The asymmetric unit is disordered in several parts. The formyl units of both the carboxylate anions are disordered over two positions; for each unit, the C—O distances involving the unprimed and primed O atom were restrained to be within 0.01 Å of each other.

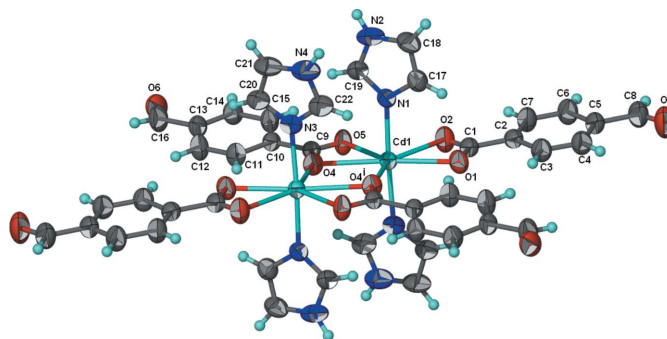


Figure 1

The molecular structure of (I). The disordered water molecule is not shown; only one of the disorder components is shown. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

Displacement parameters of the primed atoms were set equal to those of the unprimed atoms. One of the two imidazole groups is also disordered and all bond distances of each disorder component were restrained to be within 0.01 Å of each other, as were the 1,3-related distances. The displacement parameters of the primed and unprimed atoms were set to be equal. The occupancies of the formyl units and the imidazole ligand could not be refined, and the disorder components were given 0.5 occupancies. The water molecule is disordered over three positions; the occupancies were arbitrarily assigned as 1/3, and the displacement parameters of the three 1/3-occupancy O atoms were set to be identical. The carbon- and nitrogen-bound H atoms were positioned geometrically (C—H = 0.93 Å and N—H = 0.86 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms could not be placed in any chemically sensible positions on the basis of hydrogen-bonding interactions and were not included.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2006).

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