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# Aquabis(benzimidazole-$\kappa N$)bis(4-formylbenzoato)-$\kappa O;\kappa^2 O,O'$-cadmium(II) tetrahydrate

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.008 Å
$R$ factor = 0.048
$wR$ factor = 0.171
Data-to-parameter ratio = 17.4

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



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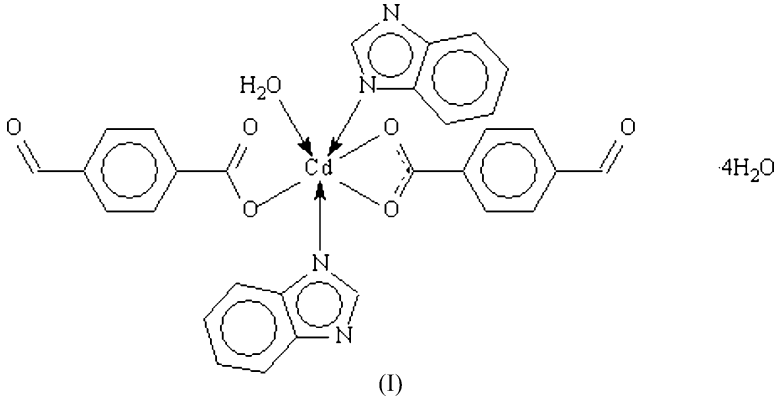
The distorted octahedral coordination of the $Cd^{II}$ atom in the title complex, $[Cd(C_8H_5O_3)_2(C_7H_6N_2)_2(H_2O)]\cdot 4H_2O$, is formed by four O atoms (two from a chelating carboxylate group, one from a unidentate carboxylate group and one from a water ligand) and two N atoms (from two *N*-heterocycles); the N atoms are *trans* to each other. In the crystal structure, molecules are linked into a three-dimensional network by intermolecular hydrogen bonds.

## Comment

The preceeding paper (Deng *et al.*, 2006) reports a related 1:2 cadmium bis(4-formylbenzoate) imidazole complex in which the $Cd^{II}$ atom is chelated by a carboxylate group; two molecules are further bridged through one of the two carboxylate groups and its symmetry-equivalent, forming a dinuclear species. The $Cd^{II}$ atom exhibits a pentagonal bipyramidal coordination, with two donor ligands occupying the axial sites. The use of a sterically more crowded benzimidazole *N*-heterocycle ligand in place of imidazole also leads to a 1:2 complex. However, the resulting title compound, (I), features only one chelating carboxylate group, the other being unidentate. Furthermore, the ligand appears to inhibit dimer formation. The disorted octahedral coordination is achieved by the inclusion of a water molecule into the coordination geometry (Fig. 1). Four O atoms form a square plane (two from a chelating carboxylate group, one from a unidentate carboxylate group and one from a water water); the two N atoms of a donor ligand are in the other two sites.




(I)

In the crystal structure, adjacent molecules are linked through uncoordinated water molecules by intermolecular hydrogen bonds bonds (Table 2), forming a three-dimensional network.

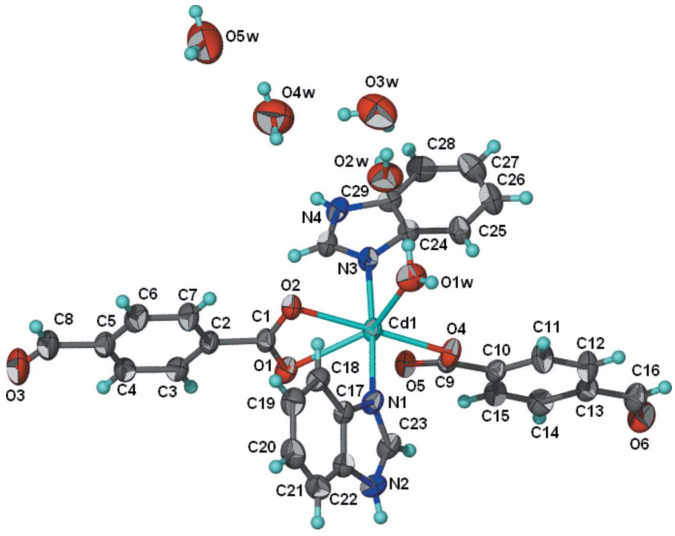



**Figure 1**
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii.

## Experimental

Cadmium diacetate dihydrate (0.133 g, 0.5 mmol) was added to a 1:1 aqueous ethanol solution (20 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) and benzimidazole (0.068 g, 1 mmol). The pH value of the mixture was about 5. The filtered solution was allowed to evaporate, and colorless prismatic crystals were isolated after several days. Elemental analysis calculated for $C_{30}H_{32}CdN_4O_{11}$: C 48.89, H 4.38, N 7.60%; found: C 48.85, H 4.33, N 7.54%.

*Crystal data*

$[Cd(C_8H_5O_3)_2(C_7H_6N_2)_2(H_2O)]\cdot 4H_2O$
$M_r$ = 737.00
Triclinic, $P\overline{1}$
$a$ = 11.294 (2) Å
$b$ = 12.656 (2) Å
$c$ = 12.936 (3) Å
$\alpha$ = 73.024 (3)°
$\beta$ = 69.403 (3)°
$\gamma$ = 70.883 (3)°
$V$ = 1602.4 (5) Å$^3$
$Z$ = 2
$D_x$ = 1.528 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.75 mm$^{-1}$
$T$ = 293 (2) K
Prism, colorless
0.38 × 0.28 × 0.19 mm

*Data collection*

Rigaku R-AXIS RAPID IP diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.459, $T_{max}$ = 0.871
15576 measured reflections
7219 independent reflections
5767 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 27.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.171
$S$ = 1.07
7219 reflections
415 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1099P)^2 + 0.2597P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.78 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.588 (3) | Cd1—O1*w* | 2.314 (3) |
| Cd1—O2 | 2.331 (3) | Cd1—N1 | 2.325 (4) |
| Cd1—O4 | 2.261 (3) | Cd1—N3 | 2.304 (4) |
| | | | |
| O1—Cd1—O2 | 53.3 (1) | O2—Cd1—N3 | 87.3 (1) |
| O1—Cd1—O4 | 126.6 (1) | O4—Cd1—O1*w* | 88.6 (1) |
| O1—Cd1—O1*w* | 143.8 (1) | O4—Cd1—N1 | 88.1 (1) |
| O1—Cd1—N1 | 79.8 (1) | O4—Cd1—N3 | 93.9 (1) |
| O1—Cd1—N3 | 97.5 (1) | O1*w*—Cd1—N1 | 94.9 (1) |
| O2—Cd1—O4 | 178.8 (1) | O1*w*—Cd1—N3 | 87.1 (1) |
| O2—Cd1—O1*w* | 91.4 (1) | N1—Cd1—N3 | 177.3 (1) |
| O2—Cd1—N1 | 90.8 (1) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*w*—H1*w*1···O4$^{i}$ | 0.86 | 1.93 | 2.774 (4) | 166 |
| O1*w*—H1*w*2···O2*w* | 0.85 | 1.89 | 2.710 (6) | 162 |
| O2*w*—H2*w*1···O6$^{ii}$ | 0.86 | 2.20 | 2.800 (6) | 127 |
| O2*w*—H2*w*2···O3*w* | 0.86 | 1.93 | 2.759 (8) | 164 |
| O3*w*—H3*w*1···O4*w* | 0.86 | 1.87 | 2.72 (1) | 170 |
| O4*w*—H4*w*1···O5*w* | 0.86 | 1.98 | 2.73 (1) | 144 |
| O5*w*—H5*w*1···O2$^{iii}$ | 0.85 | 2.20 | 2.813 (7) | 129 |
| O5*w*—H5*w*2···O2*w*$^{iii}$ | 0.86 | 2.35 | 2.82 (1) | 115 |
| N2—H2*n*···O1$^{iv}$ | 0.85 | 2.03 | 2.871 (5) | 169 |
| N4—H4*n*···O5$^{v}$ | 0.85 | 2.02 | 2.855 (5) | 166 |

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

The carbon- and nitrogen-bound H atoms were positioned geometrically (C—H = 0.93 Å and N—H = 0.85 Å) and were included in the refinement in the riding-model approximation, with $U_{iso}$(H)= 1.2$U_{eq}$(C). Those on the water molecules were positioned using the *HYDROGEN* (Nardelli, 1999) option in the *WinGX* package (Farrugia, 1999). These were not refined; their displacement parameters were similarly tied. Some short H···H atom contacts are probably an artifact of some disorder; the disorder was not modeled as the magnitude of the atomic displacement ellipsoids of the O atoms appear reasonable.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 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: *publCIF* (Westrip, 2006).

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