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trans-Diaquabis(1*H*-imidazole-4,5-dicarboxylato-κ^2N^3,O^4)cadmium(II)

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The water-coordinated Cd atom in the title compound, $[Cd(C_5H_3N_2O_4)(H_2O)_2]$, lies on an inversion centre and is *N*,*O*-chelated by imidazole-4,5-dicarboxylate anions, defining an octahedral environment. The structure is isomorphous with the Mn analogue [Ma, Chen, Chen & Liu (2003). *Acta Cryst*. C**59**, m516–m518].

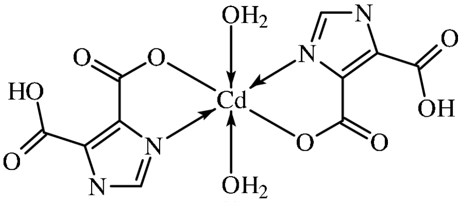
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.052
Data-to-parameter ratio = 11.6

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

Comment

Ma *et al.* (2002) described the structure of diaquabis[imidazole-4,5-dicarboxylato(1−)]manganese(II) as a three-dimensional network of $[Mn(C_5H_3N_2O_4)(H_2O)_2]$ molecules held together by hydrogen-bonding interactions involving the carboxylic acid, amino and water H atoms. The anion behaves as a chelating unit that binds through the tertiary amino and negatively charged carboxyl atoms. The present centrosymmetric Cd analogue, (I) (Fig. 1) is isomorphous, the two compounds having nearly identical unit-cell parameters.



(I)

Experimental

The pH of a solution of cadmium diacetate dihydrate (0.20 g, 1 mmol) and imidazole-4,5-dicarboxylic acid (0.23 g, 1 mmol) in water (7 ml) was adjusted to 7 with 4 *M* sodium hydroxide. The solution was then transferred into a 15 ml Teflon-lined stainless-steel bomb and heated at 433 K for 120 h. The bomb was cooled slowly to room temperature to afford well formed prismatic crystals of (I) in about 50% yield.

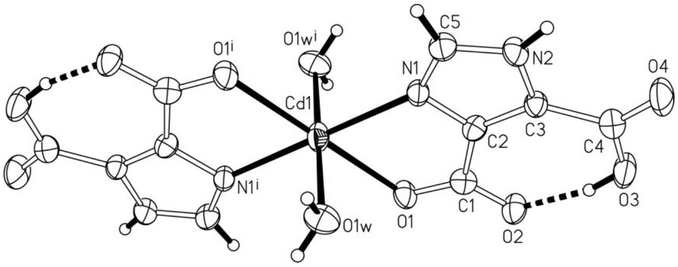


Figure 1
A view of the centrosymmetric molecule of (I), with displacement ellipsoids drawn at the 50% probability level [symmetry code: (i) $1 - x$, $1 - y$, $1 - z$].

Crystal data

[$Cd(C_5H_3N_2O_4)(H_2O)_2$]
M_r = 458.62
Monoclinic, $P2_1/n$
a = 5.0407 (7) Å
b = 23.036 (3) Å
c = 6.6601 (9) Å
β = 111.569 (2)°
V = 719.2 (2) Å^3
Z = 2
D_x = 2.118 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2270 reflections
θ = 3.4–27.0°
μ = 1.59 mm^{-1}
T = 298 (2) K
Block, colourless
0.32 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.492, $T_{\max}$ = 0.752
4035 measured reflections
1571 independent reflections
1127 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.055
$\theta_{\max}$ = 27.0°
$h = -6 \rightarrow 6$
$k = -29 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.052
S = 0.74
1571 reflections
135 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.87 e Å^{-3}
$\Delta\rho_{\min}$ = −1.00 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.260 (2)	Cd1—O1W	2.342 (2)
Cd1—O1	2.326 (2)		
N1—Cd1—N1$^{\rm i}$	180.0 (1)	O1—Cd1—O1$^{\rm i}$	180.0 (1)
N1—Cd1—O1	73.9 (1)	O1—Cd1—O1W	88.6 (1)
N1—Cd1—O1$^{\rm i}$	106.1 (1)	O1—Cd1—O1$W^{\rm i}$	91.4 (1)
N1—Cd1—O1W	84.9 (1)	O1W—Cd1—O1$W^{\rm i}$	180.0 (1)
N1—Cd1—O1$W^{\rm i}$	95.1 (1)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.85 (1)	1.67 (1)	2.503 (3)	166 (4)
O1W—H1W1···O1$^{\rm ii}$	0.83 (1)	1.93 (2)	2.721 (3)	159 (3)
O1W—H1W2···O2$^{\rm ii}$	0.84 (1)	1.96 (2)	2.766 (3)	160 (3)
N2—H2···O3$^{\rm iv}$	0.84 (1)	2.03 (1)	2.865 (3)	169 (3)

Symmetry codes: (ii) $2-x, 1-y, 1-z$; (iii) $x, y, 1+z$; (iv) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$.

The diffraction data were of sufficient quality to enable the refinement of all H atoms, which were located from a difference Fourier map. Their positional parameters were refined subject to O—H = N—H = 0.85 (1) Å and C—H = 0.95 (1) Å. The goodness-of-fit of 0.74 is somewhat low. The weighting scheme used was that suggested by *SHELXL*97 (Sheldrick, 1997), although a higher GoF could have been obtained using an alternative scheme with an additional term.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: isostructural with Mn analogue; program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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