Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

A two-dimensional cadmium(II)–iminodiacetate polymer

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Received 16 May 2005
Accepted 18 May 2005
Online 28 May 2005

The title compound, poly[[aquatri-μ_3-iminodiacetato-tricadmium(II)] trihydrate], $\{[Cd_3(C_4H_5NO_4)_3(H_2O)]\cdot 3H_2O\}_n$, consists of a polymeric Cd^{II}–iminodiacetate network and uncoordinated water molecules. One Cd atom located on a general position is surrounded by three iminodiacetate (IDA) dianions, while a second Cd atom located on a mirror plane is coordinated by three IDA dianions and one water molecule. Both Cd^{II} atoms possess distorted octahedral coordination geometries. The iminodiacetate dianion bridges neighbouring Cd^{II} atoms to form polymeric sheets.

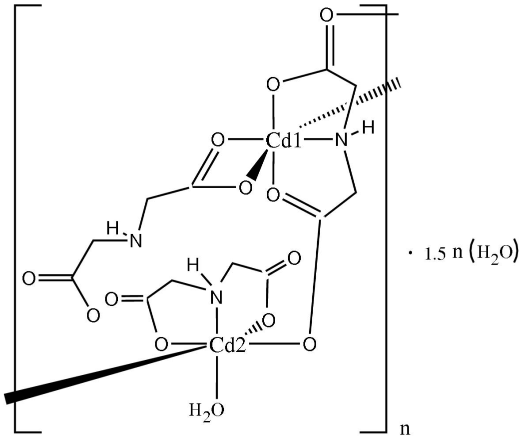
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
H-atom completeness 92%
Disorder in solvent or counterion
R factor = 0.033
wR factor = 0.061
Data-to-parameter ratio = 12.4

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

Comment

The $(C_4H_5NO_4)^{2-}$ iminodiacetate (IDA) dianion has shown various coordination modes in transition metal complexes. When it behaves as a tridentate chelating ligand, both the facial and meridional chelating configurations are possible in octahedral metal complexes, but IDA usually displays the *fac* configuration (Liu & Xu, 2004; Li *et al.*, 2003; Su & Xu, 2004; Su *et al.*, 2004). However, both *fac* and *mer* configurations appear simultaneously in the polymeric title compound, (I).



(I)

A segment of the polymeric structure of (I) is shown in Fig. 1. There are two independent Cd^{II} atoms in the crystal structure, atom Cd1 occupying a general position and atom Cd2 located on a mirror plane. Both Cd^{II} atoms display distorted octahedral coordination geometries, although they have different coordination environments.

Atom Cd1 is surrounded by three IDA ligands, of which one is *N*-monodentate, one *O*,*O*-bidentate and one *N*,*O*,*O*-tridentate. The IDA ligand containing atom N1 (N1-IDA) chelates in a tridentate fashion to atom Cd1 in the meridional

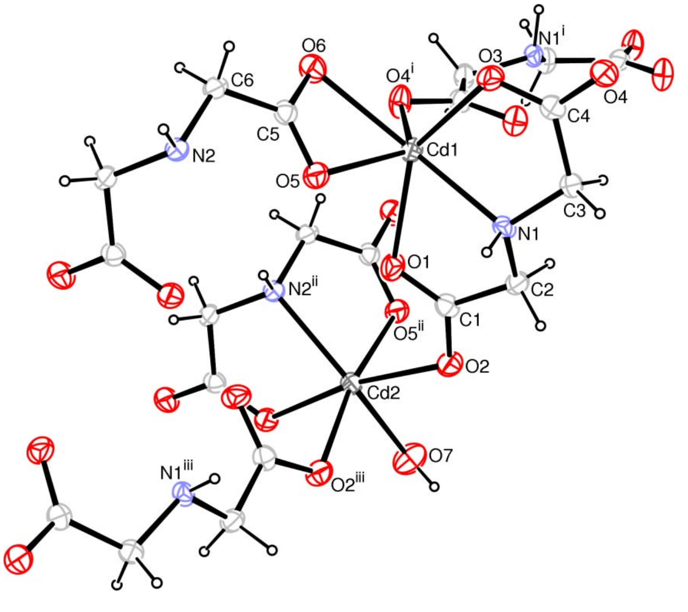


Figure 1
A segment of the polymeric complex structure of (I), showing the coordination environments around atoms Cd1 and Cd2 and the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $\frac{3}{2} - x, 1 - y, z - \frac{1}{2}$; (ii) $x, y, z - 1$; (iii) $x, \frac{3}{2} - y, z$.]

configuration, atom N1 deviating from the mean plane formed by the other eight atoms of IDA by 0.425 (4) Å. The N1^{i}-IDA ligand coordinates in an *N*-monodentate fashion to atom Cd1 [symmetry code: (i) $\frac{3}{2} - x$, $1 - y$, $z - \frac{1}{2}$]. Finally, the C5-carboxyl group of the N2-IDA ligand chelates in an *O*,*O*-bidentate fashion to atom Cd1 to complete a CdO_5N octahedral coordination. The Cd1—O4^{i} bond distance is much shorter than the other Cd1—O bonds (Table 1).

Atom Cd2 is coordinated by three IDA ligands (two *O*-monodentate and one *N*,*O*,*O*-tridentate) and one water molecule. The coordinated water molecule (O7) occupies the same mirror plane as atom Cd2. The N2^{ii}-IDA ligand [symmetry code: (ii) $x, y, z - 1$], with its N atom located on the same mirror plane, chelates to atom Cd2 in a facial configuration: the five-membered chelate ring adopts an envelope configuration, with atom N2^{ii} lying in the flap position and deviating from the mean plane formed by the other four atoms by 0.349 (6) Å. The symmetrically related N1-IDA and N1^{iii}-IDA ligands coordinate in a monodentate fashion to atom Cd2 [symmetry code: (iii) $x, \frac{3}{2} - y, z$], with a shorter Cd2—O2 bond distance than Cd2—O5. A distorted CdO_5N octahedron results from these bonding modes.

The N1-IDA and N2-IDA ligands each bridge three Cd^{II} atoms to form two-dimensional (010) polymeric sheets (Fig. 2). The uncoordinated water molecules are located between adjacent sheets and are hydrogen bonded to the polymeric complex (Table 2) to form the sandwich-like supramolecular structure (Fig. 3).

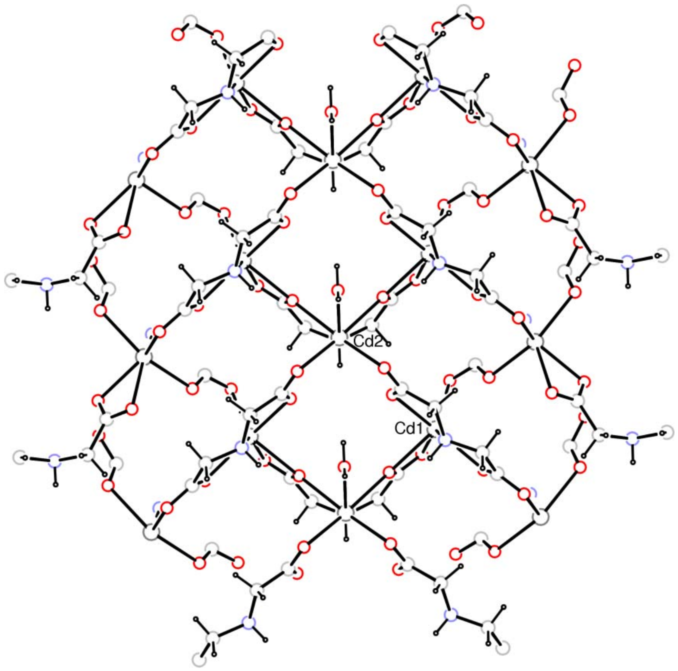


Figure 2
The two-dimensional sheet structure of (I).

Experimental

An aqueous solution (20 ml) of $CdCl_2\cdot 2H_2O$ (0.22 g, 1 mmol) was mixed with another aqueous solution (10 ml) containing iminodiacetic acid (0.14 g, 1 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 3 h. The solution was filtered after cooling to room temperature. Colourless single crystals of (I) were obtained from the filtrate after 5 d.

Crystal data

$[Cd_3(C_4H_5NO_4)_3(H_2O)]\cdot 3H_2O$
$M_r = 802.54$
Orthorhombic, *Pnma*
$a = 15.8286$ (11) Å
$b = 21.2483$ (16) Å
$c = 6.7247$ (9) Å
$V = 2261.7$ (4) Å^3
$Z = 4$
$D_x = 2.357$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9866 reflections
$\theta = 3.0$–24.0°
$\mu = 2.88$ mm^{-1}
$T = 295$ (2) K
Prism, colourless
0.32 × 0.30 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.410$, $T_{max} = 0.525$
11022 measured reflections
2051 independent reflections
2012 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 25.0°$
$h = -18 \rightarrow 17$
$k = -24 \rightarrow 25$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.061$
$S = 1.27$
2051 reflections
166 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0119P)^2 + 6.6406P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

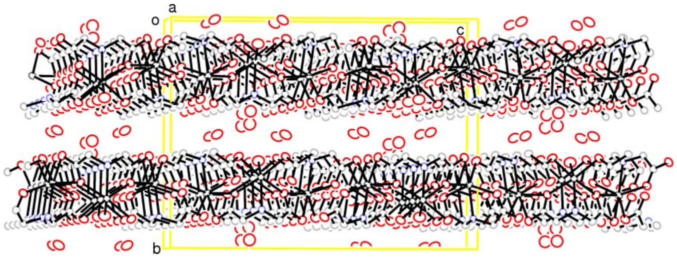


Figure 3
A molecular packing diagram for (I), viewed down [100], showing the polymeric sheets sandwiching uncoordinated water molecules. H atoms have been omitted for clarity.

Table 1
Selected bond lengths (Å).

Cd1—N1	2.296 (4)	Cd2—O2	2.259 (3)
Cd1—O1	2.377 (3)	Cd1—O3	2.341 (3)
Cd1—O4^{i}	2.232 (3)	Cd2—O2^{iii}	2.259 (3)
Cd1—O5	2.371 (3)	Cd2—O5^{ii}	2.315 (3)
Cd1—O6	2.378 (3)	Cd2—O7	2.373 (5)
Cd2—N2^{ii}	2.331 (5)		

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

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
N1—H1$\cdots$O1*W*^{iv}	0.94	2.04	2.937 (5)	159
O1*W*—H1*A*$\cdots$O2	0.96	1.79	2.719 (5)	160
O1*W*—H1*B*$\cdots$O4^{v}	0.87	2.08	2.824 (5)	142
N2—H2$\cdots$O2*WB*^{vi}	0.94	2.30	3.131 (15)	147
O7—H7*A*$\cdots$O2*WA*	0.85	1.89	2.682 (17)	155

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

The refinement showed that an uncoordinated water molecule located on a mirror plane is disordered over two sites, O2*WA* and O2*WB*. Their fractional site occupancies were refined freely and converged to 0.51 (3) and 0.59 (2), respectively. In the final cycles of refinement, the occupancies were fixed at $\frac{1}{2}$. The H atoms bound to them were not located. H atoms on the other water molecules were located in a difference Fourier map and refined as riding in their as-found positions relative to their parent atoms, with a fixed isotropic displacement parameter of 0.05 Å^2. Other H atoms were placed in calculated positions, with C—H = 0.97 Å and N—H = 0.91 Å, and included in the final cycles of refinement as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the parent atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This project was supported by the National Natural Science Foundation of China (grant No. 20443003).

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