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catena-Poly[[cadmium(II)]-μ-β-alanine-di-μ-chloro]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.032
wR factor = 0.081
Data-to-parameter ratio = 8.1

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

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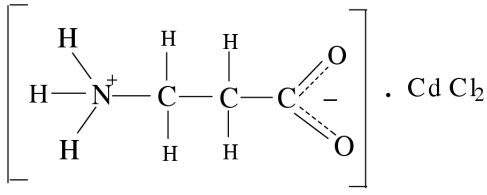
In the title compound, $[CdCl_2(C_3H_7NO_2)]_n$, the β-alanine residues exist in the zwitterionic form. The Cd atoms are coordinated by four Cl atoms and two O atoms, forming a distorted octahedral environment. These octahedra are linked through Cl—Cl edges and are bridged by the carboxyl groups of the β-alanine residues, to form a one-dimensional polymer chain that extends along [100].

Comment

β-Alanine, a variant of L-alanine, is not a constituent of proteins or enzymes, but is a component of the naturally occurring peptides carnosine and anserine, and also of pantothenic acid (vitamin B5). The redetermination of the crystal structure of β-alanine (Papavinasam *et al.*, 1986) was carried out in our laboratory. The present study reports the crystal structure of a complex of β-alanine with cadmium chloride, *viz.* *catena*-poly[[cadmium(II)]-μ-β-alanine-di-μ-chloro], (I). The crystal structures of complexes of cadmium chloride with glycine (Thulasidhass & Mohana Rao, 1980), L-alanine (Schaffers & Keszler, 1993), sarcosine (Krishnakumar *et al.*, 1996), L-proline (Yukawa *et al.*, 1983) and hydroxy-L-proline (Yukawa *et al.*, 1982) have already been reported.



(I)

β-Alanine residues exist as zwitterions. Though the space group appears to be *Pnma*, the crystal structure is correctly described in space group $Pna2_1$. Atom C3 (Fig. 1) deviates by 0.70 (2) Å from a nearly perfect plane formed by the other non-H atoms of the β-alanine residue. As a result of this deviation, an inversion centre is forbidden, lowering the overall symmetry of an otherwise symmetrical crystal structure. The torsion angles [145.0 (2), −24 (3) and 62.5 (2)°] observed in the present structure (Table 1) are distinctly different from those observed in β-alanine [−177.8, 25.3 and −154.8°].

The coordination environment around the Cd atom, involving Cl atoms and carboxyl O atoms, may be visualized as a distorted octahedron. Four Cl atoms coordinate to a Cd

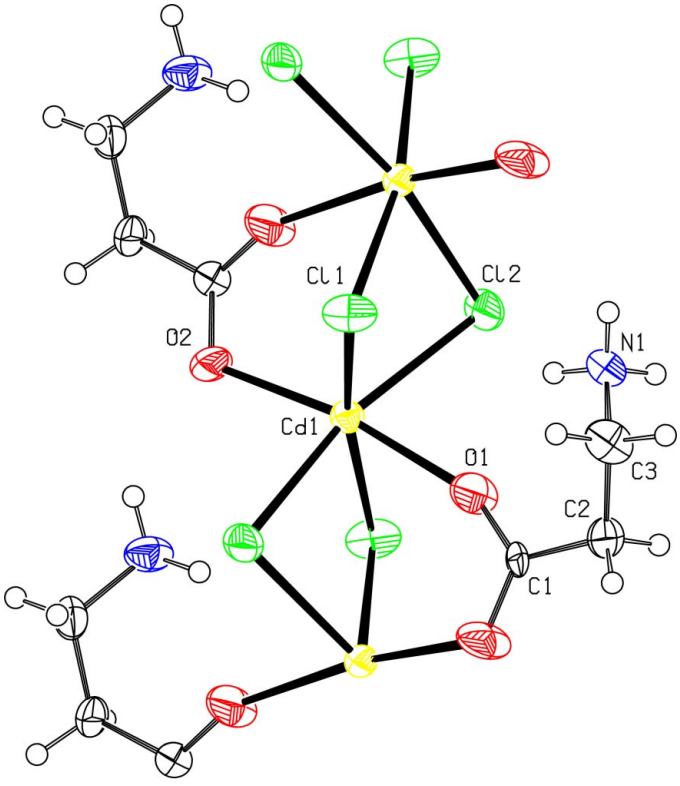


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

atom, forming a square plane (planar within 0.005 Å). These square planes extend infinitely along the shortest axis, *a*. The angle between adjacent square planes is 156.0 (1)°. These square planes are shared (spanned) by the carboxyl O atoms, which complete the octahedral coordination around the Cd atom. These polyhedra fuse directly by sharing Cl—Cl edges, forming one-dimensional polymeric chains in the [100] direction. The metal–ligand coordination observed in (I) is remarkably similar to those observed in the crystal structures of complexes of $CdCl_2$ with L-alanine, L-proline and hydroxy-L-proline, and distinctly different from glycine–$CdCl_2$ and sarcosine–$CdCl_2$.

The crystal packing of the complex is illustrated in Fig. 2. The polymeric chains form strings along the shortest axis, *a*. Alternate strings are interconnected through hydrogen bonds in which the carboxyl O and Cl atoms participate as acceptors. The crystal packing is also characterized by a head-to-tail S2 sequence, since N1—H1*A*···O2 connects two translationally related amino acids (Vijayan, 1988).

Experimental

Colourless single crystals of the title complex were grown as transparent needles from a saturated aqueous solution containing *β*-alanine and cadmium chloride in a 1:1 stoichiometric ratio.

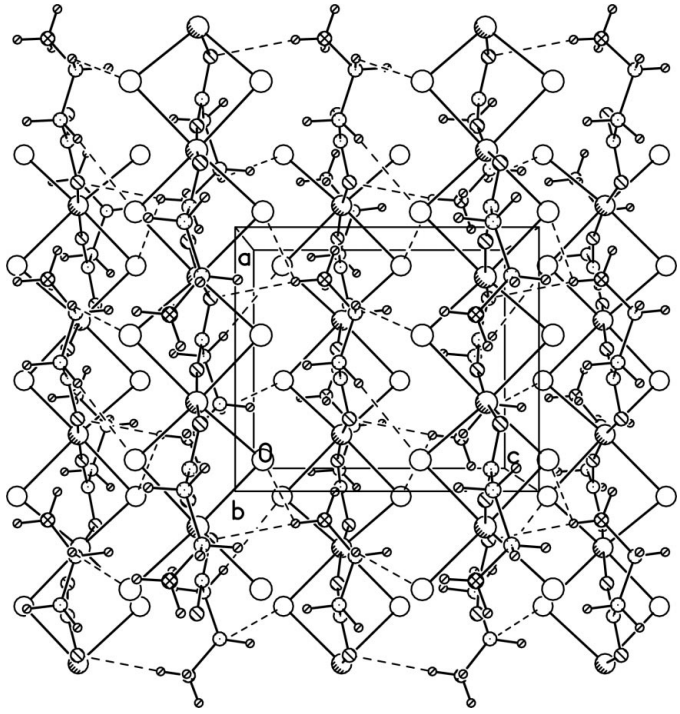


Figure 2
Crystal packing diagram, viewed down the *b* axis.

Crystal data

$[CdCl_2(C_3H_7NO_2)]$
M_r = 272.40
Orthorhombic, $Pna2_1$
a = 6.9391 (10) Å
b = 12.945 (2) Å
c = 7.9714 (10) Å
V = 716.05 (18) Å^3
Z = 4
D_x = 2.527 Mg m^{-3}
D_m = 2.53 Mg m^{-3}
D_m measured by flotation in a mixture of carbon tetrachloride and bromoform
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 12–18°
μ = 3.72 mm^{-1}
T = 293 (2) K
Hexagonal needle, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.42, T_{max} = 0.68
1727 measured reflections
673 independent reflections
652 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°
$h = 0 \rightarrow 8$
$k = -15 \rightarrow 15$
$l = -9 \rightarrow 9$
2 standard reflections
every 100 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.23
673 reflections
83 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 1.0571P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0162 (18)
Absolute structure: Flack (1983); 351 Friedel reflections
Flack parameter = 0.05 (11)

Table 1
Selected geometric parameters (Å, °).

Cd1—O2	2.278 (5)	Cl2—Cd1^{ii}	2.609 (4)
Cd1—O1^{i}	2.348 (5)	O1—C1	1.221 (8)
Cd1—Cl1^{i}	2.612 (5)	O1—Cd1^{ii}	2.348 (5)
Cd1—Cl2^{i}	2.609 (5)	O2—C1	1.259 (10)
Cd1—Cl1	2.631 (5)	C1—C2	1.520 (8)
Cd1—Cl2	2.627 (4)	C2—C3	1.498 (12)
Cl1—Cd1^{ii}	2.612 (5)		
O2—Cd1—O1^{i}	170.6 (3)	Cl1^{i}—Cd1—Cl1	92.05 (16)
O2—Cd1—Cl1^{i}	85.2 (3)	Cl2^{i}—Cd1—Cl1	167.67 (18)
O1^{i}—Cd1—Cl1^{i}	85.8 (4)	O2—Cd1—Cl2	108.8 (3)
O2—Cd1—Cl2^{i}	93.3 (3)	O1^{i}—Cd1—Cl2	80.3 (4)
O1^{i}—Cd1—Cl2^{i}	83.4 (4)	Cl1^{i}—Cd1—Cl2	166.08 (19)
Cl1^{i}—Cd1—Cl2^{i}	86.27 (6)	Cl2^{i}—Cd1—Cl2	93.17 (15)
O2—Cd1—Cl1	98.7 (3)	Cl1—Cd1—Cl2	85.52 (6)
O1^{i}—Cd1—Cl1	84.3 (4)		
O1—C1—C2—C3	−24 (3)	C1—C2—C3—N1	62.5 (17)
O2—C1—C2—C3	145.0 (15)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.89	2.53	3.227 (10)	136
N1—H1B···O2^{ii}	0.89	2.48	3.317 (16)	157
N1—H1B···Cl1^{iii}	0.89	2.69	3.212 (9)	119
N1—H1C···O1	0.89	2.10	2.732 (10)	127
N1—H1C···Cl2^{iv}	0.89	2.54	3.262 (11)	139

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

All the H atoms were placed in calculated positions and were allowed to ride on their respective parent atoms, with C—H = 0.97 Å and N—H = 0.89 Å.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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