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catena-Poly[cadmium(II)-(μ-3-ammonio-3-phenylpropanoato-κ²*O*:*O*′)-di-μ-chlorido]

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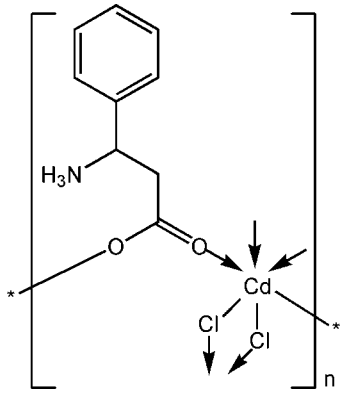
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.041; data-to-parameter ratio = 16.3.

The title compound, $[CdCl_2(C_9H_{11}NO_2)]_n$, is a coordination polymer prepared by the hydrothermal reaction of cadmium(II) chloride and 3-amino-3-phenylpropanoic acid. Geometric parameters are in the usual ranges. The cadmium cation is octahedrally coordinated by four Cl atoms at equatorial sites and two O atoms from two ligands at the axial sites. The material is composed of one-dimensional extended polymeric chains in which two Cl atoms bridge Cd atoms. The crystal structure is stabilized by an intramolecular N—H···O hydrogen bond.

Related literature

For related literature, see: Arki *et al.* (2004); Cohen *et al.* (2002); Zeller *et al.* (1965); Zhao (2007); Qu *et al.* (2004).



Experimental

Crystal data

$[CdCl_2(C_9H_{11}NO_2)]$
M_r = 348.49
Monoclinic, $P2_1/c$
a = 11.879 (2) Å
b = 6.9364 (14) Å
c = 14.072 (3) Å
β = 110.26 (3)°
V = 1087.7 (4) Å³
Z = 4
Mo $K\alpha$ radiation
μ = 2.48 mm⁻¹
T = 293 (2) K
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.592, T_{max} = 0.690
9829 measured reflections
2148 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 0.92
2148 reflections
132 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å⁻³
$\Delta\rho_{min}$ = −0.31 e Å⁻³

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···O1	0.89	2.08	2.735 (3)	130

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PRPKAPPA* (Ferguson, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2165).

References

Arki, A., Tourwe, D., Solymar, M., Fueloep, F., Armstrong, D. W. & Peter, A. (2004). *Chromatographia*, **60**, S43–S54.
Cohen, J. H., Abdel-Magid, A. F., Almond, H. R. Jr & Maryanoff, C. A. (2002). *Tetrahedron Lett.* **43**, 1977–1981.
Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Qu, Z.-R., Zhao, H., Wang, Y.-P., Wang, X.-S., Ye, Q., Li, Y.-H., Xiong, R.-G., Abrahams, B. F., Liu, Z.-G. & Xue, Z.-L. (2004). *Chem. Eur. J.* **10**, 54–60.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zeller, E. A., Ramachander, G., Fleisher, G. A., Ishimaru, T. & Zeller, V. (1965). *Biochem. J.* **95**, 262–269.
Zhao, H. (2007). *Acta Cryst.* E**63**, o3400.

supporting information

Acta Cryst. (2008). E**64**, m1085 [doi:10.1107/S1600536808023179]

catena-Poly[cadmium(II)-(*μ*-3-ammonio-3-phenylpropanoato-κ^2O:O')-di-*μ*-chlorido]

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S1. Comment

Coordination frameworks have received much attention over the past decade because of their potential applications. *β*-amino acids are important molecules due to their pharmacological properties. Recently, there is an increased interest in the enantiomeric preparation of *β*-amino acids as precursors for the synthesis of novel biologically active compounds (Arki *et al.*, 2004; Cohen *et al.*, 2002; Zeller *et al.*, 1965). We report here the crystal structure of the title compound, which was obtained by the hydrothermal reaction of cadmium chloride and 3-amino-3-phenylpropanoic acid. In the structure of the title compoud, The geometric parameters are in the usual ranges (Zhao, 2007; Qu *et al.*, 2004). The cadmium cation is octahedrally coordinated by four Cl atoms at equatorial sites and two O atoms from two ligands at at axial sites (Fig. 1). The material is composed of one-dimensional extended polymeric chains in which two Cl atoms bridges Cd atoms (Fig. 2). The crystal structure is stabilized by an intramolecular hydrogen bond, (Table 1).

S2. Experimental

A mixture of $CdCl_2$ (0.2 mmol, 0.037 g) and 3-amino-3-phenylpropanoic acid (0.2 mmol, 0.033 g) in H_2O (4 ml) was heated in Pyrex tube at 100°C for two days. After slowly cooling down to room temperature over a period of 12 h, colorless crystals of the title compound suitable for diffraction were isolated.

S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C, N atoms to which they are bonded. C—H = 0.97–0.98 Å, with $1.5U_{eq}$(methyl), C—H = 0.93 Å with U_{iso}(H) = $1.2U_{eq}$(Caromatic) and N—H = 0.89 Å with U_{iso}(H) = $1.5U_{eq}$(N).

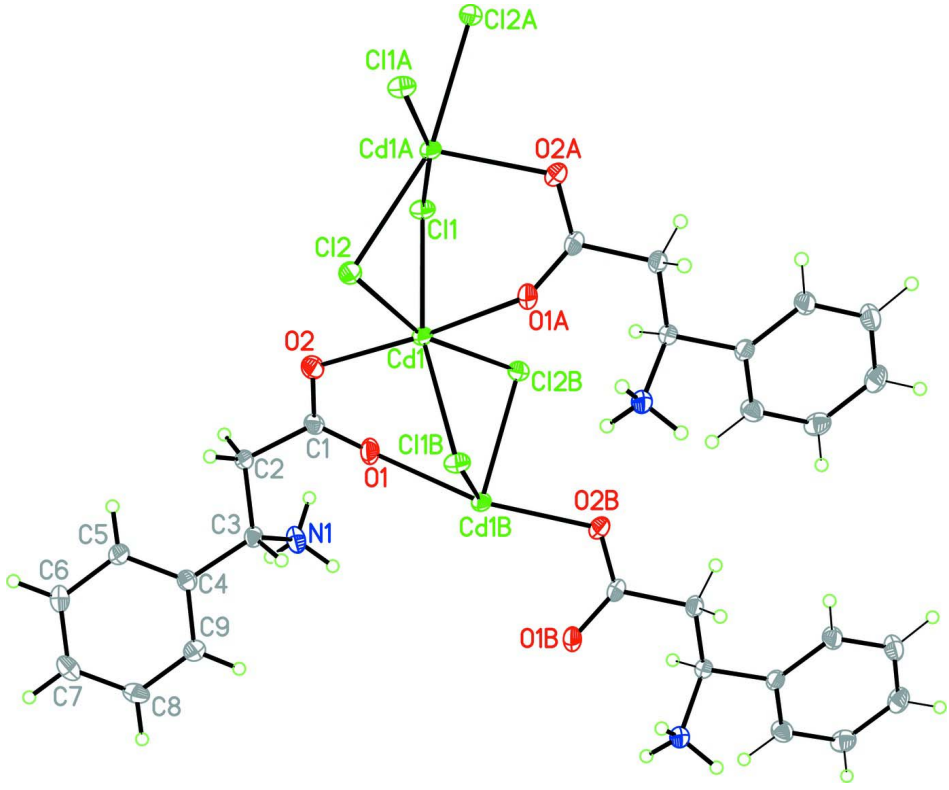

Figure 1

A partial packing diagram of the title compound, with the displacement ellipsoids were drawn at the 30% probability level. [Symmetry codes: (A) -*x*+1, *y* - 1/2, -*z* + 3/2; (B) -*x* + 1, *y* + 1/2, *z* + 3/2.]

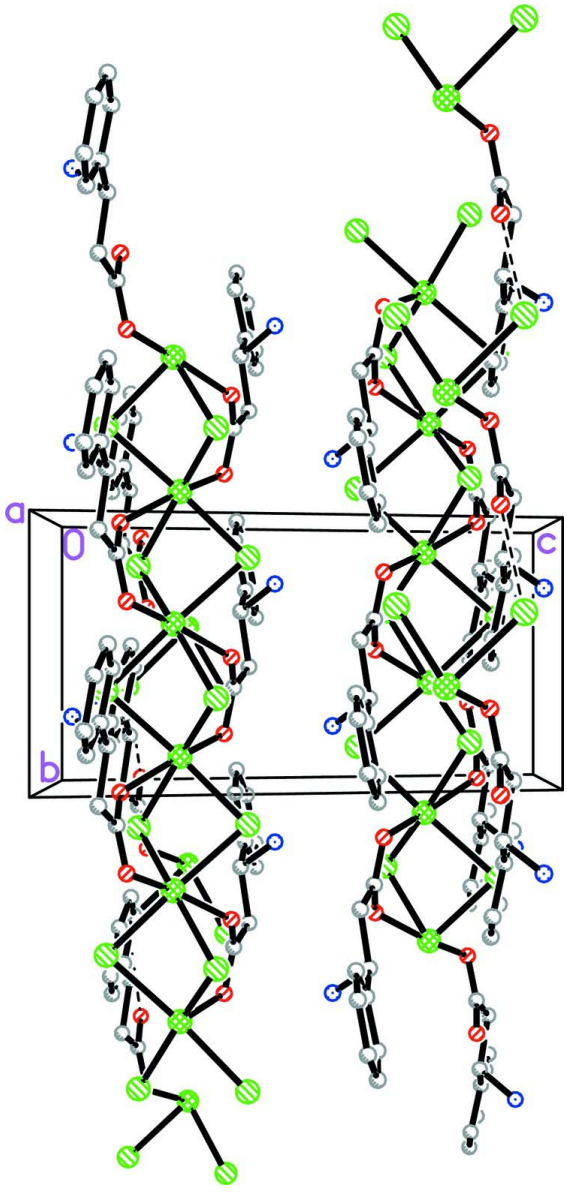

Figure 2

Packing diagram of the title compound, showing the structure along the *b* axis. H atoms have been omitted for clarity.

catena-Poly[cadmium(II)-(*μ*-3-ammonio-3-phenylpropanoato- *κ*^{2}*O*:*O*′)-di-*μ*-chlorido]

Crystal data

[$CdCl_2(C_9H_{11}NO_2)$]
M_r = 348.49
Monoclinic, $P2_1/c$
Hall symbol: -p 2ybc
a = 11.879 (2) Å
b = 6.9364 (14) Å
c = 14.072 (3) Å
β = 110.26 (3)°
V = 1087.7 (4) Å^3
Z = 4
$F(000)$ = 680
D_x = 2.128 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1979 reflections
θ = 3.1–27.5°
μ = 2.48 mm^{-1}
T = 293 K
Prism, colourless
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD Profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.592, T_{max} = 0.690

9829 measured reflections
2148 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.0°, θ_{min} = 3.1°
h = −14→14
k = −8→8
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.041
S = 0.92
2148 reflections
132 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2 + 1.2054P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0014 (2)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.523335 (14)	0.11166 (2)	0.744199 (12)	0.02328 (7)
Cl1	0.40439 (5)	−0.13994 (8)	0.60907 (4)	0.02792 (13)
Cl2	0.67267 (5)	−0.16544 (8)	0.83106 (4)	0.02717 (13)
O1	0.57035 (16)	0.4852 (3)	0.64381 (14)	0.0390 (4)
O2	0.64928 (15)	0.1924 (2)	0.65962 (13)	0.0336 (4)
N1	0.66195 (17)	0.7705 (3)	0.55775 (16)	0.0339 (5)
H1A	0.6566	0.7490	0.4940	0.051*
H1B	0.6696	0.8964	0.5705	0.051*
H1C	0.5959	0.7275	0.5670	0.051*
C1	0.6496 (2)	0.3701 (3)	0.64067 (17)	0.0248 (5)
C2	0.7528 (2)	0.4489 (3)	0.61134 (18)	0.0261 (5)
H2A	0.7376	0.4211	0.5404	0.031*
H2B	0.8263	0.3834	0.6508	0.031*
C3	0.76996 (19)	0.6662 (3)	0.62857 (17)	0.0238 (5)

H3	0.7715	0.6913	0.6975	0.029*
C4	0.8836 (2)	0.7527 (3)	0.62093 (17)	0.0243 (5)
C5	0.9706 (2)	0.6450 (3)	0.6001 (2)	0.0315 (5)
H5	0.9576	0.5147	0.5847	0.038*
C6	1.0771 (2)	0.7308 (4)	0.6019 (2)	0.0373 (6)
H6	1.1362	0.6563	0.5903	0.045*
C7	1.0959 (2)	0.9252 (4)	0.62066 (19)	0.0359 (6)
H7	1.1661	0.9831	0.6198	0.043*
C8	1.0096 (2)	1.0326 (4)	0.6407 (2)	0.0355 (6)
H8	1.0217	1.1640	0.6533	0.043*
C9	0.9049 (2)	0.9479 (4)	0.64233 (19)	0.0318 (5)
H9	0.8483	1.0219	0.6578	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02816 (10)	0.01635 (9)	0.02832 (10)	−0.00091 (7)	0.01356 (7)	−0.00123 (6)
Cl1	0.0328 (3)	0.0208 (3)	0.0266 (3)	0.0000 (2)	0.0057 (2)	0.0004 (2)
Cl2	0.0264 (3)	0.0230 (3)	0.0326 (3)	0.0018 (2)	0.0108 (2)	0.0014 (2)
O1	0.0391 (10)	0.0336 (10)	0.0582 (12)	0.0027 (8)	0.0345 (9)	0.0042 (9)
O2	0.0390 (10)	0.0263 (9)	0.0436 (10)	−0.0021 (8)	0.0244 (8)	0.0053 (8)
N1	0.0275 (10)	0.0356 (12)	0.0424 (12)	0.0052 (9)	0.0169 (9)	0.0133 (10)
C1	0.0291 (12)	0.0263 (12)	0.0220 (11)	−0.0050 (10)	0.0127 (9)	−0.0003 (9)
C2	0.0280 (12)	0.0224 (11)	0.0337 (13)	−0.0031 (9)	0.0182 (10)	−0.0014 (10)
C3	0.0250 (11)	0.0238 (11)	0.0255 (11)	0.0017 (9)	0.0127 (9)	0.0026 (9)
C4	0.0251 (11)	0.0251 (12)	0.0246 (11)	−0.0017 (9)	0.0110 (9)	0.0022 (9)
C5	0.0333 (13)	0.0250 (12)	0.0421 (14)	−0.0014 (10)	0.0205 (11)	−0.0035 (11)
C6	0.0284 (13)	0.0446 (16)	0.0444 (15)	0.0016 (12)	0.0195 (11)	−0.0013 (13)
C7	0.0278 (12)	0.0443 (16)	0.0344 (14)	−0.0108 (11)	0.0095 (11)	0.0023 (12)
C8	0.0366 (14)	0.0259 (12)	0.0401 (15)	−0.0078 (11)	0.0081 (11)	−0.0009 (11)
C9	0.0311 (13)	0.0267 (12)	0.0378 (14)	0.0016 (10)	0.0123 (11)	−0.0028 (11)

Geometric parameters (Å, º)

Cd1—O2	2.2807 (17)	C2—C3	1.529 (3)
Cd1—O1^{i}	2.3888 (18)	C2—H2A	0.9700
Cd1—Cl1^{ii}	2.5965 (8)	C2—H2B	0.9700
Cd1—Cl1	2.6072 (8)	C3—C4	1.515 (3)
Cd1—Cl2	2.6141 (8)	C3—H3	0.9800
Cd1—Cl2^{ii}	2.6880 (8)	C4—C5	1.386 (3)
Cl1—Cd1^{i}	2.5965 (8)	C4—C9	1.391 (3)
Cl2—Cd1^{i}	2.6880 (8)	C5—C6	1.391 (3)
O1—C1	1.246 (3)	C5—H5	0.9300
O1—Cd1^{ii}	2.3888 (18)	C6—C7	1.377 (4)
O2—C1	1.261 (3)	C6—H6	0.9300
N1—C3	1.509 (3)	C7—C8	1.373 (4)
N1—H1A	0.8900	C7—H7	0.9300
N1—H1B	0.8900	C8—C9	1.383 (3)

N1—H1C	0.8900	C8—H8	0.9300
C1—C2	1.524 (3)	C9—H9	0.9300
O2—Cd1—O1^{i}	166.93 (6)	C1—C2—H2A	109.0
O2—Cd1—Cl1^{ii}	98.98 (5)	C3—C2—H2A	109.0
O1^{i}—Cd1—Cl1^{ii}	79.65 (5)	C1—C2—H2B	109.0
O2—Cd1—Cl1	94.10 (5)	C3—C2—H2B	109.0
O1^{i}—Cd1—Cl1	88.67 (5)	H2A—C2—H2B	107.8
Cl1^{ii}—Cd1—Cl1	166.089 (9)	N1—C3—C4	109.76 (18)
O2—Cd1—Cl2	87.88 (5)	N1—C3—C2	109.37 (19)
O1^{i}—Cd1—Cl2	79.47 (5)	C4—C3—C2	116.91 (19)
Cl1^{ii}—Cd1—Cl2	97.59 (3)	N1—C3—H3	106.8
Cl1—Cd1—Cl2	87.56 (3)	C4—C3—H3	106.8
O2—Cd1—Cl2^{ii}	106.76 (5)	C2—C3—H3	106.8
O1^{i}—Cd1—Cl2^{ii}	86.18 (5)	C5—C4—C9	118.5 (2)
Cl1^{ii}—Cd1—Cl2^{ii}	86.24 (3)	C5—C4—C3	123.3 (2)
Cl1—Cd1—Cl2^{ii}	85.47 (3)	C9—C4—C3	118.0 (2)
Cl2—Cd1—Cl2^{ii}	164.176 (16)	C4—C5—C6	120.4 (2)
Cd1^{i}—Cl1—Cd1	85.28 (3)	C4—C5—H5	119.8
Cd1—Cl2—Cd1^{i}	83.32 (3)	C6—C5—H5	119.8
C1—O1—Cd1^{ii}	142.04 (16)	C7—C6—C5	120.5 (2)
C1—O2—Cd1	113.60 (14)	C7—C6—H6	119.7
C3—N1—H1A	109.5	C5—C6—H6	119.7
C3—N1—H1B	109.5	C8—C7—C6	119.2 (2)
H1A—N1—H1B	109.5	C8—C7—H7	120.4
C3—N1—H1C	109.5	C6—C7—H7	120.4
H1A—N1—H1C	109.5	C7—C8—C9	120.8 (2)
H1B—N1—H1C	109.5	C7—C8—H8	119.6
O1—C1—O2	124.1 (2)	C9—C8—H8	119.6
O1—C1—C2	117.9 (2)	C8—C9—C4	120.5 (2)
O2—C1—C2	118.0 (2)	C8—C9—H9	119.8
C1—C2—C3	112.72 (19)	C4—C9—H9	119.8

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, *y*+1/2, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O1	0.89	2.08	2.735 (3)	130