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Di-*μ*-chloro-bis[(2-pyridinecarboxylato-*N*,*O*)-(2-pyridinecarboxylic acid-*N*,*O*)cadmium(II)] ethanol solvate

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Key indicators

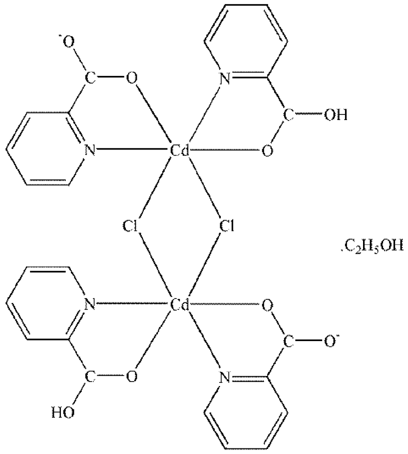
Single-crystal X-ray study
T = 296 K
Mean *σ*(C–C) = 0.008 Å
H-atom completeness 76%
Disorder in solvent or counterion
R factor = 0.035
wR factor = 0.106
Data-to-parameter ratio = 19.2

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

In the title compound, $[Cd_2Cl_2(C_6H_4NO_2)_2(C_6H_5NO_2)_2]\cdot C_2H_5OH$, each Cd atom has a distorted octahedral coordination geometry defined by two N atoms of the pyridine rings, two O atoms of the carboxylate groups and two Cl atoms. Two bridging Cl atoms and an ethanol solvent molecule lie on mirror planes. Symmetrical hydrogen bonds link the carboxylate/carboxylic acid ligands of adjacent molecules.

Comment

2-Pyridinecarboxylic acid is one of the tryptophan metabolites and up until now the crystal structures of its Ni^{II} and Zn^{II} (Takenaka *et al.*, 1970), Cu^{II} (Faure *et al.*, 1973) and Mn^{II} (Okabe & Koizumi, 1998) complexes have been determined. Kinetic studies of Co^{II}, Cu^{II} and Ni^{II} complexes in solution have also been reported (Das & Dash, 1993).



(I)

In this study, the structure of a cadmium complex, (I), of 2-pyridinecarboxylic acid has been determined. The Cd atom is coordinated octahedrally by N atoms of two pyridine rings [Cd1—N1 2.326 (5) Å and Cd1—N8 2.307 (5) Å], two O atoms of the carboxylic acid groups [Cd1—O1 2.318 (5) Å and Cd1—O3 2.334 (5) Å] and two Cl atoms [Cd1—Cl1 2.586 (2) Å and Cd1—Cl2 2.608 (2) Å]. The angles around the Cd atom are considerably distorted from ideal octahedral values of 90/180°. The main distortions are those of the chelate rings with narrow O—Cd—N angles: O1—Cd1—N1 72.3 (2)° and O3—Cd1—N8 71.3 (2)°. These values are much smaller than those observed in other metal complexes [O—Ni—N 81° and O—Zn—N 80° (Takenaka *et al.*, 1970), and O—Cu—N 83.6 (1)° (Faure *et al.*, 1973)] and similar to those in the Mn

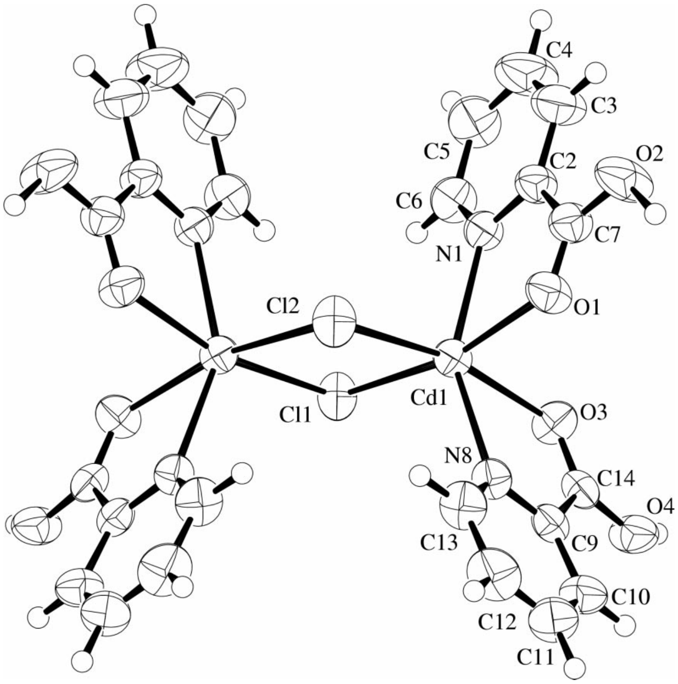


Figure 1
*ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. Ellipsoids for non-H atoms correspond to 50% probability.

complex [O2—Mn1—N1 74.61 (7)° and O4—Mn1—N2 73.00 (7)°]. The 2-pyridinecarboxylic acid and 2-pyridinecarboxylate ligands lie roughly perpendicular to one another, a typical torsion angle being O1—Cd1—O3—C14 of 87.5 (5), and all corresponding pairs of ligand atoms lie in *cis* positions. The carboxyl group is nearly coplanar with the pyridine ring plane; O1—C7—C2—N1 −3.7 (10)° and O3—C14—C9—N8 3.4 (9)°.

In the crystal packing, the complex molecules are bridged *via* carboxylic H atoms. One H atom bonds to each carboxylate group of two adjacent complex molecules, so that two carboxylate anions share the positive charge of one H^+.

Experimental

A single colorless crystal was obtained by slow evaporation of a 90% ethanol–water solution of a 4:1 molar ratio mixture of 2-pyridinecarboxylic acid and $CdCl_2{\cdot}2.5H_2O$ at room temparature.

Crystal data

$[Cd_2Cl_2(C_6H_4NO_2)_2(C_6H_5NO_2)_2]{\cdot}C_2H_6O$
$M_r = 840.29$
Orthorhombic, *Pbcm*
$a = 9.891\ (2)$ Å
$b = 15.443\ (1)$ Å
$c = 20.664\ (2)$ Å
$V = 3156\ (1)$ Å^3
$Z = 4$
$D_x = 1.768$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 14.7$–$14.9°$
$\mu = 1.57$ mm^{-1}
$T = 296.2$ K
Plate, colorless
$0.50 \times 0.20 \times 0.15$ mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.525$, $T_{max} = 0.790$
3725 measured reflections
3725 independent reflections
2525 reflections with $F^2 > 2\sigma(F^2)$
$\theta_{max} = 27.5°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 20$
$l = 0 \rightarrow 26$
3 standard reflections every 150 reflections intensity decay: 1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.106$
$S = 1.58$
3725 reflections
194 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + \{0.03[\mathrm{Max}(F_o^2,0) + 2F_c^2]/3\}^2]$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -1.09$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—Cl1	2.588 (1)	Cd1—O3	2.332 (3)
Cd1—Cl2	2.608 (1)	Cd1—N1	2.326 (4)
Cd1—O1	2.313 (3)	Cd1—N8	2.309 (4)
Cl1—Cd1—Cl2	87.07 (4)	O1—Cd1—O3	93.0 (1)
Cl1—Cd1—O1	166.57 (9)	O1—Cd1—N1	72.0 (1)
Cl1—Cd1—O3	92.41 (8)	O1—Cd1—N8	86.3 (1)
Cl1—Cd1—N1	95.63 (9)	O3—Cd1—N1	91.1 (1)
Cl1—Cd1—N8	107.04 (10)	O3—Cd1—N8	71.2 (1)
Cl2—Cd1—O1	90.61 (9)	N1—Cd1—N8	151.5 (1)
Cl2—Cd1—O3	166.10 (9)	Cd1—Cl1—Cd1^{i}	93.35 (5)
Cl2—Cd1—N1	102.8 (1)	Cd1—Cl2—Cd1^{i}	92.43 (5)
Cl2—Cd1—N8	95.61 (10)		

Symmetry code: (i) $x, y, \frac{3}{2} - z$.

All H atoms were initially located from difference Fourier maps. All except those on carboxylate groups were positioned with ideal geometry.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *TEXSAN*; molecular graphics: *ORTEP* II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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