Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[[tris(pyridine-κN)cadmium(**II**)]-μ-{2-[3-(1-carboxylatomethyl)-4-nitrophenyl]-propionato-$\kappa^2 O,O'$}] dihydrate]

Shan Gao,[a] Li-Hua Huo,[a] Xian-Fa Zhang[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Chemical Technology, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 25 October 2004
Accepted 29 October 2004
Online 6 November 2004

The dicarboxylate dianion in the title compound, $[Cd(C_5H_5N)_3(C_{11}H_9NO_6)]\cdot 2H_2O$, uses its carboxylatomethyl arm to chelate to one Cd atom and the 1-carboxylatoethyl arm to bind to another Cd atom through only one terminal O atom, giving rise to a polymeric chain that runs along $[10\overline{1}]$. The octahedral geometry of the Cd atom is completed by the N atoms of three pyridine N-atom donors.

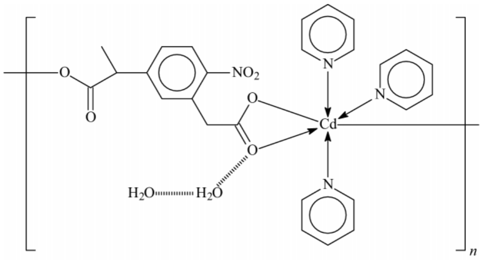
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.037
wR factor = 0.094
Data-to-parameter ratio = 17.3

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

Comment

We have recently synthesized 2-(3-carboxymethyl-4-nitrophenyl)propionic acid (Huo *et al.*, 2004) for complexation studies with metal systems. In the title cadmium derivative, the dicarboxylate dianion uses its acetate arm to chelate to one Cd atom and the propionate arm to bind to another Cd atom through only one terminal O. The six-coordinate geometry is distorted owing to the proximity of the uncoordinated O atom (Fig. 1). In the acetate arm, the C—O single and double bonds are not significantly different [1.254 (3) and 1.241 (4) Å], as are those in the propionate arm [1.249 (4) and 1.236 (4) Å]. Nevertheless, if the shorter of the pair of bonds is regarded as the double bond, then the water molecule O1*w* forms hydrogen bonds to the carbonyl O atom of the same dianion. On the other hand, the O2*w* water molecule forms hydrogen bonds to the O1*w* O atom and also to the uncoordinated carbonyl O atom (Table 2). The resulting structure assumes a chain motif along $[10\overline{1}]$. The monodentate/bidentate nature of the dianion contrasts with the monodentate nature of both arms in the tripyridinecadmium benzene-1,3-dioxyacetate complex; the six-coordinate geometry is completed by a water ligand that engages in hydrogen-bonding interactions (Gao *et al.*, 2004).



(I)

The tripyridine adduct of cadmium bis(4-hydroxybenzoate) also displays a chelating carboxylate anion and a unidentate carboxylate anion; the compound crystallizes as a pyridine solvate (Shnulin *et al.*, 1981).

Experimental

The title complex was prepared by the addition of 2-(3-carboxymethyl-4-nitrophenyl)propionic acid (5.06 g, 20 mmol) (Gao *et al.*, 2004) and pyridine (1.5 ml) to an aqueous solution of cadmium nitrate tetrahydrate (6.17 g, 20 mmol). The resulting mixture was heated for 30 min. Yellow crystals separated from the solution after several days. Analysis calculated for $C_{26}H_{28}CdN_4O_8$: C 49.03, H 4.43, N 8.80%; found: C 49.08, H 4.51 N 8.84%.

Crystal data

$[Cd(C_5H_5N)_3(C_{11}H_9NO_6)]\cdot 2H_2O$
$M_r = 636.92$
Monoclinic, $P2_1/n$
$a = 9.748\ (2)$ Å
$b = 19.923\ (4)$ Å
$c = 14.598\ (3)$ Å
$\beta = 95.92\ (3)^\circ$
$V = 2820\ (1)$ Å^3
$Z = 4$
$D_x = 1.500$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 23092 reflections
$\theta = 3.2$–27.5°
$\mu = 0.83$ mm^{-1}
$T = 295\ (2)$ K
Prism, yellow
0.35 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.594$, $T_{max} = 0.865$
25939 measured reflections
6413 independent reflections
4950 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5^\circ$
$h = -10 \rightarrow 12$
$k = -25 \rightarrow 25$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.094$
$S = 1.04$
6413 reflections
371 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 1.0608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.63$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.328 (2)	Cd1—N1	2.364 (3)
Cd1—O2	2.579 (2)	Cd1—N2	2.403 (3)
Cd1—O3^i	2.293 (2)	Cd1—N3	2.330 (3)

O1—Cd1—O2	52.75 (7)	O2—Cd1—N3	101.64 (9)
O1—Cd1—O3^i	137.18 (7)	O3^i—Cd1—N1	86.50 (9)
O1—Cd1—N1	97.66 (9)	O3^i—Cd1—N2	137.08 (8)
O1—Cd1—N2	85.65 (8)	O3^i—Cd1—N3	94.37 (9)
O1—Cd1—N3	90.01 (9)	N1—Cd1—N2	84.35 (9)
O2—Cd1—O3^i	84.75 (7)	N1—Cd1—N3	167.75 (9)
O2—Cd1—N1	90.61 (9)	N2—Cd1—N3	86.74 (9)
O2—Cd1—N2	137.06 (8)		

Symmetry code: (i) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H1w1···O2	0.85 (1)	2.08 (2)	2.882 (4)	159 (4)
O1w—H1w2···O4	0.85 (1)	2.04 (1)	2.851 (3)	160 (3)
O2w—H2w1···O1w	0.86 (1)	2.00 (1)	2.860 (4)	176 (4)
O2w—H2w2···O3^i	0.86 (1)	1.98 (2)	2.812 (4)	165 (4)

Symmetry code: (i) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$.

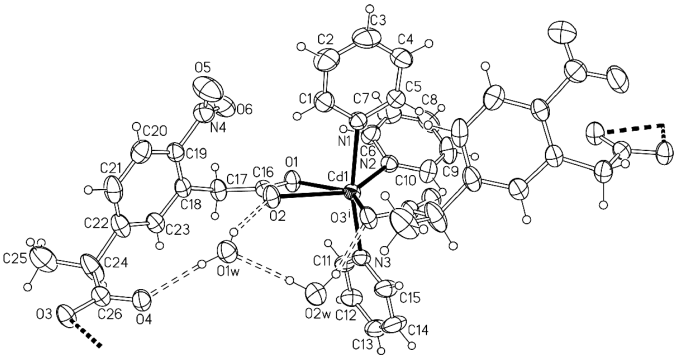


Figure 1
*ORTEP*II (Johnson, 1976) plot of a portion of the polymeric structure of (I) with ellipsoids shown at the 30% probability level. H atoms are drawn as spheres of arbitrary radii. Broken lines indicate hydrogen bonds.

The structure is disordered in the methyl substituent of the 1-carboxylatoethyl arm of the dicarboxylate ligand. The methyl C atom (C25) was refined as two atoms of 0.5 site occupancy, as the occupancy could not be refined; the C24—C25 and C24—C25′ distances were restrained to 1.50 (1) Å and the displacement parameters of the unprimed and primed atoms were made equal to each other. The vibration of the C24 and C25 atoms was restrained to be approximately isotropic. The H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ (aromatic); C–H 0.98 Å and $U_{iso} = 1.2U_{eq}(C)$ (methine); C—H = 0.97 Å and $U_{iso} = 1.2U_{eq}(C)$ (methylene); C–H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ (methyl)], and were included in the refinement in the riding-model approximation. The water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); 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.

We thank the National Natural Science Foundation of China (No. 20101003), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054G036) and the University of Malaya for supporting this study.

References

Gao, S., Liu, J.-W. & Ng, S. W. (2004). *Appl. Organomet. Chem.* **18**, 413–414.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Huo, L.-H., Gao, S., Zhao, H., Zain, S. M. & Ng, S. W. (2004). *Acta Cryst.* E**60**, o1394–o1396.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Shnulin, A. N., Nadzhafov, G. N. & Mamedov, Kh. S. (1981). *Zh. Strukt. Khim.* **22**, 106–113.

Acta Cryst. (2004). E**60**, m1788–m1789 Gao *et al.* • $[Cd(C_5H_5N)_3(C_{11}H_9NO_6)]\cdot 2H_2O$ **m1789**