

**catena-Poly[[[triaquacadmium(II)]- $\mu$ -3-carboxylato-phenoxyacetato- $\kappa^3 O^3, O^{3'}:O''$ ] sesquihydrate]**Shan Gao<sup>a</sup> and Seik Weng Ng<sup>b\*</sup><sup>a</sup>College of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

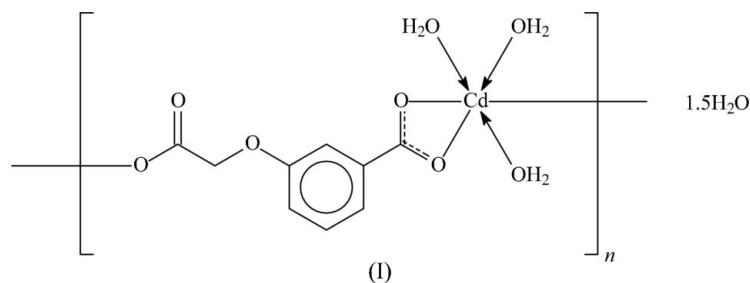
Correspondence e-mail: seikweng@um.edu.my

Received 7 November 2005  
Accepted 21 November 2005  
Online 23 December 2005**Key indicators**Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(C-C) = 0.004$  Å  
H-atom completeness 81%  
Disorder in solvent or counterion  
 $R$  factor = 0.028  
 $wR$  factor = 0.067  
Data-to-parameter ratio = 15.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The dicarboxylate ligand in the title compound,  $[Cd(C_9H_6O_5)(H_2O)_3] \cdot 1.5H_2O$ , bridges triaquacadmium groups into a linear chain; the carboxylate arm that is directly connected to the aromatic ring behaves as a chelate, whereas the carboxylate arm of the oxyacetate portion binds in a monodentate mode. The octahedral environment of cadmium is distorted towards a pentagonal bipyramid, owing to a long  $Cd \cdots O$  interaction of 2.721 (2) Å.

**Comment**

A recent study of the cadmium derivative of 4-carboxyphenoxyacetic acid describes the isolation of a triaqua compound whose seven-coordinate metal exists in a pentagonal-bipyramidal environment (Gao *et al.*, 2005). Both carboxylate arms of the dicarboxylate function in the chelating mode, with the four  $Cd-O$  bond distances ranging from 2.356 (2) to 2.444 (2) Å. The corresponding 3-carboxyphenoxyacetic acid also affords a triaquacadmium compound. However, probably owing to the greater flexibility of the ligand, the packing is less efficient, so that the compound crystallizes with one-and-a-half uncoordinated water molecules, (I) (Fig. 1). Compound (I) exists as a linear chain that propagates along the longest axis of the unit cell. Of the two carboxylate arms, that connected to the aromatic ring functions as a chelate, whereas that belonging to the oxyacetate portion is only monodentate. However, a long-range interaction between  $Cd1$  and  $O5$  is sufficiently close [2.721 (2) Å] to distort the octahedral geometry to a pentagonal bipyramid. The chains are linked by hydrogen bonds (Table 2) into a three-dimensional network.

**Experimental**

Cadmium dinitrate tetrahydrate (0.62 g, 2 mmol) and 3-carboxyphenoxyacetic acid (0.39 g, 2 mmol) were dissolved in a small volume of water (30 ml); 0.2 M sodium hydroxide was added in drops to the solution until it showed a pH of 6. The solution was set aside for the formation of colourless prisms; crystallization took several weeks. CH analysis, calculated for  $C_9H_{15}O_9Cd$ : C 27.89, H 3.90%; found: C 27.16, H 4.03%.

Crystal data

[Cd(C<sub>9</sub>H<sub>6</sub>O<sub>5</sub>)(H<sub>2</sub>O)<sub>3</sub>].1.5H<sub>2</sub>O  
*M<sub>r</sub>* = 387.61  
 Triclinic, *P* $\bar{1}$   
*a* = 7.029 (1) Å  
*b* = 8.829 (2) Å  
*c* = 11.720 (2) Å  
 $\alpha$  = 80.62 (3)°  
 $\beta$  = 72.66 (3)°  
 $\gamma$  = 76.52 (3)°  
*V* = 671.7 (2) Å<sup>3</sup>

*Z* = 2  
*D<sub>x</sub>* = 1.916 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 5430 reflections  
 $\theta$  = 3.1–27.5°  
 $\mu$  = 1.67 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Block, colourless  
 0.36 × 0.25 × 0.18 mm

Data collection

Rigaku RAXIS-RAPID IP diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.460, *T<sub>max</sub>* = 0.753  
 5896 measured reflections

2969 independent reflections  
 2671 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.021  
 $\theta_{max}$  = 27.5°  
*h* = -9 → 9  
*k* = -11 → 11  
*l* = -15 → 14

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.028  
*wR* (*F*<sup>2</sup>) = 0.067  
*S* = 1.05  
 2969 reflections  
 193 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.544P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.71 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.57 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—O1	2.445 (2)	Cd1—O1 <i>w</i>	2.337 (3)
Cd1—O2	2.301 (2)	Cd1—O2 <i>w</i>	2.268 (2)
Cd1—O4 <sup>i</sup>	2.281 (2)	Cd1—O3 <i>w</i>	2.399 (2)
O1—Cd1—O2	55.0 (1)	O2—Cd1—O3 <i>w</i>	95.7 (1)
O1—Cd1—O4 <sup>i</sup>	144.6 (1)	O4 <sup>i</sup> —Cd1—O1 <i>w</i>	92.8 (1)
O1—Cd1—O1 <i>w</i>	97.7 (1)	O4 <sup>i</sup> —Cd1—O2 <i>w</i>	131.2 (1)
O1—Cd1—O2 <i>w</i>	83.8 (1)	O4 <sup>i</sup> —Cd1—O3 <i>w</i>	88.2 (1)
O1—Cd1—O3 <i>w</i>	87.2 (1)	O1 <i>w</i> —Cd1—O2 <i>w</i>	83.1 (1)
O2—Cd1—O4 <sup>i</sup>	90.6 (1)	O1 <i>w</i> —Cd1—O3 <i>w</i>	169.9 (1)
O2—Cd1—O1 <i>w</i>	94.3 (1)	O2 <i>w</i> —Cd1—O3 <i>w</i>	88.7 (1)
O2—Cd1—O2 <i>w</i>	138.2 (1)		

Symmetry code: (i) *x*, *y*, *z* + 1.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1 <i>w</i> —H1 <i>w</i> 1...O4 <i>w</i>	0.85	2.27	3.015 (8)	147
O1 <i>w</i> —H1 <i>w</i> 1...O4 <i>w</i> <sup>v</sup>	0.85	1.83	2.593 (8)	148
O1 <i>w</i> —H1 <i>w</i> 2...O4 <sup>ii</sup>	0.85	1.95	2.732 (3)	153
O2 <i>w</i> —H2 <i>w</i> 1...O3 <i>w</i> <sup>iii</sup>	0.85	2.09	2.841 (3)	147
O2 <i>w</i> —H2 <i>w</i> 2...O5 <sup>iv</sup>	0.85	2.02	2.821 (4)	157
O3 <i>w</i> —H3 <i>w</i> 2...O1 <i>w</i> <sup>v</sup>	0.85	2.21	2.959 (3)	147
O3 <i>w</i> —H3 <i>w</i> 1...O2 <sup>vi</sup>	0.85	1.84	2.684 (3)	175

Symmetry codes: (ii) -*x* + 2, -*y* + 1, -*z* + 1; (iii) -*x* + 1, -*y* + 2, -*z* + 2; (iv) -*x* + 1, -*y* + 2, -*z* + 1; (v) *x* - 1, *y*, *z*; (vi) -*x* + 1, -*y* + 1, -*z* + 2.

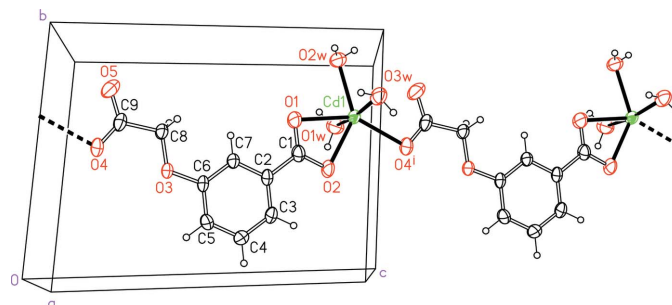


Figure 1

A plot of a portion of the chain structure of (I). The disordered uncoordinated water molecules are not shown. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) *x*, *y*, 1 + *z*.]

The carbon-bound H atoms were positioned geometrically [C—H 0.93 or 0.97 Å] and were included in the refinement in the riding-model approximation, with *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C). The H atoms of the coordinated water molecules were similarly treated [O—H 0.85 Å, *U<sub>iso</sub>*(H) = 1.5*U<sub>eq</sub>*(O)]; these were rotated to fit the electron density.

Of the two independent uncoordinated water molecules, one is disordered over two positions (O4*w* and O4*w*<sup>'</sup>), while the other (O5*w*) is disordered over an inversion centre. A consideration of possible hydrogen-bonding interactions led to the assignment of half occupancies for these atoms. H atoms could not be placed in any chemically sensible positions owing to the disorder. Atom O4*w* is 3 Å from O5*w*<sup>ii</sup> while O4*w*<sup>'</sup> is 2.7 Å from O5*w* [symmetry code: (ii) 3 - *x*, 2 - *y*, 1 - *z*].

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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

References

Gao, S., Liu, J.-W., Huo, L.-H. & Zhao, J.-G. (2005). *Acta Cryst.* E61, m1092–m1094.  
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.  
 Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
 Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.  
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.