

Ying-Hui Xiao,<sup>a</sup> 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

**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
 H-atom completeness 81%  
 Disorder in solvent or counterion  
 R factor = 0.047  
 wR factor = 0.173  
 Data-to-parameter ratio = 16.5

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

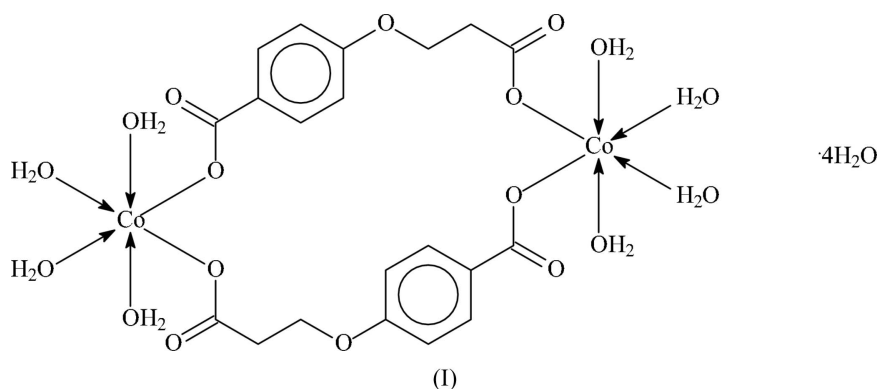
**Bis[ $\mu$ -3-(4-carboxylatophenoxy)propionato- $\kappa^2\text{O}:\text{O}'$ ]bis[tetraaquacobalt(II)] tetrahydrate**

In the title compound,  $[\text{Co}_2(\text{C}_{10}\text{H}_8\text{O}_5)_2(\text{H}_2\text{O})_8]\cdot 4\text{H}_2\text{O}$ , two tetraaquacobalt(II) cations are bridged by two 3-(4-carboxylatophenoxy)propionate dianions across a center of inversion, giving rise to a dinuclear molecule; the coordinating O atoms that comprise the octahedral coordination polyhedron around the metal are *cis* to each other. Hydrogen bonds link the dinuclear molecules into a three-dimensional network. The disordered uncoordinated water molecules occupy cavities within the framework.

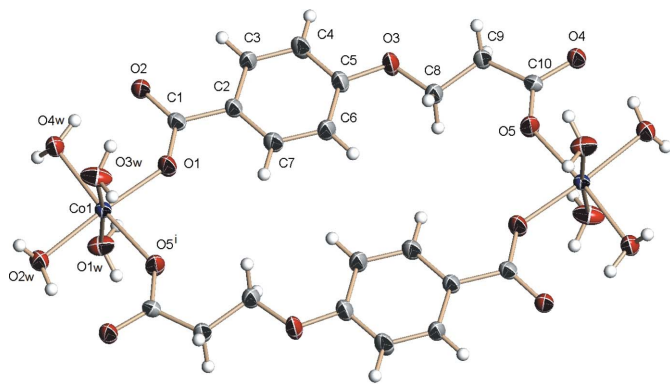
Received 28 July 2006  
 Accepted 16 August 2006

**Comment**

Our studies have addressed the metal derivatives of carboxyphenoxyacetic acids. For 4-carboxyphenoxyacetic acid, the cobalt(II) derivatives that have been characterized by X-ray crystallography include the 4,4'-bipyridine adduct (Deng *et al.*, 2005) and the 1,10-phenanthroline adduct (Gao *et al.*, 2005). The tetraaquabis(4-carboxyphenoxyacetato)cobalt(II) homolog, whose structure has been reported previously (Kennard *et al.*, 1984), consists of a discrete centrosymmetric molecule whose metal atom is covalently linked to the aliphatic carboxyl group instead of the aromatic one. This feature is also noted in the structure of tetraaquabis(3-carboxyphenoxyacetato)cobalt(II) (Li *et al.*, 2004).



The inclusion of another methylene linkage in the dianion leads to the formation of a centrosymmetric dinuclear molecule which crystallizes as a tetrahydrate, (I) (Fig. 1). The dianion functions in a bridging mode and binds covalently through the aromatic and aliphatic carboxyl groups. The two Co—O bonds, which are *cis* to each other around the Co atom, are not statistically distinguishable. Hydrogen bonds involving the coordinated water molecules link the dinuclear molecules



**Figure 1**

Plot of the dinuclear title compound; the disordered water molecules are not shown. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. [Symmetry code: (i)  $2 - x, 1 - y, 1 - z$ .]

into a three-dimensional network (Table 2). There are cavities within the network which are occupied by the uncoordinated water molecules; however, the role of these molecules is unclear as they are disordered.

## Experimental

Cobalt(II) acetate trihydrate (2.28 g, 10 mmol) was added to a hot aqueous solution of 4-carboxyphenoxypropionic acid (2.10 g, 10 mmol) (Gao & Ng, 2006). Sodium hydroxide (0.1 M) was added dropwise until the solution registered a pH of 6. Pink crystals separated from the filtered solution after several days. As the CH elemental percentages of the bulk crystals did not fit the expected  $C_{20}H_{40}O_{22}Co_2$  formulation, the crystal selected for the diffraction study is probably not representative of the bulk compound.

### Crystal data

$[Co_2(C_{10}H_8O_5)_2(H_2O)_8] \cdot 4H_2O$   
 $M_r = 750.38$   
 Monoclinic,  $P2_1/c$   
 $a = 18.277$  (4) Å  
 $b = 7.281$  (2) Å  
 $c = 11.303$  (2) Å  
 $\beta = 96.84$  (2)°  
 $V = 1493.4$  (5) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.669$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 1.20$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 Block, pink  
 $0.37 \times 0.29 \times 0.18$  mm

### Data collection

Rigaku RAXIS-RAPID IP diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{min} = 0.651, T_{max} = 0.795$

14137 measured reflections  
 3422 independent reflections  
 2336 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.036$   
 $\theta_{max} = 27.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.173$   
 $S = 1.15$   
 3422 reflections  
 208 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2 + 4.709P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.47$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.00$  e Å<sup>-3</sup>

**Table 1**  
Selected geometric parameters (Å, °).

Co1—O1	2.020 (3)	Co1—O2w	2.119 (3)
Co1—O5 <sup>i</sup>	2.055 (3)	Co1—O3w	2.086 (4)
Co1—O1w	2.096 (3)	Co1—O4w	2.141 (3)
O1—Co1—O5 <sup>i</sup>	87.5 (1)	O5 <sup>i</sup> —Co1—O4w	174.6 (1)
O1—Co1—O1w	91.2 (2)	O1w—Co1—O2w	86.3 (1)
O1—Co1—O2w	175.8 (1)	O1w—Co1—O3w	173.5 (1)
O1—Co1—O3w	94.9 (2)	O1w—Co1—O4w	89.3 (1)
O1—Co1—O4w	87.6 (1)	O2w—Co1—O3w	87.7 (1)
O5 <sup>i</sup> —Co1—O1w	92.9 (2)	O2w—Co1—O4w	95.8 (1)
O5 <sup>i</sup> —Co1—O2w	89.3 (1)	O3w—Co1—O4w	88.8 (1)
O5 <sup>i</sup> —Co1—O3w	89.5 (2)		

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

**Table 2**  
Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1w—H1w1 $\cdots$ O4 <sup>ii</sup>	0.85	2.02	2.828 (5)	158
O1w—H1w2 $\cdots$ O2 <sup>iii</sup>	0.85	1.96	2.774 (5)	159
O2w—H2w1 $\cdots$ O5w	0.85	2.03	2.804 (8)	150
O2w—H2w2 $\cdots$ O4 <sup>i</sup>	0.85	1.94	2.722 (4)	153
O3w—H3w1 $\cdots$ O2 <sup>iv</sup>	0.85	2.09	2.858 (5)	151
O3w—H3w2 $\cdots$ O4 <sup>v</sup>	0.85	1.94	2.737 (5)	156
O4w—H4w1 $\cdots$ O2	0.85	1.89	2.682 (4)	154
O4w—H4w2 $\cdots$ O5w <sup>vi</sup>	0.85	2.01	2.850 (8)	171

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

The carbon-bound H atoms were positioned geometrically ( $C-H = 0.93-0.97$  Å) and were included in the refinement in the riding-model approximation, with  $U(H) = 1.2U_{eq}(C)$ . The H atoms of the coordinated water molecules were placed at chemically sensible positions on the basis of hydrogen bonds, but these were not refined; their displacement parameters were similarly tied. The two uncoordinated water molecules are disordered over three positions; each was about 2 Å from the other two. As the occupancies of O5w', O5w'' and O5w''' refined to 0.56, 0.59 and 0.57; each position was then assigned a two-thirds site occupancy. The final difference Fourier map had a large hole at 1.44 Å from H6. H atoms could not be placed in any chemical sensible positions owing to the disorder.

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: *ORTEP* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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

## References

- Deng, Z.-P., Gao, S., Huo, L.-H. & Zhao, J.-G. (2005). *Acta Cryst.* **E61**, m2550–m2552.  
 Gao, S., Huo, L.-H., Gu, C.-S., Liu, J.-W. & Zhao, J.-G. (2005). *Acta Cryst.* **E61**, m496–m498.  
 Gao, S. & Ng, S. W. (2006). *Acta Cryst.* **E62**, o3420–o3421.  
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

- Johnson, C. K. (1976). *ORTEP II*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- Kennard, C. H. L., Smith, G., O'Reilly, E. J. & Manoharan, P. T. (1984). *Inorg. Chim. Acta*, **82**, 35–40.
- Li, S.-J., Gu, C.-S., Gao, S., Zhao, H., Zhao, J.-G. & Huo, L.-H. (2004). *Chin. J. Struct. Chem.* **23**, 835–838.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSK (2002). *CrystalStructure*. Rigaku/MSK Inc. The Woodlands, Texas, USA.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.