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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.041  
 $wR$  factor = 0.096  
Data-to-parameter ratio = 14.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Hexaaquacadmium(II) bis{[*N*-(2-oxidobenzyl-  
idene)alanyl-glycinato]cuprate(II)} dodecahydrate

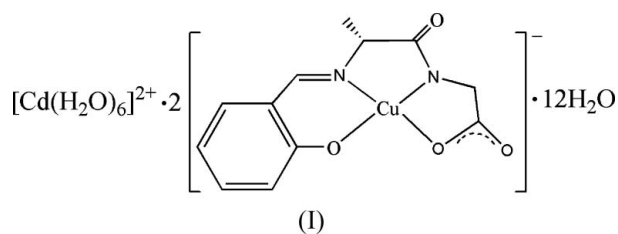
In the title compound,  $[\text{Cd}(\text{H}_2\text{O})_6][\text{Cu}(\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_4)]_2 \cdot 12\text{H}_2\text{O}$ , the  $\text{Cd}^{2+}$  ion lies on an inversion center and the coordination by six aqua ligands is slightly distorted octahedral. The  $\text{Cu}^{\text{II}}$  atom has a square-planar coordination with two N and two O atoms of the tetradentate Schiff base ligand  $L^{3-}$ , which was derived from alanyl-glycine and salicylaldehyde. The  $[\text{Cd}(\text{H}_2\text{O})_6]^{2+}$  cations and  $[\text{CuL}]^-$  anions each form columns along the  $c$  axis; these are well segregated from each other.

Received 30 May 2006

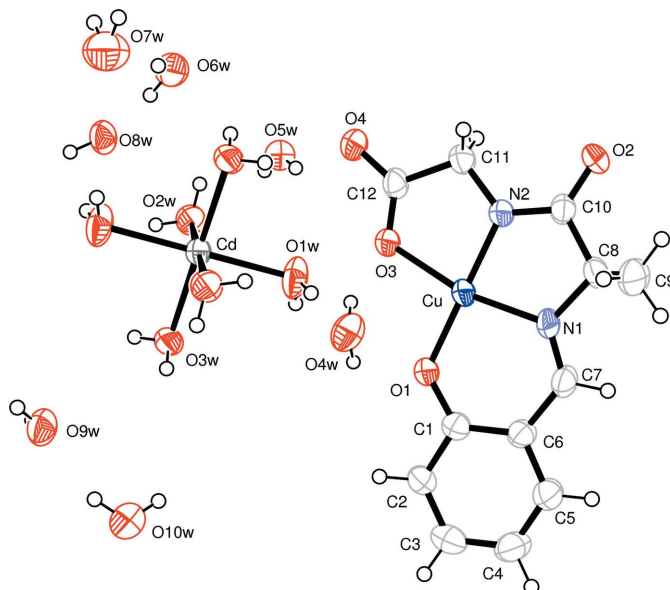
Accepted 12 June 2006

## Comment

We are making a systematic investigation of metal complexes of Schiff bases derived from simple peptides, to which little attention has been given, and have recently reported a series of  $\text{Cu}^{\text{II}}$  complexes of Schiff base ligands resulting from the condensation of glycyl-glycine with salicylaldehyde (Zou *et al.*, 2003, 2004; Liu *et al.*, 2004). In these complexes, hydrogen bonds and  $\pi$ - $\pi$  stacking interactions generally exist. Here we report the synthesis and the structure of the title compound, (I).



The asymmetric unit of (I) consists of one  $[\text{CuL}]^-$  anion ( $\text{H}_3\text{L}$  is a Schiff base derived from alanyl-glycine and salicylaldehyde), one half-cation ( $\text{Cd}/\text{O1W}/\text{O2W}/\text{O3W}$ ), five uncoordinated water molecules ( $\text{O4W}$ ,  $\text{O6W}$ ,  $\text{O8W}$ ,  $\text{O9W}$  and  $\text{O10W}$ ) in general positions and half each of two uncoordinated water molecules on twofold axes ( $\text{O5W}$  and  $\text{O7W}$ ).  $[\text{CuL}]^-$  shows approximately square-planar coordination. The deprotonated Schiff base is a triple negatively charged tetradentate ligand, coordinating to the  $\text{Cu}^{\text{II}}$  ion *via* one phenolate O atom ( $\text{O1}$ ), one imine N atom ( $\text{N1}$ ), one deprotonated amide N atom ( $\text{N2}$ ), and one carboxylate O atom ( $\text{O3}$ ). The benzene ring ( $\text{C1}-\text{C6}$ ) and the  $\text{O1}/\text{C1}/\text{C6}/\text{C7}/\text{N1}/\text{Cu}$  chelate ring are almost coplanar, with a dihedral angle of  $1.0$  ( $1$ )°. The  $\text{Cd}^{\text{II}}$  atom lies on an inversion center and the coordination by six aqua ligands is slightly distorted octahedral (Table 1). The anions and cations each form columns along the  $c$  axis; these are well segregated from each other.  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bonds (Table 2) play an important role in the stabilization of the crystal structure.



**Figure 1**  
The structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are related to labeled atoms by the symmetry code (1 - x, 1 - y, 1 - z).

## Experimental

Alanylglycine (5 mmol), salicylaldehyde (5 mmol) and LiOH (10 mmol) were dissolved and refluxed in MeOH/H<sub>2</sub>O (30 ml, 1:1 v/v); CuCl<sub>2</sub>·2H<sub>2</sub>O (5 mmol) was then added to the solution and the resulting solution was adjusted to pH 9–11. Finally, CdCl<sub>2</sub>·6H<sub>2</sub>O (5 mmol) was added. The precipitate was recrystallized from water. Violet crystals of (I) suitable for X-ray diffraction were obtained after one week (yield 42% based on CuCl<sub>2</sub>·2H<sub>2</sub>O).

### Crystal data

[Cd(H <sub>2</sub> O) <sub>6</sub> ][Cu(C <sub>12</sub> H <sub>11</sub> N <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O]	$V = 4378.2$ (13) Å <sup>3</sup>
$M_r = 1058.22$	$Z = 4$
Monoclinic, $C2/c$	$D_x = 1.605$ Mg m <sup>-3</sup>
$a = 28.635$ (5) Å	Mo $K\alpha$ radiation
$b = 11.815$ (2) Å	$\mu = 1.53$ mm <sup>-1</sup>
$c = 14.584$ (3) Å	$T = 298$ (2) K
$\beta = 117.458$ (3)°	Block, violet
	$0.30 \times 0.20 \times 0.15$ mm

### Data collection

Bruker SMART APEX CCD diffractometer	10785 measured reflections
$\varphi$ and $\omega$ scans	3893 independent reflections
Absorption correction: multi-scan (SHELXTL; Bruker, 2000)	2766 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.70$ , $T_{\max} = 0.79$	$R_{\text{int}} = 0.065$
	$\theta_{\text{max}} = 25.1^\circ$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2]$
$wR(F^2) = 0.096$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3893 reflections	$\Delta\rho_{\text{max}} = 0.79$ e Å <sup>-3</sup>
261 parameters	$\Delta\rho_{\text{min}} = -0.56$ e Å <sup>-3</sup>

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

Cu—O1	1.872 (3)	Cd—O1W	2.240 (3)
Cu—N2	1.874 (3)	Cd—O3W	2.270 (3)
Cu—N1	1.926 (3)	Cd—O2W	2.300 (3)
Cu—O3	1.987 (3)		
O1—Cu—N2	179.37 (16)	N1—Cu—O3	166.70 (13)
O1—Cu—N1	95.91 (14)	O1W—Cd—O3W	89.52 (11)
N2—Cu—N1	83.93 (15)	O1W—Cd—O2W	90.25 (12)
O1—Cu—O3	97.30 (12)	O3W—Cd—O2W	84.19 (11)
N2—Cu—O3	82.85 (13)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1A <sup>(i)</sup> ···O3	0.85	2.19	2.703 (4)	118
O1W—H1B <sup>(i)</sup> ···O4W	0.85	1.98	2.692 (5)	140
O2W—H2A <sup>(i)</sup> ···O5W	0.85	2.20	2.746 (4)	122
O2W—H2B <sup>(i)</sup> ···O8W	0.85	2.32	2.740 (4)	111
O3W—H3A <sup>(i)</sup> ···O6W <sup>(i)</sup>	0.85	2.10	2.774 (4)	136
O3W—H3B <sup>(i)</sup> ···O4 <sup>(i)</sup>	0.85	1.96	2.723 (4)	149
O4W—H4A <sup>(i)</sup> ···O7W <sup>(i)</sup>	0.85	2.33	2.836 (6)	119
O4W—H4B <sup>(i)</sup> ···O2W <sup>(ii)</sup>	0.85	2.28	3.124 (5)	175
O5W—H5A <sup>(i)</sup> ···O9W <sup>(i)</sup>	0.85	2.45	2.826 (4)	108
O6W—H6A <sup>(i)</sup> ···O10W <sup>(iii)</sup>	0.85	2.25	2.750 (5)	118
O6W—H6B <sup>(i)</sup> ···O8W	0.85	1.91	2.749 (5)	168
O7W—H7A <sup>(i)</sup> ···O10W <sup>(iii)</sup>	0.85	2.10	2.813 (5)	142
O8W—H8A <sup>(i)</sup> ···O2 <sup>(iv)</sup>	0.85	1.86	2.689 (5)	163
O8W—H8B <sup>(i)</sup> ···O1 <sup>(i)</sup>	0.85	2.02	2.771 (4)	147
O9W—H9D <sup>(i)</sup> ···O2 <sup>(v)</sup>	0.85	2.21	2.643 (4)	111
O9W—H9E <sup>(i)</sup> ···O4 <sup>(i)</sup>	0.85	2.11	2.812 (5)	139
O10W—H10A <sup>(i)</sup> ···O6W <sup>(i)</sup>	0.85	2.00	2.803 (5)	157
O10W—H10B <sup>(i)</sup> ···O9W	0.85	1.92	2.711 (4)	155

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

The water H atoms were located in difference Fourier maps, while other H atoms were positioned geometrically; they were constrained as riding atoms, with O—H = 0.85 Å, C—H = 0.93–0.97 Å, and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C}, \text{O})$  for the methyl group and water molecules.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This work was supported by the National Natural Science Foundation of China.

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