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Key indicators

Single-crystal X-ray study  
 T = 298 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
 R factor = 0.045  
 wR factor = 0.103  
 Data-to-parameter ratio = 14.9

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

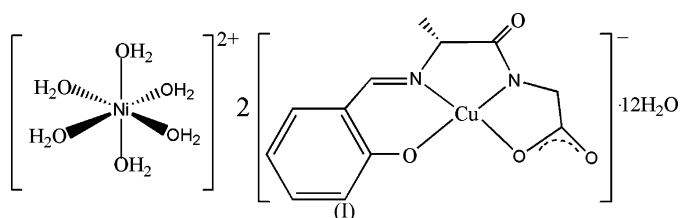
Hexaaquanickel(II) bis{[N-(2-hydroxybenzyl-  
 idene)alanyl-glycinato]cuprate(II)} dodecahydrate

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The crystal structure of the title compound,  $[\text{Ni}(\text{H}_2\text{O})_6][\text{Cu}(\text{C}_{12}\text{H}_{11}\text{N}_2\text{O}_4)]_2 \cdot 12\text{H}_2\text{O}$ , consists of  $\text{Cu}^{\text{II}}$  complex anions,  $\text{Ni}^{\text{II}}$  complex cations and solvent water molecules. The  $\text{Cu}^{\text{II}}$  ion is located on a general position and coordinated by a Schiff base ligand with a square-planar  $\text{CuN}_2\text{O}_2$  geometry. The  $\text{Ni}^{\text{II}}$  ion is located on an inversion center and coordinated by six water molecules in an octahedral geometry.

Comment

As part of our ongoing investigation on metal complexes with Schiff bases, we present here the structure of the title compound, (I).



The crystal structure of (I) consists of  $\text{Cu}^{\text{II}}$  complex anions,  $\text{Ni}^{\text{II}}$  complex cations and solvent water molecules (Fig. 1). The  $\text{Cu}^{\text{II}}$  ion is located on a general position and coordinated by a trivalent Schiff base anion, N-(hydroxybenzylidene)alanyl-glycinate, with a square-planar  $\text{CuN}_2\text{O}_2$  geometry (Table 1). The  $\text{Ni}^{\text{II}}$  ion is located on an inversion center and coordinated by six water molecules in an octahedral geometry.

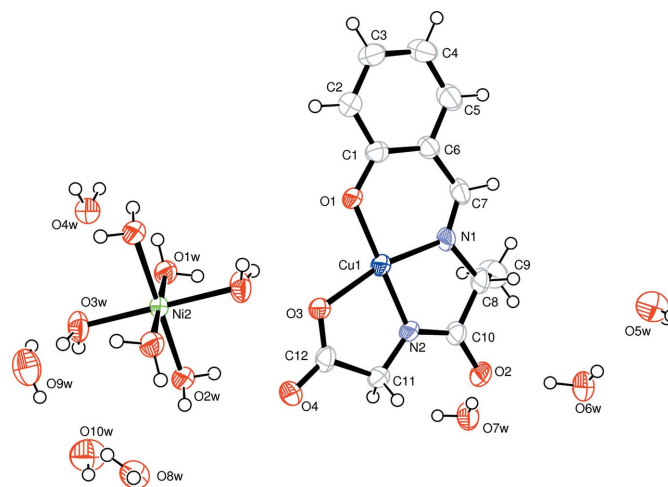


Figure 1  
 The asymmetric unit of (I), together with additional aqua ligands to complete the coordination of Ni2, with 50% probability displacement ellipsoids (arbitrary spheres for H atoms). Unlabeled atoms are related to labeled atoms by  $x + 1, -y + 1, -z + 1$ .

The extensive hydrogen-bonding network (Table 2) helps to stabilize the crystal structure.

### Experimental

A methanol/water solution (30 ml, *v/v* 1:1) containing alanylglycine (5 mmol), salicylaldehyde (5 mmol) and LiOH (10 mmol) was refluxed for 30 min. CuCl<sub>2</sub>·2H<sub>2</sub>O (5 mmol) in water (15 ml) was added and the resulting solution was adjusted to pH 10 with NaOH solution. After stirring at room temperature for 4 h, Ni(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O (5 mmol) in water (5 ml) was added to the solution with stirring. A violet precipitate appeared immediately. After stirring for 30 min, the precipitate was filtered off and recrystallized from water. Single crystals of (I) were obtained after one week.

#### Crystal data

[Ni(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]	<i>V</i> = 4279 (3) Å <sup>3</sup>
<i>M<sub>r</sub></i> = 1004.53	<i>Z</i> = 4
Monoclinic, <i>C2/c</i>	<i>D<sub>x</sub></i> = 1.559 Mg m <sup>-3</sup>
<i>a</i> = 28.314 (9) Å	Mo <i>Kα</i> radiation
<i>b</i> = 11.792 (4) Å	<i>μ</i> = 1.51 mm <sup>-1</sup>
<i>c</i> = 14.407 (5) Å	<i>T</i> = 298 (2) K
<i>β</i> = 117.17 (1)°	Block, violet
	0.30 × 0.20 × 0.15 mm

#### Data collection

Bruker SMART APEX CCD diffractometer	10637 measured reflections
<i>φ</i> and <i>ω</i> scans	3879 independent reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 2002)	2660 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T<sub>min</sub></i> = 0.70, <i>T<sub>max</sub></i> = 0.79	<i>R<sub>int</sub></i> = 0.078
	<i>θ<sub>max</sub></i> = 25.2°

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	H-atom parameters constrained
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.045	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0438 <i>P</i> ) <sup>2</sup> ]
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.103	where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
<i>S</i> = 0.93	(Δ/ <i>σ</i> ) <sub>max</sub> = 0.001
3879 reflections	Δ <i>ρ</i> <sub>max</sub> = 0.64 e Å <sup>-3</sup>
261 parameters	Δ <i>ρ</i> <sub>min</sub> = -0.41 e Å <sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Cu1—O1	1.870 (2)	Ni2—O1 <i>W</i>	2.063 (3)
Cu1—O3	1.989 (2)	Ni2—O2 <i>W</i>	2.059 (2)
Cu1—N1	1.926 (3)	Ni2—O3 <i>W</i>	2.033 (2)
Cu1—N2	1.873 (3)		

**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>A</i> ···O7 <i>W</i> <sup>i</sup>	0.82	1.96	2.732 (4)	156
O1 <i>W</i> —H1 <i>B</i> ···O4 <i>W</i>	0.83	1.97	2.781 (3)	168
O2 <i>W</i> —H2 <i>A</i> ···O8 <i>W</i>	0.85	2.09	2.754 (4)	135
O2 <i>W</i> —H2 <i>B</i> ···O4	0.84	1.98	2.735 (4)	149
O3 <i>W</i> —H3 <i>A</i> ···O9 <i>W</i>	0.92	1.85	2.733 (4)	159
O3 <i>W</i> —H3 <i>B</i> ···O3 <sup>ii</sup>	0.90	1.86	2.722 (4)	159
O4 <i>W</i> —H4 <i>A</i> ···O6 <i>W</i> <sup>iii</sup>	0.79	2.04	2.808 (3)	167
O5 <i>W</i> —H5 <i>A</i> ···O8 <i>W</i> <sup>iv</sup>	0.85	1.99	2.759 (5)	150
O5 <i>W</i> —H5 <i>B</i> ···O8 <i>W</i> <sup>v</sup>	0.83	2.03	2.814 (5)	156
O6 <i>W</i> —H6 <i>A</i> ···O2	0.84	1.81	2.648 (4)	178
O6 <i>W</i> —H6 <i>B</i> ···O5 <i>W</i>	0.82	2.07	2.714 (4)	135
O7 <i>W</i> —H7 <i>A</i> ···O2	0.85	1.85	2.697 (4)	179
O7 <i>W</i> —H7 <i>B</i> ···O1 <sup>vi</sup>	0.86	1.91	2.750 (4)	166
O8 <i>W</i> —H8 <i>B</i> ···O7 <i>W</i> <sup>vii</sup>	0.86	2.23	2.748 (5)	119
O9 <i>W</i> —H9 <i>D</i> ···O1 <i>W</i> <sup>viii</sup>	0.85	2.36	3.114 (4)	149
O9 <i>W</i> —H9 <i>E</i> ···O10 <i>W</i>	0.85	2.04	2.877 (5)	165
O10 <i>W</i> —H10 <i>A</i> ···O5 <i>W</i> <sup>ix</sup>	0.85	2.03	2.813 (5)	153

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

Water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(O). Methyl H atoms were placed in calculated positions with C—H = 0.96 Å and the torsion angle was refined to fit the electron density; *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C). Other H atoms were placed in calculated positions with C—H = 0.93–0.98 Å, and refined in riding mode; *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE-Plus* (Bruker, 2003); data reduction: *SAINTE-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*.

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