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# A Cu–Mn complex of a Schiff base containing alanylglycine: hexaaquamanganese(II) bis{[*N*-(2-oxidobenzylidene)alanylglycinato]cuprate(II)} dodecahydrate

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**Key indicators**

Single-crystal X-ray study
*T* = 295 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.034
*wR* factor = 0.080
Data-to-parameter ratio = 14.2

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



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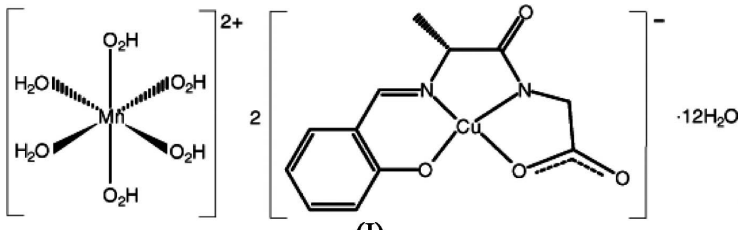
In the title compound, $[Mn(H_2O)_6][Cu(C_{12}H_{11}N_2O_4)]_2\cdot 12H_2O$, the Cu atom has a square-planar coordination with two N and two O atoms of the tetradentate Schiff base ligand. The centrosymmetric cation $[Mn(H_2O)_6]^{2+}$ and anion $[CuL]^-$ (*L* is a Schiff base derived from alanylglycine and salicylaldehyde) occupy a stacking structure within well separated columns along the *c* axis.

## Comment

The title compound, (I), is one of the copper(II) Schiff base complexes derived from alanylglycine and salicylaldehyde. The study of copper(II) Schiff base complexes formed between pyridoxal or analogs and amino acids or small peptides (Koh *et al.*, 1996) is a subject of considerable interest owing to their structural and magnetic properties, and potential antimicrobial, anti-inflammatory and antipyretic activities, together with a superoxide dismutase-like activity (Garcia-Raso *et al.*, 1999).




(I)

The complex crystallizes in the monoclinic space group *C*2/*c*. The asymmetric unit consists of one $[CuL]^-$ anion (*L* is a Schiff base derived from alanylglycine and salicylaldehyde), one half-cation (Mn1, O1*W*, O2*W*, O3*W*), five uncoordinated water molecules in general positions and two uncoordinated water molecules (O4*W* and O9*W*) in special positions. $[CuL]^-$ has an approximately square-planar structure. The deprotonated Schiff base ligand is a triple negatively charged quadridentate ONNO chelant, coordinating to the $Cu^{II}$ ion *via* one phenol O atom (O1), one deprotonated amide N atom (N2), one imine N atom (N1) and one carboxylate O atom (O3). The O1—Cu1—N2 angle of 179.15 (8)° is nearly linear. The benzene ring (C1–C6) and the O1/C1/C6/C7/N1/Cu1 ring are almost coplanar, with a small dihedral angle of 1.13 (10)°. The $Mn^{II}$ ion lies on an inversion center and exhibits essentially octahedral coordination by six aqua ligands.

The anions and cations form well separated columns along the *c* axis in the stacking structure of (I). Intermolecular hydrogen bonds play an important role in the stabilization of the whole structure (Table 2) .

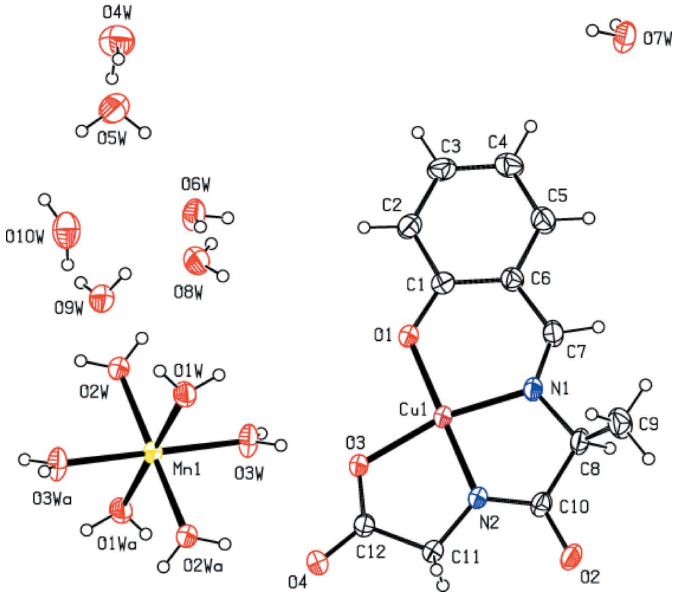



**Figure 1**
View of the structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

## Experimental

The title compound, (I), was prepared from the copper(II) Schiff base complex [Cu*L*] with manganese perchlorate, as described previously (Liu *et al.*, 2004). Suitable crystals of (I) were obtained by evaporation of an aqueous solution. Analysis calculated for $C_{24}H_{58}Cu_2MnN_4O_{26}$: C 28.80, H 5.84, N 5.60%; found: C 28.74, H 5.90, N 5.54%.

### *Crystal data*

$[Mn(H_2O)_6][Cu(C_{12}H_{11}N_2O_4)]_2\cdot 12H_2O$
$M_r$ = 1000.78
Monoclinic, $C2/c$
$a$ = 28.479 (6) Å
$b$ = 11.781 (2) Å
$c$ = 14.483 (3) Å
$\beta$ = 117.280 (10)°
$V$ = 4318.8 (15) Å$^3$
$Z$ = 4
$D_x$ = 1.539 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 1.35 mm$^{-1}$
$T$ = 295 (2) K
Block, red–violet
0.50 × 0.35 × 0.20 mm

### *Data collection*

Bruker SMART APEX CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.551, $T_{max}$ = 0.774
12220 measured reflections
4719 independent reflections
3482 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 27.1°

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.080
$S$ = 0.93
4719 reflections
333 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.8677 (16) | O2—C10 | 1.258 (3) |
| Cu1—O3 | 1.9869 (18) | O3—C12 | 1.275 (3) |
| Cu1—N1 | 1.925 (2) | O4—C12 | 1.235 (3) |
| Cu1—N2 | 1.8698 (19) | N1—C8 | 1.478 (3) |
| Mn1—O3*W* | 2.141 (3) | N1—C7 | 1.267 (3) |
| Mn1—O1*W* | 2.190 (2) | N2—C11 | 1.434 (3) |
| Mn1—O2*W* | 2.1721 (18) | N2—C10 | 1.304 (4) |
| O1—C1 | 1.321 (3) | | |
| O1—Cu1—O3 | 97.25 (7) | Cu1—N1—C7 | 124.95 (18) |
| O1—Cu1—N1 | 95.87 (8) | Cu1—N1—C8 | 114.08 (15) |
| O1—Cu1—N2 | 179.15 (8) | C7—N1—C8 | 120.8 (2) |
| O3—Cu1—N1 | 166.79 (7) | C10—N2—C11 | 123.33 (19) |
| O3—Cu1—N2 | 83.03 (8) | Cu1—N2—C10 | 119.20 (15) |
| N1—Cu1—N2 | 83.83 (9) | Cu1—N2—C11 | 117.18 (17) |
| O2*W*$^i$—Mn1—O3*W* | 90.33 (8) | O1—C1—C2 | 118.6 (2) |
| O3*W*—Mn1—O3*W*$^i$ | 180 | O1—C1—C6 | 124.4 (2) |
| O2*W*—Mn1—O3*W* | 89.67 (8) | N1—C7—C6 | 125.4 (3) |
| O1*W*$^i$—Mn1—O2*W* | 85.14 (7) | N1—C8—C9 | 112.4 (2) |
| O1*W*—Mn1—O2*W* | 94.86 (7) | N1—C8—C10 | 108.0 (2) |
| O1*W*—Mn1—O3*W* | 88.91 (9) | O2—C10—N2 | 125.7 (2) |
| O1*W*—Mn1—O1*W*$^i$ | 180 | O2—C10—C8 | 119.7 (2) |
| O2*W*—Mn1—O3*W*$^i$ | 90.33 (8) | N2—C10—C8 | 114.6 (2) |
| O1*W*$^i$—Mn1—O3*W* | 91.09 (9) | N2—C11—C12 | 107.98 (19) |
| O2*W*—Mn1—O2*W*$^i$ | 180 | O3—C12—O4 | 124.0 (2) |
| Cu1—O1—C1 | 125.71 (17) | O3—C12—C11 | 117.4 (2) |
| Cu1—O3—C12 | 114.25 (17) | O4—C12—C11 | 118.7 (2) |

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

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O9*W* | 0.75 (3) | 2.03 (3) | 2.767 (3) | 173 (3) |
| O1*W*—H1*A*···O9*W* | 0.75 (3) | 2.03 (3) | 2.767 (3) | 173 (3) |
| O1*W*—H1*B*···O7*W*$^{ii}$ | 0.83 (4) | 1.91 (3) | 2.724 (3) | 168 (3) |
| O2*W*—H2*A*···O8*W* | 0.79 (2) | 1.98 (2) | 2.759 (3) | 172 (3) |
| O2*W*—H2*B*···O4$^i$ | 0.79 (2) | 1.93 (2) | 2.722 (3) | 179 (4) |
| O3*W*—H3*A*···O10*W*$^{iii}$ | 0.76 (3) | 1.96 (3) | 2.724 (4) | 179 (4) |
| O3*W*—H3*B*···O3 | 0.81 (3) | 1.91 (3) | 2.714 (3) | 174 (3) |
| O4*W*—H4*W*···O5*W* | 0.98 (4) | 1.85 (4) | 2.808 (4) | 168 (4) |
| O5*W*—H5*A*···O8*W*$^{iv}$ | 0.86 (5) | 1.97 (5) | 2.797 (4) | 164 (5) |
| O5*W*—H5*B*···O6*W* | 0.80 (5) | 1.95 (5) | 2.718 (4) | 159 (5) |
| O6*W*—H6*A*···O2$^v$ | 0.75 (4) | 1.90 (4) | 2.653 (3) | 177 (1) |
| O6*W*—H6*B*···O4$^{vi}$ | 0.79 (3) | 2.00 (3) | 2.789 (3) | 179 (5) |
| O7*W*—H7*A*···O2$^{vii}$ | 0.79 (3) | 1.90 (3) | 2.689 (3) | 174 (3) |
| O7*W*—H7*B*···O1$^v$ | 0.76 (4) | 2.01 (4) | 2.765 (3) | 174 (3) |
| O8*W*—H8*A*···O5*W*$^{viii}$ | 0.78 (4) | 1.97 (4) | 2.734 (4) | 167 (4) |
| O8*W*—H8*B*···O7*W*$^{ii}$ | 0.76 (3) | 1.99 (3) | 2.749 (4) | 174 (3) |
| O9*W*—H9*W*···O6*W* | 0.78 (3) | 2.03 (3) | 2.803 (3) | 174 (3) |

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

The water H atoms were located in difference maps and refined freely [O—H = 0.75 (3)–0.98 (4) Å]. The other H atoms were placed in geometrically idealized positions with C—H distances in the range 0.93–0.98 Å and constrained to ride on their parent atoms with $U_{iso}$(H) = 1.2–1.5$U_{eq}$(C).

Data collection: *SMART* for WNT/2000 (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Bruker, 2000); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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