Acta Cryst. (1980). B**36**, 1645–1646

[(*R*,*S*)-*N*,*N'*-Ethylenebis(serinato)]copper(II) Monohydrate

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(*Received* 28 *January* 1980; *accepted* 3 *March* 1980)

Abstract. $C_8H_{14}CuN_2O_6.H_2O$, $[Cu(C_8H_{14}N_2O_6)].H_2O$, $M_r = 315.8$, monoclinic, $P2_1/c$, $a = 10.516$ (3), $b = 12.204$ (3), $c = 15.631$ (3) Å, $\beta = 143.88$ (2)°, $U = 1182.5$ Å^3, $Z = 4$, $D_m = 1.73$, $D_x = 1.77$ Mg m^{-3}, Cu $K\alpha$ ($\lambda = 1.5418$ Å), $\mu = 2.98$ mm^{-1}. $R = 0.05$ for 1342 independent reflections. Cu is coordinated by two N atoms of imino groups, two O atoms of carboxylate groups and a water molecule in a square-pyramidal polyhedron.

Introduction. As part of the study of chelate-ring conformation in the complexes of amino acid derivatives by theoretical force-field (Pavelčík & Majer, 1978*a*) and X-ray methods (Pavelčík & Majer, 1978*b*) we have investigated the title compound, [Cu(ebser)].H_2O. Crystals were kindly supplied by Dr M. Kotouček. The crystal used for structure determination was of irregular shape (0·275 × 0·250 × 0·175 mm). The intensities of 1424 independent reflections ($0 < 2\theta \leq 115°$) were collected on a Syntex $P2_1$ diffractometer with graphite-monochromated Cu $K\alpha$ radiation and the θ–2θ technique at a scan rate varying from 4·88 to 29·3° min^{-1} in 2θ. The background was measured at each end of the scan for one half the scan time. Two standard reflections monitored after every 98 scans, showed that no correction for instrument instability or crystal decay was required. 1342 reflections with $I > 1.96\sigma(I)$ were considered observed. The intensities were corrected for Lorentz and polarization factors but not for absorption or extinction. The structure was solved by Patterson and Fourier methods. A difference synthesis showed the positions of all the H atoms, including those of the water molecule. The structure was refined by block-diagonal least squares with anisotropic thermal parameters for non-hydrogen atoms and isotropic for H. The function $\sum w(|F_o| - |F_c|)^2$ was minimized; a weighting scheme $w^{-1} = \sigma^2(|F_o|) + (C|F_o|)^2$, where $\sigma(|F_o|)$ is derived from counting statistics and $C = 0.03$, was employed. C was adjusted so that a constant value of $\langle w(|F_o| - |F_c|)^2\rangle$ was obtained in different $|F_o|$ intervals. The final $R = \sum|\Delta F|/\sum|F_o| = 0.0502$ for the observed reflections used in the refinement and 0·0529 including the zero-weighted reflections. The corresponding $R_w = [\sum w|\Delta F|^2/\sum w|F_o|^2]^{1/2} = 0.076$ and

Table 1. *Final atomic coordinates for the nonhydrogen atoms* (×10^4) *with e.s.d.'s in parentheses*

	x	*y*	*z*
Cu(1)	3069 (1)	1932 (0)	1817 (1)
O(1)	2448 (4)	2507 (2)	335 (3)
O(2)	3324 (5)	2244 (3)	−543 (4)
O(3)	8262 (4)	2373 (3)	2645 (3)
O(4)	56 (5)	1852 (2)	559 (3)
O(5)	−2165 (5)	837 (3)	133 (3)
O(6)	3039 (5)	−890 (2)	3990 (3)
O(7)	3817 (5)	3355 (3)	3013 (4)
N(1)	5924 (5)	1550 (3)	2843 (4)
N(2)	3579 (5)	703 (3)	2917 (3)
C(1)	3608 (7)	2085 (3)	370 (5)
C(2)	5408 (7)	1294 (3)	1649 (5)
C(3)	7357 (7)	1291 (4)	2145 (5)
C(4)	−348 (7)	1050 (4)	822 (5)
C(5)	1470 (7)	233 (3)	2018 (4)
C(6)	1417 (7)	−122 (4)	2916 (5)
C(7)	6857 (7)	640 (4)	3848 (5)
C(8)	5068 (7)	−47 (4)	3265 (5)

Table 2. *Interatomic distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Cu–N(1)	2·006 (6)	C(3)–O(3)	1·435 (6)
Cu–N(2)	2·001 (4)	C(4)–O(4)	1·259 (8)
Cu–O(1)	1·961 (4)	C(4)–O(5)	1·247 (10)
Cu–O(4)	1·963 (6)	C(4)–C(5)	1·540 (7)
Cu–O(7)	2·181 (4)	C(5)–N(2)	1·479 (9)
C(1)–O(1)	1·283 (10)	C(5)–C(6)	1·511 (11)
C(1)–O(2)	1·215 (9)	C(6)–O(6)	1·408 (6)
C(1)–C(2)	1·548 (6)	C(7)–N(1)	1·474 (6)
C(2)–N(1)	1·497 (8)	C(7)–C(8)	1·518 (11)
C(2)–C(3)	1·495 (13)	C(8)–N(2)	1·487 (10)
N(1)–Cu–N(2)	87·2 (2)	C(2)–C(1)–O(2)	120·0 (6)
N(1)–Cu–O(1)	83·3 (2)	O(1)–C(1)–O(2)	124·3 (6)
N(1)–Cu–O(4)	162·2 (2)	C(1)–C(2)–C(3)	113·9 (5)
N(1)–Cu–O(7)	103·3 (2)	C(1)–C(2)–N(1)	108·3 (5)
N(2)–Cu–O(1)	152·4 (2)	C(3)–C(2)–N(1)	112·9 (5)
N(2)–Cu–O(4)	85·3 (2)	C(2)–C(3)–O(3)	108·0 (5)
N(2)–Cu–O(7)	101·5 (2)	C(5)–C(4)–O(4)	119·0 (5)
O(1)–Cu–O(4)	96·2 (2)	C(5)–C(4)–O(5)	116·5 (5)
O(1)–Cu–O(7)	105·9 (2)	O(4)–C(4)–O(5)	124·4 (6)
O(4)–Cu–O(7)	94·1 (2)	C(4)–C(5)–C(6)	111·9 (5)
Cu–N(1)–C(2)	104·5 (4)	C(4)–C(5)–N(2)	109·9 (5)
Cu–N(1)–C(7)	107·8 (4)	C(6)–C(5)–N(2)	112·4 (5)
Cu–N(2)–C(5)	108·6 (4)	C(5)–C(6)–O(6)	112·3 (5)
Cu–N(2)–C(8)	104·3 (4)	N(1)–C(7)–C(8)	110·0 (5)
Cu–O(1)–C(1)	114·1 (4)	C(7)–C(8)–N(2)	108·0 (5)
Cu–O(4)–C(4)	114·1 (4)	C(2)–N(1)–C(7)	115·5 (5)
C(2)–C(1)–O(1)	115·7 (5)	C(5)–N(2)–C(8)	115·9 (5)

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0·081. The maximum peak in the final difference synthesis was 0·038 e Å^{-3}. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). All crystallographic calculations were performed with the NRC program package (Ahmed, 1970) on a Siemens 4004/150 computer. Atomic coordinates for nonhydrogen atoms are listed in Table 1, bond distances and angles in Table 2, and selected torsion angles in Table 3.*

Discussion. [Cu(ebser)].H_2O (Fig. 1) is both quadridentate and five-coordinate, with a water molecule, O(7), filling the apical position of a square-pyramidal polyhedron. The Cu atom is shifted by 0·381 (1) Å from the basal plane O(1), N(1), N(2), O(4) towards the water molecule. The ligand forms an ethylenediamine and two glycine-type chelate rings. Hydroxyl groups do not take part in the coordination.

Table 3. *Selected torsion angles* (°)

Cu–N(1)–C(2)–C(1)	36·9 (5)	Cu–N(2)–C(5)–C(4)	−18·4 (6)
N(1)–C(2)–C(1)–O(1)	−22·3 (7)	N(2)–C(5)–C(4)–O(4)	14·2 (8)
C(2)–C(1)–O(1)–Cu	−5·6 (5)	C(5)–C(4)–O(4)–Cu	−1·9 (7)
C(1)–O(1)–Cu–N(1)	22·7 (3)	C(4)–O(4)–Cu–N(2)	−7·6 (4)
O(1)–Cu–N(1)–C(2)	−32·7 (2)	O(4)–Cu–N(2)–C(5)	14·7 (3)
C(1)–C(2)–C(3)–O(3)	61·6 (5)	C(4)–C(5)–C(6)–O(6)	178·5 (3)
N(1)–C(2)–C(3)–O(3)	−62·5 (5)	N(2)–C(5)–C(6)–O(6)	−57·4 (5)
C(1)–C(2)–N(1)–C(7)	155·1 (6)	C(4)–C(5)–N(2)–C(8)	−135·4 (5)
C(2)–N(1)–C(7)–C(8)	−87·6 (8)	C(5)–N(2)–C(8)–C(7)	166·0 (4)
Cu–N(1)–C(7)–C(8)	28·8 (6)	Cu–N(2)–C(8)–C(7)	46·6 (4)
N(2)–Cu–N(1)–C(7)	−2·0 (2)	N(1)–Cu–N(2)–C(8)	−25·0 (3)
N(1)–C(7)–C(8)–N(2)	−51·5 (6)		

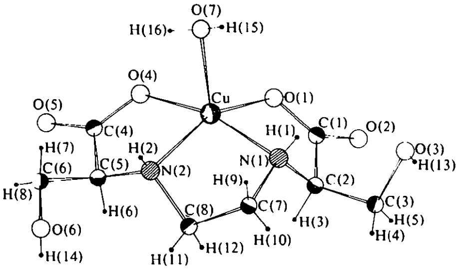

Fig. 1. A perspective drawing of [Cu(ebser)] H_2O and the numbering scheme of the atoms.

Table 4. *Hydrogen-bond contacts* (X—H$\cdots$$Y$) <3 Å

N(2)$\cdots$O(6^{iii})	2·880 (4) Å	O(7)$\cdots$O(2^{iv})	2·789 (9) Å
O(3)$\cdots$O(1^{i})	2·678 (5)	O(7)$\cdots$O(5^{i})	2·680 (7)
O(6)$\cdots$O(3^{ii})	2·692 (5)		

The equivalent positions are: (i) $x + 1, \frac{1}{2} - y, z + \frac{1}{2}$; (ii) $1 - x, y + \frac{1}{2}, \frac{1}{2} - z$; (iii) $1 - x, -y, 1 - z$; (iv) $x, \frac{1}{2} - y, z + \frac{1}{2}$.

Intramolecular bond lengths and angles are normal and similar to those in [Cu(ser)$_2$].H_2O (van der Helm & Franks, 1969). Significant angular distortions occur only at the secondary N atoms: C(2)–N(1)–C(7) 115·5°, C(5)–N(2)–C(8) 115·9°. Strain-free angles at these atoms would be expected to be close to 109·5°. The two amino acid moieties show several dissimilarities. The two side-chain hydroxyl groups have different conformations relative to the N and COO$^-$ groups (Fig. 1). O(3) has a *gauche–gauche* configuration relative to these two groups; O(6) adopts a *gauche–anti* configuration. This feature was also observed in [Pd(L-ser)$_2$] (Vagg, 1979).

As is evident from Fig. 1 and Table 3, all the chelate rings are considerably puckered. The conformation of the ethylenediamine chelate ring is closer to an envelope than the usual *gauche* conformation: C(8) deviates from the plane of the remaining atoms by 0·61 (1) Å. Both glycine rings have asymmetric envelope conformations.

The molecules are hydrogen bonded to each other *via* their hydroxyl groups, the water molecule and an imino group (Table 4).

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* Lists of structure factors, thermal parameters and H positions have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35184 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.