metal-organic papers

Bis{[2-hydroxy-κO-1,1-bis(hydroxymethyl)-ethylamino-κN]acetato-κO}copper(II)

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The title compound, [Cu(C$_6$H$_{12}$NO$_5$)$_2$], was prepared from copper(II) acetate and N-[2-hydroxy-1,1-bis(hydroxymethyl)-ethyl]glycine. The copper ion is coordinated by two N and four O atoms from two N-[2-hydroxy-1,1-bis(hydroxymethyl)-ethyl]glycine ligands, forming a distorted octahedral geometry. Extensive intermolecular hydrogen bonding is observed in the crystal structure.

Comment

Copper ions play a very important role in the functions of enzymes in many biological and chemical systems. Copper ions are mainly coordinated by the N and O atoms of the amino acid in the reaction of amino acids and copper ions (Tanaka *et al.*, 2002; Mizutani *et al.*, 1999). The organic ligand N-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]glycine possesses not only a carboxyl group and an amino group but also three hydroxyl groups. These hydroxyl groups could coordinate to copper ions and form extensive hydrogen bonds. Here, the synthesis and structure of the title complex, (I), are presented.

(I)
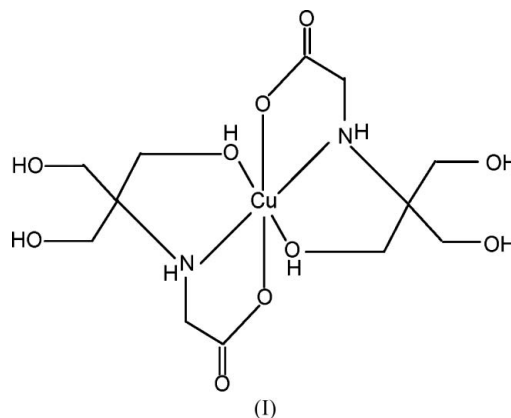
The structural analysis of the title complex (Fig. 1 and Table 1) reveals that each ligand acts as a tridentate ligand coordinating to the copper ion center through the amine N atom, one carboxylate O and one hydroxyl O atom. Four O and two N atoms complete the distorted octahedral coordination of the central copper ion, of which O1, O6, N1 and N2 constitute the equatorial plane; the axial positions are occupied by atoms O3 and O8. The bond lengths Cu—O3 and Cu—O8 are 2.302 (2) and 2.329 (2) Å, respectively. The long axial Cu—O bonds (Table 1) demonstrate the typical Jahn–Teller effect which leads to an elongated octahedron. N—H⋯O and O—H⋯O hydrogen bonds between adjacent molecules are found in the title complex, as shown in Fig. 2; the corresponding hydrogen-bonding information is listed in Table 2.
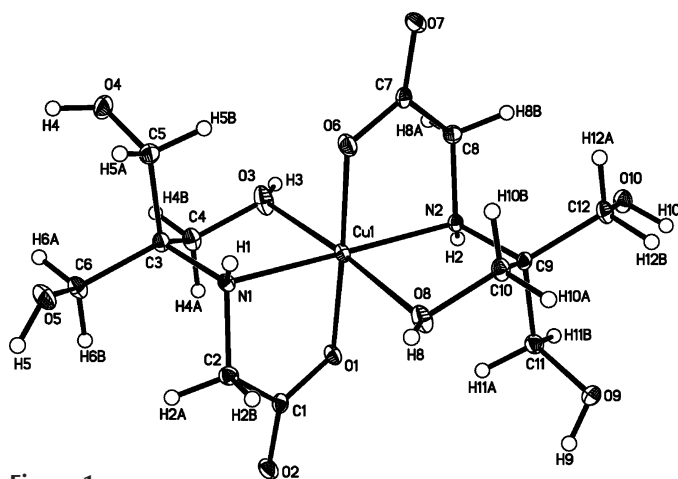
Figure 1
The molecular structure of the title complex, (I).Displacement ellipsoids are drawn at the 30% probability level.
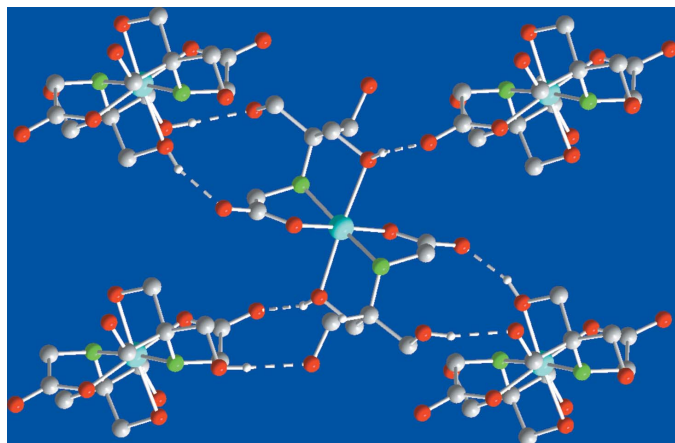

Figure 2
Hydrogen-bonding interactions (dashed lines) in (I).

Experimental

The title compound was prepared by refluxing and stirring *N*-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]glycine (0.02 mol) and copper(II) acetate (0.04 mol) for 3.5 h in 50 ml of H_2O. The reaction mixture was filtered, and the filtrate was then kept at room temperature for several days, giving rise to blue crystals suitable for X-ray analysis.

Crystal data

$[Cu(C_6H_{12}NO_5)_2]$	$D_x = 1.757$ Mg m^{-3}
$M_r = 419.87$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1891
$a = 14.343$ (2) Å	reflections
$b = 9.1271$ (17) Å	$\theta = 2.8–26.2°$
$c = 12.2913$ (18) Å	$\mu = 1.44$ mm^{-1}
$\beta = 99.460$ (6)°	$T = 293$ (2) K
$V = 1587.2$ (5) Å^3	Block, blue
$Z = 4$	$0.32 \times 0.22 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	2798 independent reflections
	2127 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.038$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -10 \rightarrow 17$
$T_{min} = 0.680$, $T_{max} = 0.791$	$k = -10 \rightarrow 10$
7959 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.042$	$+ 0.0974P]$
$wR(F^2) = 0.118$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
2798 reflections	$\Delta\rho_{max} = 2.01$ e Å^{-3}
258 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O6	1.956 (2)	Cu1—N2	2.044 (3)
Cu1—O1	1.976 (2)	Cu1—O3	2.302 (2)
Cu1—N1	2.039 (3)	Cu1—O8	2.329 (2)
O6—Cu1—N1	93.64 (10)	O1—Cu1—N2	99.12 (10)
O1—Cu1—N1	83.95 (10)	O3—Cu1—O8	175.27 (7)
O6—Cu1—N2	83.30 (10)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1$\cdots$O5^i	0.77 (4)	2.24 (4)	3.004 (3)	178 (2)
N2—H2$\cdots$O9^{ii}	0.87 (4)	2.10 (3)	2.942 (4)	163 (2)
O3—H3$\cdots$O2^{iii}	0.84 (4)	1.80 (4)	2.606 (3)	161 (2)
O4—H4$\cdots$O7^{iv}	0.85 (3)	2.02 (3)	2.865 (4)	177 (2)
O4—H4$\cdots$O6^{iv}	0.85(3)	2.44 (3)	2.945 (2)	119 (2)
O5—H5$\cdots$O4^v	0.842 (12)	1.993 (18)	2.809 (3)	163 (2)
O5—H5$\cdots$O6^i	0.842 (12)	2.65 (4)	3.104 (3)	115 (2)
O8—H8$\cdots$O7^{vi}	0.84 (3)	1.86 (3)	2.664 (3)	162 (2)
O9—H9$\cdots$O10^{vi}	0.85 (2)	1.92 (2)	2.772 (2)	179 (2)
O10—H10$\cdots$O1^{vii}	0.84 (3)	1.98 (3)	2.826 (3)	177 (2)
O10—H10$\cdots$O2^{vii}	0.84 (3)	2.63 (2)	3.206 (4)	125 (2)

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

N– and O-bound H atoms were located in difference Fourier maps and refined isotropically. C-bound H atoms were positioned geometrically, with C—H = 0.97 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. The highest density peak is located at (0.2359, 0.4993, 0.9941) and the deepest hole at (0.2654, 0.0152, 0.1138).

Data collection: *SMART* (Bruker 1998); cell refinement: *SAINT* (Bruker 1999); data reduction: *SAINT* (Bruker 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 1999); software used to prepare material for publication: *SHELXTL*.

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