

The distortion of the square pyramid is also important, but less severe than that of the trigonal bipyramid. The four basal atoms N(1), N(2), Br(1) and Br(2) deviate strongly from coplanarity by 0.240, -0.247, -0.183 and 0.190 Å, respectively, while the Cu atom deviates from this plane by 0.252 Å in the direction of the apical Br atom. The dihedral angle between the unweighted mean planes N(1)-Cu-N(2) and Br(1)-Cu-Br(2) is 24.9°, thus indicating a distortion towards tetrahedrality, which is quite common in '4 + 1' complexes. The distances and angles of the di-2-pyridylmethane ligand are comparable with those found by us for chloro(di-2-pyridylmethane)-(di-2-pyridylmethanol)copper(II) perchlorate (Garland, Le Marouille, Spodine & Manzur, 1986).

The structure of the dibromo(di-2-pyridylmethane)-copper(II) complex is similar to that found in the bis[dibromo(4-methyloxazole)copper(II)] complex (Marsh *et al.*, 1982), in the sense that all metal-ligand distances are comparable. However, in their case the Cu atom deviates from the basal plane of the pyramid by 0.309 Å, and the in-plane Br(1)-Cu-Br(2) angle is 157.15 (4)°.

This research was supported in part by the Departamento de Desarrollo de Investigacion y Bibliotecas, Universidad de Chile (Q 1872-8634) and the Fondo Nacional (project No. 1081). In addition, MTG thanks the Facultad de Ciencias Fisicas y Matematicas,

Universidad de Chile, for a leave of absence. ES acknowledges the financial support of the PNUD-UNESCO program.

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## Structure of *catena*-Bis[4-(2-aminoethyl)imidazole-*N*<sup>3</sup>,*N*<sup>8</sup>]- $\mu$ -chloro-copper(II) Chloride Dihydrate\*

BY ANDRZEJ WOJTCZAK†

*Department of Mineralogy and Crystallography, Institute of Chemistry, N. Copernicus University, ul. Gagarina 7, 87-100 Toruń, Poland*

AND MARIUSZ JASKÓLSKI AND ZOFIA KOSTURKIEWICZ

*Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, ul. Grunwaldzka 6, 60-780 Poznań, Poland*

(Received 12 December 1985; accepted 21 October 1986)

**Abstract.** [CuCl(C<sub>5</sub>H<sub>9</sub>N<sub>3</sub>)<sub>2</sub>]<sub>2</sub>Cl<sub>2</sub>·2H<sub>2</sub>O, *M*<sub>r</sub> = 392.77, monoclinic, *P*2<sub>1</sub>/*c*, *a* = 9.727 (2), *b* = 10.463 (2), *c* = 18.022 (3) Å,  $\beta$  = 114.83 (1)°, *V* = 1664.6 (6) Å<sup>3</sup>,

*Z* = 4, *D*<sub>m</sub> = 1.570 (1), *D*<sub>x</sub> = 1.567 Mg m<sup>-3</sup>,  $\lambda$ (Mo *K* $\alpha$ ) = 0.71069 Å,  $\mu$  = 1.680 mm<sup>-1</sup>, *F*(000) = 812, room temperature, *R* = 0.0424 for 1936 observed reflections. The Cu<sup>2+</sup> ions are located at two independent centers of symmetry (000 and 0½0). Two bidentate histamine ligands form a square-planar environment around the Cu<sup>2+</sup> ions. The coordination sphere is

\* Presented at the 28th Crystallographic Symposium of the Polish Academy of Sciences, Wrocław, 25 June 1985.

† To whom correspondence should be addressed.

expanded to a square bipyramid by Cl<sup>-</sup> ions bridging central Cu<sup>2+</sup> ions. Polymeric chains are extended along the *y* axis. Only one of the two Cl<sup>-</sup> ions is coordinated to Cu<sup>2+</sup>.

**Introduction.** Histamine, a small-molecule tissue hormone, is formed in living organisms as a result of enzymatic decarboxylation of histidine. It plays an important role in many physiological processes, e.g. it is a vasodilator and a stimulator of gastric secretion, mediates symptoms of allergy, and affects the central nervous system. The histamine moiety is also an important part of the active site of metalloproteins and metal-protein complexes. For these reasons, histamine complexes with biologically important metals are studied. Some of them contain Cu<sup>2+</sup> as the central ion (Bonnet & Jeannin, 1970; Głowska, Gałdecki, Kazimierzak & Maśliński, 1980). The present paper describes the structure of [CuCl(C<sub>5</sub>H<sub>9</sub>N<sub>3</sub>)<sub>2</sub>]Cl·2H<sub>2</sub>O.

**Experimental.** Crystals (plates) from water, density by flotation, 15 reflections with  $17 < 2\theta < 27^\circ$  used to obtain lattice parameters, 3147 reflections with  $2\theta \leq 50^\circ$  (*h*: ±11, *k*: 12, *l*: 21) collected on a Syntex P<sub>2</sub> diffractometer from a 0.3 × 0.5 × 0.5 mm crystal, graphite-monochromated Mo K $\alpha$  radiation, profile analysis according to Lehmann & Larsen (1974), 2702 unique reflections,  $R_{\text{int}} = 0.0172$ , no significant intensity variations for two checks (0 $\bar{2}$ 1 and 206) monitored every 100 reflections, no absorption corrections. Structure solved by direct methods with MULTAN80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980),  $\sum w(\Delta F)^2$  minimized in anisotropic full-matrix least-squares refinement using SHELX76 (Sheldrick, 1976), 1936 observed reflections,  $I \geq 1.96\sigma(I)$ ,  $w = \sigma^{-2}(F)$  from counting statistics, H-atom positions from  $\Delta\rho$  map and not refined, extinction  $x = 0.00637(10)$  in  $F'_c = F_c(1 - 0.0001x F_c^2/\sin\theta)$ , final  $R = 0.0424$ ,  $wR = 0.0403$ ,  $S = 8.457$ ,  $|\Delta/\sigma|_{\text{max}}$  in the final refinement cycle 0.043 except 0.104 for extinction correction  $x$ ,  $\Delta\rho_{\text{max}} = 0.75$ ,  $\Delta\rho_{\text{min}} = -0.51 \text{ e } \text{\AA}^{-3}$ , scattering factors from *International Tables for X-ray Crystallography* (1974). Other programs used: PLUTO78 (Motherwell & Clegg, 1978) and those described by Jaskólski (1982), RIAD32 computer.

**Discussion.** The atomic parameters and bond lengths and angles are given in Tables 1 and 2.\* The numbering scheme is shown in Fig. 1.

\* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, details of hydrogen bonds and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43538 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

In the reported structure, histamine exists in the N<sup>π</sup>-H tautomeric form (IUPAC-IUB Commission on Biochemical Nomenclature, 1970) considered to be active on H<sub>2</sub> receptors. The same tautomeric form was also found in other complexes (Bonnet & Jeannin, 1970; Głowska *et al.*, 1980; Wojtczak, Jaskólski & Kosturkiewicz, 1985) except for [Ni(NCS)<sub>4</sub>(C<sub>5</sub>-H<sub>10</sub>N<sub>3</sub><sup>+</sup>)<sub>2</sub>] where N<sup>π</sup>-H histamine acts as a monodentate ligand (Wojtczak, Jaskólski & Kosturkiewicz, 1983).

Table 1. Final fractional coordinates and equivalent isotropic thermal parameters ( $\text{\AA}^2$ )

$$U_{\text{eq}} = (U_{11} \times U_{22} \times U_{33})^{1/3}$$

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{eq}}$
Cu(1)	0.0	0.0	0.0	0.0269 (3)
N(1)	0.2462 (5)	0.1287 (5)	-0.1268 (3)	0.042 (2)
C(2)	0.1217 (6)	0.0835 (6)	-0.1224 (3)	0.035 (2)
N(3)	0.1450 (5)	0.0612 (4)	-0.0456 (3)	0.029 (2)
C(4)	0.2935 (6)	0.0949 (5)	0.0003 (3)	0.027 (2)
C(5)	0.3576 (6)	0.1369 (6)	-0.0483 (3)	0.034 (2)
C(6)	0.3671 (6)	0.0774 (6)	0.0910 (3)	0.032 (2)
C(7)	0.3359 (6)	-0.0553 (6)	0.1157 (3)	0.034 (2)
N(8)	0.1755 (5)	-0.0661 (5)	0.1033 (3)	0.032 (2)
Cu(2)	0.0	0.5000	0.0	0.0264 (3)
N(11)	0.2411 (5)	0.6356 (5)	0.2364 (3)	0.033 (2)
C(12)	0.1177 (6)	0.5872 (6)	0.1761 (3)	0.035 (2)
N(13)	0.1432 (5)	0.5647 (4)	0.1106 (2)	0.028 (2)
C(14)	0.2918 (6)	0.5995 (5)	0.1307 (3)	0.026 (2)
C(15)	0.3531 (6)	0.6452 (6)	0.2085 (3)	0.032 (2)
C(16)	0.3661 (6)	0.5786 (6)	0.0750 (3)	0.030 (2)
C(17)	0.3367 (6)	0.4433 (6)	0.0403 (4)	0.036 (2)
N(18)	0.1771 (5)	0.4310 (4)	-0.0207 (3)	0.031 (2)
Cl(1)	0.0004 (2)	0.2490 (1)	0.06503 (9)	0.0372 (5)
Cl(2)	0.2255 (2)	0.5007 (2)	-0.19775 (9)	0.0460 (5)
O(1)	0.2762 (5)	0.2674 (4)	0.2385 (2)	0.051 (2)
O(2)	0.2780 (5)	0.7290 (4)	0.3884 (2)	0.050 (2)

Table 2. Bond lengths ( $\text{\AA}$ ) and bond angles ( $^\circ$ ) with their e.s.d.'s

Cu(1)-N(3)	2.012 (4)	Cu(2)-N(13)	2.010 (4)
Cu(1)-N(8)	2.046 (5)	Cu(2)-N(18)	2.041 (4)
Cu(1)-Cl(1)	2.856 (2)	Cu(2)-Cl(1)	2.875 (2)
N(1)-C(2)	1.333 (7)	N(11)-C(12)	1.335 (7)
C(2)-N(3)	1.327 (6)	C(12)-N(13)	1.325 (6)
N(3)-C(4)	1.375 (6)	N(13)-C(14)	1.383 (6)
C(4)-C(5)	1.344 (7)	C(14)-C(15)	1.359 (7)
C(5)-N(1)	1.376 (7)	C(15)-N(11)	1.381 (7)
C(4)-C(6)	1.496 (7)	C(14)-C(16)	1.479 (7)
C(6)-C(7)	1.527 (8)	C(16)-C(17)	1.525 (8)
C(7)-N(8)	1.485 (7)	C(17)-N(18)	1.484 (7)
N(8)-Cu(1)-N(3)	91.1 (2)	N(18)-Cu(2)-N(13)	90.8 (2)
Cl(1)-Cu(1)-N(3)	89.8 (1)	Cl(1)-Cu(2)-N(13)	91.2 (1)
Cl(1)-Cu(1)-N(8)	94.5 (1)	Cl(1)-Cu(2)-N(18)	84.0 (1)
C(2)-N(3)-Cu(1)	129.8 (4)	C(12)-N(13)-Cu(2)	129.2 (4)
C(4)-N(3)-Cu(1)	125.1 (3)	C(14)-N(13)-Cu(2)	124.1 (3)
C(7)-N(8)-Cu(1)	122.3 (3)	C(17)-N(18)-Cu(2)	122.3 (4)
C(5)-N(1)-C(2)	107.7 (4)	C(15)-N(11)-C(12)	108.0 (4)
N(3)-C(2)-N(1)	111.2 (5)	N(13)-C(12)-N(11)	110.6 (5)
C(4)-N(3)-C(2)	105.0 (4)	C(14)-N(13)-C(12)	106.6 (4)
C(5)-C(4)-N(3)	110.4 (5)	C(15)-C(14)-N(13)	108.7 (5)
C(4)-C(5)-N(1)	105.6 (5)	C(14)-C(15)-N(11)	106.1 (5)
C(6)-C(4)-N(3)	121.7 (5)	C(16)-C(14)-N(13)	122.6 (5)
C(6)-C(4)-C(5)	127.8 (5)	C(16)-C(14)-C(15)	128.6 (5)
C(7)-C(6)-C(4)	111.6 (5)	C(17)-C(16)-C(14)	110.8 (5)
N(8)-C(7)-C(6)	110.4 (5)	N(18)-C(17)-C(16)	110.0 (5)

The bond lengths and angles in the imidazole rings of the histamine ligands are comparable with those found in imidazole or histamine complexes (Głowiak & Wnęk, 1985*a,b*; Clegg, Acott & Garner, 1984; Wojtczak *et al.*, 1983, 1985; and references cited therein). However, the angles are different from those found in histaminium or imidazolium cations, imidazolate anions and imidazole (Yamane, Ashida & Kakudo, 1973; Bonnet & Jeannin, 1972; Fuess, Hohlwein & Mason, 1977; Freeman, Huq, Rosalky & Taylor, 1975; Kolks & Lippard, 1984; Ivarsson, Lundberg & Ingri, 1972; Craven, McMullan, Bell & Freeman, 1977; and references cited therein). The average difference between the two C—N—C angles in the imidazole moiety is 0.5 (2), 0.6 (5), 2.0 (2) and 1.9 (1)° for cations, anions, complexes and imidazole, respectively. The average differences between the two imidazole C—C—N angles are 0.5 (2), 0.6 (7), 2.8 (3) and 3.7 (1)°, respectively. The average values of the N—C—N angle are 108.7 (1), 111.4 (1), 112.0 (1) and 112.2 (3)° for cation, complex, imidazole and anion, respectively. These facts suggest that the geometry of the imidazole ring depends on what bonds are formed by the imidazole N atoms. It should be pointed out that the values cited above for the imidazole molecule refer in fact to hydrogen-bonded imidazole entities with N(3) atoms acting as hydrogen-bond acceptors (N...H 1.83 Å, Craven *et al.*, 1977). We may therefore conclude that the influence of the coordinate N(3)—M bond on the geometry of the imidazole ring is very similar to that of the N(3)...H hydrogen bond. It is also worth noting that in histamine (Bonnet & Ibers, 1973), where there is no such hydrogen bond, the value of the N—C—N angle [112.3 (2)°] is shifted further away from that characterizing the imidazolium cation.

Both imidazole rings are planar ( $\chi^2$  0.25 and 3.33).

Bond lengths and angles in the side chains are similar to those found in other histamine complexes, *e.g.* Wojtczak *et al.* (1983, 1985).

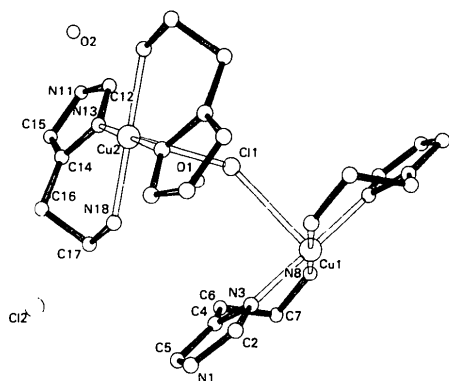


Fig. 1. Fragment of the polymeric Cu(1)—Cl(1)—Cu(2) chain with the numbering scheme.

The side-chain conformation of the histamine ligands is synclinal, the torsion angles C(4)—C(6)—C(7)—N(8) and C(5)—C(4)—C(6)—C(7) being  $-71.7$  (5),  $-129.3$  (6)° and  $72.6$  (6),  $128.4$  (6)° for the two ligands, respectively. Their absolute values are similar to those found by Wojtczak *et al.* (1985) in  $[\text{Ni}(\text{NCS})_2 \cdot (\text{C}_5\text{H}_9\text{N}_3)_2]$  [74.0 (4), 135.0 (4)° and 74.5 (4), 129.7 (4)°].

Each histamine molecule forms two coordinate bonds to the  $\text{Cu}^{2+}$  ion *via* the  $\text{N}^\pi$  atom of the imidazole ring and the amino group of the side chain. The Cu—N(8) bond lengths [2.046 (5) and 2.041 (4) Å] are similar to those found by Bonnet & Jeannin (1970) and Camerman, Camerman & Sarkar (1976). Also the Cu—N(3) bonds [2.012 (4), 2.010 (4) Å] are similar to those found in the above structures. The four N atoms coordinated to  $\text{Cu}^{2+}$  form a square-planar environment around the central ion. The coordination sphere is completed by two  $\text{Cl}(1)^-$  ions to form a square bipyramid [Cu—Cl distances 2.875 (2), 2.856 (2) Å]. Such a geometry (elongated axial bonds, Procter, Hathaway & Nicholls, 1968) of the coordination sphere seems to be a result of the Jahn—Teller effect. The  $\text{Cl}(1)^-$  ions form bridges between  $\text{Cu}^{2+}$  ions, the Cu—Cl—Cu angle being  $131.78$  (5)°.

The structure contains a three-dimensional network of hydrogen bonds (Fig. 2) involving  $\text{N}^\pi$ —H, amino, water and C(12)—H groups as donors and water O atoms and  $\text{Cl}^-$  ions as acceptors. The two  $\text{N}^\pi$ —H groups form hydrogen bonds to the water O atoms [N(1)...O(1)( $x, \frac{1}{2}-y, z-\frac{1}{2}$ ) 2.785 (7), N(11)...O(2) 2.787 (7) Å]. The C(12)—H group forms a hydrogen bond to the  $\text{Cl}(2)^-$  ion, the C—H...Cl distance being 2.616 (2) Å. This C atom is located between N atoms N(13) (coordinated to  $\text{Cu}^{2+}$ ) and N(11)—H (a hydrogen-bond donor) and is therefore particularly likely to become a hydrogen-bond donor (Taylor & Kennard, 1982). This above C—H...Cl hydrogen bond is linear, the C—H...Cl angle being  $175.1$  (3)°. The amino groups act as donors in N...Cl hydrogen bonds [N(8)...Cl(2)( $x, \frac{1}{2}-y, \frac{1}{2}+z$ ) 3.478 (5), N(18)...Cl(1) 3.347 (5), N(18)...Cl(2) 3.492 (4) Å]. Water O—H

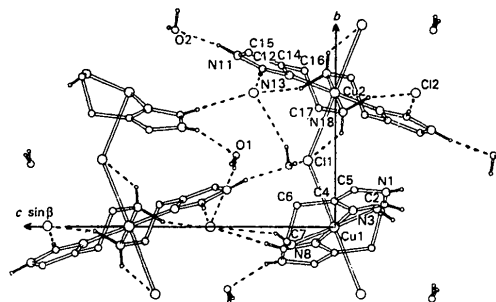


Fig. 2. Crystal-structure projection down the *a* axis. Dotted lines indicate the hydrogen bonds.

groups form O...Cl hydrogen bonds [O(1)...Cl(2)( $x, \frac{1}{2}-y, \frac{1}{2}+z$ ) 3·148 (5), O(2)...Cl(1)( $-x, \frac{1}{2}+y, \frac{1}{2}-z$ ) 3·160 (4), O(2)...Cl(2)( $x, \frac{3}{2}-y, \frac{1}{2}+z$ ) 3·163 (4) Å]. The Cl(1)<sup>-</sup> ion participates in two coordinate and two hydrogen bonds, whereas the Cl(2)<sup>-</sup> ion acts as an acceptor in as many as five hydrogen bonds.

This research was partly supported by project RP.II.10.

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*Acta Cryst.* (1987). **C43**, 648–651

## Structures of Ethylenediaminetetraacetato(3-) Metal Complexes. I. Complexes with Co, Mg and Cd Metals

BY X. SOLANS AND M. FONT-BARDÍA

*Dpto Cristalografía y Mineralogía, Universidad de Barcelona, Grand Via 585, 08007-Barcelona, Spain*

M. AGUILÓ

*Cristalografía, Fac. Químicas, Universidad de Barcelona, Pza Imperial Tarraco 1, Tarragona, Spain*

AND M. AROSTEGUI AND J. OLIVA

*Dpto Farmacia, Universidad de Barcelona, Diagonal 645, 08028-Barcelona, Spain*

(Received 20 May 1986; accepted 17 November 1986)

**Abstract.** (I): Hexaaquacobalt(II) aqua[ethylenediaminetetraacetato(3-)]cobaltate(II) dihydrate, [Co(H<sub>2</sub>O)<sub>6</sub>][Co(C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>)(H<sub>2</sub>O)]<sub>2</sub>·2H<sub>2</sub>O,  $M_r = 935.4$ , monoclinic,  $C2/c$ ,  $a = 13.842$  (3),  $b = 9.402$  (2),  $c = 27.936$  (4) Å,  $\beta = 90.80$  (2)°,  $V = 3635$  (2) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 1.709$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 1.512$  mm<sup>-1</sup>,  $F(000) = 1932$ ,  $T = 288$  K. (II): Tetra-

aquabis{aqua[ethylenediaminetetraacetato(3-)]cadmium(II)-O,O'}cadmium(II) tetrahydrate, [Cd{Cd-(C<sub>10</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>)(H<sub>2</sub>O)}<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>}.4H<sub>2</sub>O,  $M_r = 1095.8$ , monoclinic,  $P2_1/c$ ,  $a = 12.054$  (2),  $b = 16.457$  (2),  $c = 9.118$  (1) Å,  $\beta = 91.11$  (2)°,  $V = 1808.4$  (7) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 2.012$  Mg m<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71069$  Å,  $\mu = 1.843$  mm<sup>-1</sup>,  $F(000) = 1092$ ,  $T = 288$  K.  $R = 0.054$