Structure of Dichloroaquo-(2,9-dimethyl-1,10-phenanthroline)copper(II), an Example of a Triangular Bipyramidal Copper(II) Complex

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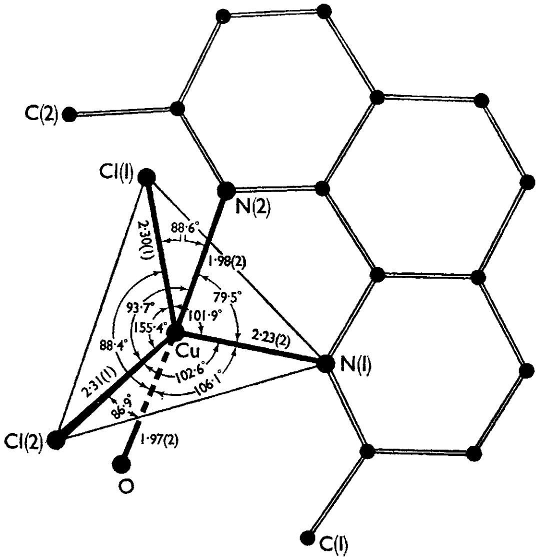
THE methyl groups of the ligand 2,9-dimethyl-1,10-phenanthroline (dmp) may sterically hinder other co-ordinating ligands surrounding a metal atom. So far, tetrahedral co-ordination has been found in the case of $M^{II}Cl_2(dmp)$, where M^{II} = Fe, Co, β-Ni,[1] and Zn.[2] However, with $CuCl_2(dmp),H_2O$, a triangular bipyramid arrangement is reported for the copper atom.

Green prismatic crystals of $CuCl_2(dmp),H_2O$,[3] were grown from methanol. *Crystal data*: $C_{14}H_{14}CuCl_2ON_2$: M, 361; monoclinic; $a = 9{\cdot}88 \pm 0{\cdot}01$; $b = 8{\cdot}17 \pm 0{\cdot}02$; $c = 9{\cdot}53 \pm 0{\cdot}02$ Å; $\beta = 105{\cdot}5 \pm 0{\cdot}5°$; $U = 742$ Å^3; $D_m = 1{\cdot}58$ (by flotation); $Z = 2$; $D_c = 1{\cdot}61$; $F_{(000)} = 366$; space group $P2_1(C_2^2)$ or $P2_1/m$ (C_{2h}^2), Cu-K_α radiation, nickel-filtered, single-crystal oscillation and Weissenberg photographs. 1176 nonzero reflections were recorded from six levels (h0l to h5l), on multiple-film Weissenberg photographs. Systematic absences indicated that the space group was either $P2_1$ or $P2_1/m$. An intensity distribution curve[4] based on general reflections indicated no centre of symmetry, so that $P2_1$ was used.

Copper atomic co-ordinates were obtained from a three-dimensional Patterson synthesis. The other atoms, except for hydrogen, were located in subsequent Fourier syntheses. Three cycles of full-matrix least-squares refinement, using individual isotropic temperature factors, gave an R value of 11·3%.

The co-ordination around the copper atom (Figure) is best described as "triangular bipyramidal", because of the large Cl–Cu–Cl angle (155·4°) in the triangular plane, rather than trigonal bipyramidal, as in the case of iodobis-(2,2′-bipyridyl)copper(II) iodide.[5] The most unusual



FIGURE

feature is the difference between the equatorial (2·23 Å) and axial (1·98 Å) Cu–N bonds. This elongation of the equatorial bond is probably caused by the interaction (3·27 Å) of the methyl group (C-1) in the (dmp) with the water molecule. A similarly distorted arrangement has been reported for trichlorobiquinolylgold(III).[6]

(*Received, October 2nd*, 1967; *Com.* 1043.)

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