CRYSTALLOGRAPHIC AND ESR STUDY OF THE TETRAIMINE MACROCYCLIC Cu(II) COMPLEX
PURE AND DILUTED IN THE ISOMORPHIC Ni(II) COMPLEX.

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The single crystal ESR spectrum of the tetra-imine macrocyclic Cu(II) complex
\[ \text{Cu} \left( C_{10}H_{20}N_{8} \right) \text{Cl} Cl \] pure and diluted in the ana-
logous Ni(II) complex as well as the crystal
structures of these two compounds have been de-
termined.
Both crystallize in the triclinic system (Space
Group P \(\bar{1}\)) with \(Z = 2\) and the following pa-
rameters:
\[ [\text{Ni} \left( C_{10}H_{20}N_{8} \right) \text{Cl} Cl] : a = 7.523, b = 9.502, c = 11.447 \ \AA, \alpha = 95.82, \beta = 108.01, \gamma = 98.62^\circ \]
\[ [\text{Cu} \left( C_{10}H_{20}N_{8} \right) \text{Cl} Cl] : a = 7.574, b = 9.548, c = 11.469 \ \AA, \alpha = 96.31, \beta = 107.19, \gamma = 99.67^\circ \]

Due to the presence in the crystallographic cell of only two molecules re-
lated by a centre of inversion, the molecular g-values could be directly
determined from the single crystal measurement of the pure copper complex.
One finds: \(g_1 = 2.183, g_2 = 2.066, g_3 = 2.047\) with the corresponding eigen-
vectors directed \(\sim\) along the bond directions.

The g-values found in the magnetically diluted complex (prepared with the
\(63^\text{Cu}\) isotope) are practically the same, within experimental error: \(g_1 = 2.178, g_2 = 2.066, g_3 = 2.048\).

Here, moreover, the hyperfine interaction with the \(63^\text{Cu}\) nucleus could be
measured: \(A_1 = 175, A_2 = 48, A_3 = 22\) gauss and also the superhyperfine in-
teraction with the four nitrogen ligands: \(A_1 = 16, A_2 = 14, A_3 = 13\) gauss.

The g-eigenvectors are \(\sim\) along the bond directions whereas the hyperfine
eigenvectors are oriented along the bisectors of the bonds in the basic
plane of the coordination pyramid.
The measured values of the ESR quantities could be reproduced theoretically
in the frame of an AOM model with the following parameter values:
\[ (e_\pi)^N_{1,10} = 7680 \text{ cm}^{-1}, (e_\sigma)^N_{5,14} = 8000 \text{ cm}^{-1}, (e_\sigma)^{\text{Cl}} = 2000 \text{ cm}^{-1}, (e_\pi)^{\text{Ni}} = 1000 \text{ cm}^{-1}, (e_\pi)^{\text{Cl}} = 500 \text{ cm}^{-1}, \gamma_{\text{Cu}} = 500 \text{ cm}^{-1}, \nu = 300.10^{-4} \text{ cm}^{-1} \] and
\(\kappa = 0.3\).