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BONDING IN d^{10} TRANSITION METAL COMPLEXES

A thesis submitted by

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ABSTRACT

The infra red, Raman and nuclear quadrupole resonance (n.q.r.) spectra of several complexes of copper(I), silver(I) and gold(I) are reported. These are interpreted in terms of the structures of the complexes and the various possible bonding schemes for these d^{10} transition elements. To interpret the n.q.r. spectra the contributions to the field gradient at the copper nucleus of the various orbitals in the copper atoms are calculated and the Townes and Dailey approximations are reevaluated. From this the s-d mixing theory of Orgel is chosen as the most satisfactory description of the bonding in these complexes. This theory is extended to cover several other geometries besides the $D_{\infty h}$ geometry for which it was originally derived.

ABBREVIATIONS

The following abbreviations are used in describing Raman and Infra red bands:

w = weak

m = medium

s = strong

v = very

sh = shoulder

The organic groups methyl, ethyl, n-butyl and phenyl are often abbreviated to Me, Et, Bu and Ph respectively.

The tetranuclear compounds formed between the copper(I) halides and various phosphines and arsines are frequently referred to as tetrakis(halophosphinecopper(I)) or tetrakis(haloarsine-copper(I)) $((\text{Cu}(\text{PR}_3)\text{X})_4$ and $(\text{Cu}(\text{AsR}_3)\text{X})_4$) for the sake of brevity and to avoid implications as to their structures which may not be correct.