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Exchange Interactions in Tetranuclear Copper(II) Complexes

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A good description of the exchange effect from the experimental point of view is only possible using relatively simple systems. The two spin case (*e.g.* Cu(II)) is the simplest one, nevertheless it also poses a number of problems. If more than two paramagnetic centres are coupled, then the problems become even more complicated. On the other hand when one has more than two centres, the chances of transferring the linear case to a three-dimensional case are increased. The latter case is far more important for the problems in question.

In copper(II) the number of centres are equal to 4 and thus one of the possible molecular shapes is the tetranuclear cuban-like type. The main part of the contribution is concentrated around our present knowledge of the exchange effect in this type of tetranuclear Cu(II) complex.

The exchange pathway runs along the diamagnetic bridge ligands. When one considers the lowest symmetry case C_1, 6 different exchange integrals for describing the exchange effect are required. The simplest description still needs two independent integrals.

In principle, the tetranuclear cuban type structures can be divided into two different types. Type I forms a tetrameric unit, consisting of two weakly coupled Cu_2O_2 dimers. The coupling occurs perpendicular to the plane of the ring. Type II can be derived from a boat like eight membered Cu_4O_4 ring. In the case of the former type of structure there is an overall antiferromagnetic effect and in the latter type one finds an overall ferromagnetism. There is a continuous series of examples verified between the two types in the groups of aminoalcohol or iminoalcohol ligands.

The greatest point of interest at present is the question of which geometrical factors (bond lengths, bond angles) determine the strength and the sign of the exchange effect. These relationships for the tetrameric cuban type clusters known up to the present time are presented. Moreover, the strength and the sign of the exchange integrals depend also on the type of ligands near the paramagnetic centre, *e.g.* saturated or unsaturated groups. This relates to the fact that the energy level of each paramagnetic center depends upon its chemical surrounding.

In this contribution we present examples which can explain the relation between the changes in the chemical structure and the strength of the exchange effect. A good example is the change of the molecular structure and also the exchange integrals under the influence of different solvents. This relates to the fact that the different interaction energies between the exchange coupled molecule and the solvent cause different modifications with different magnetic behavior. The aim of this contribution is to explain these small effects.