The Explanation of the Significant Differences in Antiferromagnetic Interactions between Two Homologous Tetranuclear Copper(II) Complexes: A Theoretical Study

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The influence of overlap interactions between the bridging ligands and the metal d orbitals on the super-exchange coupling constant has been studied by means of ab-initio Restricted Hartree-Fock molecular orbital calculations. The interaction between the magnetic d orbitals and the HOMOs of the pyrazolate nitrogens has been investigated in homologous tetranuclear copper(II) complexes which have significantly different $-2J$ values (the energy separation between the spin – triplet and spin – singlet states).

Key words: Tetranuclear Copper(II) Complex; Antiferromagnetic Coupling; Overlap Interaction; Countercomplementary Effect; Ab-initio Restricted Hartree-Fock Molecular Orbital Calculation.