

# The Reason of the Significant Differences in Antiferromagnetic Interactions between Homologous $\mu$ -Acetato-Bridged Dicopper(II) Complexes: A Theoretical Study

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

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