

Abstract

The **copper complex** of a tetradentate ligand based on dehydroacetic acid 1 has been prepared and its crystal structure redetermined, showing a copper pair. EPR **spectroscopy** shows that the dimeric structure is preserved in **CH₂Cl₂** and CH₃CN (triplet signal with $D = 480 \pm 50$ MHz, $E = 50 \pm 25$ MHz), but complex 1 is converted into a **monomer** in coordinating **solvents** (MeOH, DMF and DMSO). By DFT calculations it is seen that the copper ion geometry in the monomer is essentially square planar in MeOH and DMF, but evolves towards square pyramidal in DMSO due to solvent ligation in axial position. The hydroxyl of the **methanol** molecules are involved in **hydrogen bonds** with the carbonyl oxygen of the ligand. Complex 1 displays a quasi-reversible reduction wave at $E_{1/2} = -0.86$ V vs. Fc⁺/Fc, which is assigned to the Cu^{II}/Cu^I redox couple. It catalyzes the aerobic oxidation of benzylalcohol, with a conversion that reaches 70% after 2 h, by using a loading of 1 mol%.