

ABSTRACT

Zinc and copper are essential trace elements that are extremely important for all living things. The fundamental motive for vast interest in their coordination chemistry stems from the need for a deeper understanding of their biological role. A review of the literature revealed that the chemistry of zinc(II) and copper(II) with quinaldinate (anion of quinoline-2-carboxylic acid) is not well understood. Therefore, the reactions of zinc(II) and copper(II) quinaldinate with cyclic amines and amino alcohols were investigated. Systems with zinc(II) and amines in three different nitriles (acetonitrile, propionitrile and benzonitrile) showed that zinc(II) can catalyze the reaction between a cyclic amine and a nitrile, yielding an amidine. A variety of products have been prepared: neutral complexes with quinaldinate and coordinated amines or amidines and ionic compounds. The latter consisted of a protonated amine or amidine and an anionic homoleptic complex with three quinaldinates. Analogous reactions with copper(II) quinaldinate led to the isolation of complexes with coordinated amines. In the case of copper(II), oxidation-reduction reactions occurred in some cases. In the case of piperidine, the reduction was indeed proved by the crystal structure of a polycyclic piperidine compound. Reactions with amino alcohols led to structurally very diverse copper(II) compounds: mononuclear, binuclear and also one-dimensional polymeric species with amino alcohols or amino alcoholates. Zinc(II) systems with amino alcohols have shown that the amino alcohols can decompose to ammonia under forcing conditions. The rich structural diversity of the products confirmed the high coordination flexibility of the two metal ions. The same ligands can react differently in the presence of zinc(II) or copper(II), with the reaction conditions also playing an important role. More than a hundred compounds with nitrogen- and oxygen-donor ligands were synthesized and characterized by different physicochemical methods: infrared spectroscopy, nuclear magnetic resonance spectroscopy, elemental analysis, high-resolution mass spectrometry and single crystal X-ray structural analysis. In collaboration with the research group of Dr. Joaquín López-Serrano (University of Seville), theoretical DFT calculations were performed for some compounds, mainly to compare their relative stabilities. In collaboration with the research group of Dr. Rodolphe Clérac (University of Bordeaux), the magnetic properties of copper(II) compounds with quinaldinate and amino alcohol ligands were measured and analyzed.

Keywords: coordination chemistry, zinc(II), copper(II), quinaldinate, cyclic amines, amidines, amino alcohols, crystal structures, theoretical calculations, magnetic properties.