

Zinc halide complexes of imidazolidine-2-thione and its derivatives: X-ray structures, solid state, solution NMR and antimicrobial activity studies

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The preparation and characterization of zinc complexes of formula ZnL_2X_2 ($X = Cl$ and Br), with $L = 1,3$ -diazinane-2-thione (Diaz), 1,3-diazipane-2-thione (Diap), imidazolidine-2-thione (Imt) and its methyl and *n*-propyl substituted derivatives, are described. The complexes dichlorobis(1-methylimidazolidine-2-thione-*S*)-zinc(II) (**1**) and dichlorobis(1-propylimidazolidine-2-thione-*S*)-zinc(II) (**2**) have been characterized by single-crystal X-ray methods. Both complexes adopt distorted tetrahedral geometry. Only intramolecular hydrogen bonding interactions are observed in **1** and **2**. Solution and solid state ^{13}C NMR show a significant shift of the C=S carbon resonance of the ligands, while other resonances are relatively unaffected, indicating that most likely the solid state structure is maintained in solution. Antimicrobial activity studies of the free ligands and their complexes show that ligands exhibit substantial antibacterial activities compared to the complexes.

Keywords: Zinc; Imidazolidine-2-thione; Crystal structure; MAS NMR; Antibacterial activity

1. Introduction

Thiol groups provide biological targets for metal ions, both essential (e.g. Zn in zinc fingers, Fe in iron–sulfur proteins) and toxic (e.g. Ni, Cd, Pb, exerting their deleterious effects in part through inhibition of thiol enzymes or substitution of essential metals in their thiolate binding sites) [1, 2]. It is therefore important to understand the nature of binding of these metal ions with thiols.

Complexes of heterocyclic ligands such as imidazolidine-2-thione (Imt) and its derivatives with metal ions are of special interest in bioinorganic chemistry because of the search for simple model compounds of metal-proteins [3–7]. In view of this, Cu(I), Au(I), Ag(I), Cd(II), Hg(II), Pd(II) complexes with these ligands have been widely investigated [8–11]. These ligands exist in the N=C–SH and N=C=S forms exhibiting thiol-thione equilibrium [12, 13]. However, it has been established that the thione form dominates in the solid state [14]. We have studied extensively the interaction

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