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New cadmium chloride complexes with imidazolidine-2-thione and its derivatives: X-ray structures, solid state and solution NMR and antimicrobial activity studies

Mohammed I.M. Wazeer *, Anvarhusein A. Isab *, Mohammed Fettouhi *

Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

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Abstract

Reactions of imidazolidine-2-thione (Imt), 1,3-diazinane-2-thione (Diaz) and 1,3-diazipane-2-thione (Diap) with cadmium(II) chloride in methanol result in the formation of 2:1 complexes. Both solid state and solution NMR, in addition to X-ray structures, confirm the exocyclic sulfur atom to be the donor in all cases. Cadmium shielding tensors and anisotropies were calculated from the solid-state NMR spectra. The X-ray structures of two complexes $(NMeImt)_2CdCl_2$ and $(NEtImt)_2CdCl_2$ reveal distorted tetrahedral geometries. Antimicrobial activity studies show that the $Cd(Diap)_2Cl_2$ complex exhibits substantial antibacterial activities compared to the corresponding Zn(II) complex.

Keywords: Cadmium(II) complexes; Thiones; CP MAS NMR studies; Crystal structure; Antimicrobial activity

1. Introduction

It is well known that cadmium is a highly toxic metal and a potent carcinogen. However, its mechanism of action is still unclear [1]. The molecular architectures of coordination compounds have proven very useful, giving several molecular geometric shapes and coordination polymers [2]. Many industrial and medicinal uses have been detailed for these compounds, including the vulcanisation of diene rubbers [3] and the treatment of hyperthyroidism [4].

Thiolate complexes are of great importance from a bioinorganic point of view, mainly due to the presence of thiolate donors in the coordination sphere of many metal ions in very diverse metalloproteins [5,6]. Thione ligands are also important and the coordination chemistry of imidazolidine-2-thione and its derivatives with various metal ions has been studied extensively [7]. The interest in the interaction of Cd(II) with sulfur containing ligands arises for two main reasons: their non-linear optical properties and the convenient preparation of semi-conducting materials based on CdS through the thermal decomposition of these complexes [8].

^{113}Cd NMR spectroscopy is a sensitive probe for the number and type of coordinating groups around a cadmium ion and can be particularly useful in the study of proteins. Further, Cd^{2+} may often be exchanged for other divalent metals such as Zn^{2+}, Cu^{2+}, Hg^{2+}, Mn^{2+} and Mg^{2+} in proteins and ^{113}Cd NMR spectroscopy has developed into a useful probe of metal environments in metal proteins [9]. A number of research workers have been using ^{113}Cd NMR as a 'spin spy' in the study of zinc containing proteins. The strategy here is to replace the zinc, which is a spectroscopically silent metal, with cadmium, which has a good spectroscopic handle, and use NMR to explore the properties of the proteins [10]. However, recent advances [11] in NMR techniques to observe quadrupolar nuclei enable ^{67}Zn observation.

* Corresponding authors. Fax: +966 3 8604277.
E-mail addresses: miwazeer@kfupm.edu.sa (M.I.M. Wazeer), aisab@kfupm.edu.sa (A.A. Isab), fettouhi@kfupm.edu.sa (M. Fettouhi).

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