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# Complexations of $Hg(CN)_2$ with imidazolidine-2-thione and its derivatives: Solid state, solution NMR and antimicrobial activity studies

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## Abstract

The preparation and characterization of new mercuric complexes of formula $L_2Hg(CN)_2$ with L being imidazolidine-2-thione (Imt) and its substituted derivatives, 1,3-diazinane-2-thione (Diaz), 1,3-diazipane-2-thione (Diap), are described. The solution and solid-state $^{13}$C NMR show a significant shift of the $>$C=S carbon resonance of the ligands, while the other resonances are relatively unaffected, indicating that most likely the solid-state structure is maintained in solution as well. The principal components of the $^{199}$Hg shielding tensors were determined from solid-state NMR data. Antimicrobial activity studies of the free ligands and their complexes show that ligands exhibit substantial antibacterial activities compare to their Hg(II) complexes.

*Keywords:* Mercuric cyanide complexes; Imidazolidine-2-thione; CP MAS NMR; Antibacterial activity

## 1. Introduction

Systems that employ cyanometalate building blocks in concert with simple metal ions or their coordinatively unsaturated complexes to create multidimensional networks were among the first prepared coordination polymers to be studied and are of great current interest [1,2].

Alteration of the metal center in $[M(CN)_n]^{x-}$ building blocks and the consequent adjustment of the geometric, magnetic, and electronic properties provide the control and flexibility required to assemble solids with tunable properties [3,4]. Cyanometalates have also been employed extensively to generate inclusion compounds, clathrates, and zeolite-type systems that act as ion exchangers, molecular sieves, or materials for storing gases [5–8].

We have been utilizing monocyanometalate complexes such as Ag(I) and Au(I) to complex with = imidazolidine-2-thione and selones and their derivatives. Both of these metalcyano complexes resulted in a linear geometry with *trans* cyano and thiones ligands with metal in the center [9–11]. For the Au(I) complexes, it was observed that they dissociate in solution when dissolved, this is due to the formation constants of $Au(CN)_2{}^-$ is extremely high compare to the $Au(thione)_2{}^+$ complexes [9,12]. However, thione-Ag-CN complexes remain undissociated when dissolved in solution [9].

In this report, we extend our studies of cyanometalate complexes where metal is Hg(II), our studies of the complexation of $L_2Hg(CN)_2$ (where L = imidazolidine-2-thione and its derivatives) and compare the solution as well as solid NMR chemical shifts with previously reported similar studies [13,14].

The solution as well as the solid-state NMR studies have been reported here. The reason for this study is to see if $CN^-$ ligand can be dissociated as seen in our previous studies [9–11] for Au(I) and to correlate the Hg–S bonding with other biological Hg-thiolate complexes [15,16].

Unlike solution chemical shifts, solid-state NMR results can be correlated directly with structural determinations. This technique has the advantage that it provides information about the three principal components of the chemical shift tensor [17,18]. From this analysis, we get information referring to the nature and disposition of coordinating ligands [19]. Selected compounds are characterized by $^{199}$Hg and $^{13}$C MAS NMR to explore the dependence of the NMR properties on mercury coordination

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