

Solid state and solution NMR studies of some new complexes of mercury selenocyanate with imidazolidine-2-thione and its derivatives

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(Received 27 November 2006; in final form 15 February 2007)

Reactions of imidazolidine-2-thione (Imt), 1,3-diazinane-2-thione (Diaz) and 1,3-diazepane-2-thione (Diap) with mercury(II) selenocyanate in acetonitrile resulted in formation of 2:1 complexes. Both solid state and solution NMR, confirm the exocyclic sulfur atom to be the donor in all cases. ^{199}Hg shielding tensors and anisotropies were calculated from the solid-state NMR spectra. Based on the solid NMR data a distorted tetrahedral disposition of ligands around mercury is proposed.

Keywords: Mercury(II) complexes; Selenocyanate complexes; Imidazolidine-2-thione; CP MAS NMR studies

1. Introduction

There is considerable interest in solution as well as solid state NMR of heavy metal nuclei, which include the ^{199}Hg NMR [1–3]. A significant number of these studies involve complexes with thiolate ligands, the main interest in this group of compounds being the important role played by such ligands in biological chemistry [4]. We recently reported the solid state NMR of some Hg-selone complexes [5, 6]. These studies resulted in correlation between the ^{199}Hg solid-state NMR parameters and structures of complexes. Such correlations are of value in the investigation of mercury coordination environments where structural data are not readily obtainable by other methods [7]. Since several mercury containing thiolates as well as other complexes are polymeric [8], it was considered desirable to try to establish a more quantitative relationship between solid state NMR and structural parameters and to use this to assist in the interpretation of the data obtained for mercury complexes involving a wider variety of complexes [9].

We have chosen to study a series of complexes of $\text{Hg}(\text{SeCN})_2$ with thione ligands. Thiones, which are less basic than thiolate, are of interest because of their similar bonding nature with mercury compared to thiolates that have biological significance [10, 11].

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