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Synthesis, X-ray structure and ^{199}Hg, ^{77}Se CP MAS NMR studies on the first tris(imidazolidine-2-selone) mercury complex: {Chloro-tris[*N*-methyl-2(3H)-imidazolidine-2-selone] mercury(II)}chloride

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Abstract

A novel cationic Hg(II) complex has been synthesized with *N*-methyl-imidazolidine-2-selone ligand. The tris(*N*-Methyl-imidazolidine-2-selone) mercury(II) complex, $[(MeImSe)_3HgCl]^+Cl^-$ (**1**), has been characterized by single crystal X-ray analysis and CP MAS ^{199}Hg and ^{77}Se NMR.

Keywords: Crystal structure; CP MAS ^{199}Hg NMR; ^{77}Se NMR; *N*-methyl-imidazolidine-2-selone; Hg(II) complex

Thiolate complexes are of great importance from a bio-inorganic point of view, mainly due to the presence of thiolate donors in the co-ordination sphere of many metal ions in very diverse metalloproteins [1]. Thione ligands are also important and the coordination chemistry of imidazolidine-2-thione and its derivatives with various metal ions have been studied extensively [2]. The nd^{10} metal ions bind almost exclusively to the sulfur atom of these ligands. It is surprising that analogous selone ligand-containing complexes have not received much attention. However, Devillanova et al. [3] have reported the synthesis of the imidazolidine-2-selone (ImSe) with Zn(II), Cd(II) and Hg(II) complexes. Based on IR studies, they proposed that M(II) is bonded to the Se atom of the ligand, forming $M(ImSe)_2Cl_2$ type tetrahedral structures. Recently, the complex [1,3-dimethyl-2(3*H*)-imidazoleselone]zinc(II) was reported and prepared by direct reaction of $ZnCl_2$ and the ligand in boiling acetonitrile. This complex was found to be a potential zinc selenide synthon [4]. In this paper, we report for the first time a tris(*N*-methyl-imidazolidine-2-selone) (MeImSe) complex with $HgCl_2$, forming $[(MeImSe)_3HgCl]^+Cl^-$ (**1**). To the best of our knowledge, it is the first example of a tris(imidazolidine-2-selone) mercury complex. The X-ray structure of the title compound is the first X-ray structure ever reported for a mercury complex containing imidazolidine selone ligands. The ^{199}Hg CP MAS NMR data are the first ever reported for a selone mercury complex.

Direct reaction of $HgCl_2$ and MeImSe [5] in hot acetonitrile leads to the formation of an air-stable crystalline 1:3 addition product in reasonably good yield [6]. The crystal structure of the title compound is depicted in Fig. 1, the selected bond lengths and bond angles are given in the figure caption [7]. The sole X-ray structure known so far in literature is the one of a selenourea cationic complex $[MeHgSeC(NH_2)_2]^+$ [8]. The title $[(MeImSe)_3HgCl]^+$ complex exhibits a distorted pseudo-tetrahedral geometry as

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