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X-ray structure and ^{77}Se, ^{31}P and ^{13}C MAS NMR of the dinuclear complex 1,2-*bis*(selenourea)-1\κSe, 2\κSe-1,2-*bis*(trimethylphosphine)digold(I) chloride

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Abstract

The single crystal X-ray structure of the compound $[(Me_3P\text{-}Au\text{-}Selenourea)_2^{2+}\ 2Cl^-]$ has been determined. The $[Me_3P\text{-}Au\text{-}(selenourea)]$ units are dimerized and adopt a binuclear structure characterized by a metal–metal interaction (Au–Au:3.0386(5) Å) and a torsion angle of 69.71(2)°. Hydrogen bonding takes place between the selenourea ligands and the chloride ions. The principal components of the ^{77}Se, ^{31}P and ^{13}C shielding tensors were determined from solid-state NMR data.

Keywords: Crystal structure; Gold complex; Selenourea; MAS NMR

1. Introduction

There has been a considerable recent interest in the study of gold(I) phosphine complexes of the type R_3PAuL, because of the successful use of auranofin for the treatment of rheumatoid arthritis [1,2]. In addition, auranofin and a number of gold(I) complexes of Ph_3P have been reported to have anticancer activity [3,4]. We have been investigating the coordination chemistry of >C=S and >C=Se ligands with d^{10} metal ions in an attempt to examine their mode of binding and to study their physical properties. In this regard, we have recently reported the characterization of several R_3PAuTu complexes (Tu, thiourea) [5]. Numerous studies have shown, that heavy metal toxicity is lower in the case of selenium based gold drugs and understanding the structure of such complexes will help in the characterization of their biochemical mechanism [6]. In this context and since the crystallographic data related to Au–selenourea complexes are relatively scarce [7], we have undertaken the X-ray structure determination, as well as the solid state NMR characterization of the title compound $[(Me_3P\text{-}Au\text{-}SeU)_2^{2+}\ 2Cl^-]$ (where SeU = selenourea). We report herein its X-ray crystal structure and the results of the ^{77}Se, ^{31}P and ^{13}C solid state NMR investigations.

2. Experimental

Selenourea (Seu) MeOD, Me_2S and all solvents were obtained from Fluka-Aldrich Chemical Co., Germany. $HAuCl_4 \cdot 3H_2O$ and trimethylphosphine were obtained from Strem Chemical Co., USA.

2.1. Synthesis of the complex

The title compound was prepared as reported earlier [8]. Single crystals suitable for X-ray diffraction analysis were grown from an acetonitrile solution.

2.2. X-ray data collection and structure determination

A colorless octahedral crystal of the complex $[(Me_3P\text{-}Au\text{-}SeU)_2^{2+}\ 2Cl^-]$ was mounted on a glass fiber.

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