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Complexation of Zn(II), Cd(II) and Hg(II) with thiourea and selenourea: A ^{1}H, ^{13}C, ^{15}N, ^{77}Se and ^{113}Cd solution and solid-state NMR study

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Zinc(II), cadmium(II) and mercury(II) complexes of thiourea (TU) and selenourea (SeU) of general formula $M(TU)_2Cl_2$ or $M(SeU)_2Cl_2$ have been prepared. The complexes were characterized by elemental analysis and NMR (^{1}H, ^{13}C, ^{15}N, ^{77}Se and ^{113}Cd) spectroscopy. A low-frequency shift of the C=S resonance of thiones in ^{13}C NMR and high-frequency shifts of N–H resonances in ^{1}H and ^{15}N NMR are consistent with sulfur or selenium coordination to the metal ions. The Se nucleus in $Cd(SeU)_2Cl_2$ in ^{77}Se NMR is deshielded by 87 ppm on coordination, relative to the free ligand. In comparison, the analogous Zn(II) and Hg(II) complexes show deshielding by 33 and 50 ppm, respectively, indicating that the orbital overlap of Se with Cd is better. Principal components of ^{77}Se and ^{113}Cd shielding tensors were determined from solid-state NMR data.

Keywords: Thiourea; Selenourea; Zn(II), Cd(II), Hg(II) complexes; NMR; CP MAS NMR

1. Introduction

Coordination compounds formed by bidentate thiourea (TU) with d^{10} metal ions (Zn^{2+}, Cd^{2+}, Hg^{2+}) have recently received renewed attention. This arises for two main reasons: their nonlinear optical properties [1,2], and the convenient preparation of semiconducting materials based on CdS through thermal decomposition of the complexes [3,4].

Most of the compounds reported in the present paper have been studied by X-ray crystallography and FT-Raman spectroscopy [5]. Marcos *et al.* [6], for example, have reported X-ray structure determinations of bis(TU) cadmium halides. These complexes have tetrahedral geometry where Cd is surrounded by two halides and by two TU bonded via S. We recently reported the complexation of thiourea with silver(I) in solution, studied using ^{13}C and ^{109}Ag NMR spectroscopy [7]. The study provided

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