

Complexation of Zn(II), Cd(II) and Hg(II) with thiourea and selenourea: A ^1H , ^{13}C , ^{15}N , ^{77}Se and ^{113}Cd solution and solid-state NMR study. Isab, Anvarhusein A.; Wazeer, Mohammed I. M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. *Journal of Coordination Chemistry* (2005), 58(6), 529-537. Publisher: Taylor & Francis Ltd.,

Abstract

Zn(II), Cd(II) and Hg(II) complexes of $\text{M}(\text{TU})_2\text{Cl}_2$ (TU = thiourea) or $\text{M}(\text{SeU})_2\text{Cl}_2$ (SeU = selenourea) were prepared. The complexes were characterized by elemental analysis and NMR (^1H , ^{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 ^1H and ^{15}N NMR are consistent with S or Se coordination to the metal ions. The Se nucleus in $\text{Cd}(\text{SeU})_2\text{Cl}_2$ 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.