IR Spectroscopy of Two Polymorphs of Copper(I) Thiocyanate and of Complexes of Copper(I) Thiocyanate with Thiourea and Ethylenethiourea

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 75th birthday

Syntheses and infrared spectroscopic studies are reported for two different polymorphs of copper(I) thiocyanate and for adducts of copper(I) thiocyanate with thiourea ('tu') and ethylenethiourea ('etu' = imidazolidine-2-thione; $(CH_2NH)_2CS$)). These include the previously reported complex CuSCN/etu (1 : 2), which has a trigonal monomeric structure, and CuSCN/etu (1 : 1), which has a three-dimensional polymeric structure. A mechanochemical/infrared study of the CuSCN : tu (1 : 2) system showed that no 1 : 2 complex exists in this case, the product being a mixture of a 1 : 3 complex and a novel 1 : 0.5 complex. The latter complex was prepared both mechanochemically and from solution, and characterized by infrared and solid-state ^{65}Cu broadline NMR spectroscopy. Diagnostic ligand and metal-ligand bands in the IR and far-IR spectra are assigned for both polymorphs of CuSCN and for all of the complexes studied and are discussed in relation to the structures of the complexes.

Key words: Copper(I), Thiourea, Infrared Spectroscopy