Syntheses, Structures and Vibrational Spectroscopy of Some Adducts of Copper(I) Cyanide with Unidentate Organic Nitriles

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Dedicated to Professor Hubert Schmidbaur on the occasion of his 70th birthday

A number of adducts of copper(I) cyanide, CuCN, have been synthesized by crystallization from its solutions in various unidentate organic nitriles, RCN. Low temperature single crystal X-ray structure determinations are recorded for a number of these, of the form CuCN : RCN (m : n) for R = Me, Et (m : n = 1 : 1), and Ph, *o*-tolyl (3:2). The 1 : 1 adduct with acetonitrile is a two-dimensional polymeric web, (CN)Cu(μ-CN)$_2$Cu(NC) units being linked by the peripheral nitrogen and carbon atoms, with a fourth coordination site about each copper having MeCN pendant. The other three adducts are one-dimensional polymers, the propionitrile adduct being of the form …Cu(NCEt)CNCu(NCEt)CN… with trigonal planar copper, the bridging cyanide groups being replaced in the benzo- and *o*-toluo nitrile adducts by linear $Cu(CN)_2^-$ moieties. The vibrational spectra of bulk samples are largely consistent with the single crystal structural results, but reveal the possible existence of adducts of higher CuCN content in the case of the CuCN/benzonitrile system.

Key words: Copper Cyanide, Nitrile, Structure, Infrared Spectroscopy, Raman Spectroscopy