Structural chemistry of CuCN network solids with N-alkylethanolamine cation guests

P Corfield[1], L Rachid[2], D Garcia[2], F Elali[2], G Contrera[2]
[1]Chemistry, Fordham Univ, Bronx, NY, [2]Fordham University, Bronx, NY
pcorfield@fordham.edu

We present structural data and chemical decomposition studies for seven CuCN network structures that include protonated alkylethanolamine derivatives as guest cations. Each 3D anionic polymeric structure is built from cyanide-bridged Cu atoms and is distinct from the others. All structures include cuprophilic pairs of Cu atoms as a building block, with Cu … Cu distances ranging from 2.46 to 2.73 Å. A typical unit is shown. Most Cu pairs have one or two μ3-CN groups bridging the pair of Cu atoms, but in one case there appears to be no such bridge. There appears to be some correlation between Cu … Cu distance and number of bridging pairs. Charge balance is provided by the protonated ethanolamine derivatives, but in two cases, the ethanolamine has apparently reacted with an aqueous CN- ion to form a cyclic oxazolidin cation. It is intriguing that thermogravimetric studies show a common theme of a mass decrease at 200-300oC that corresponds to the ethanolamine free base plus one HCN molecule to form CuCN. However, we have found no evidence for formation of the cyclic oxazolidine compound in the vapor phase in subsequent sublimation experiments. Conditions favoring formation of these cyclic compounds are under investigation.

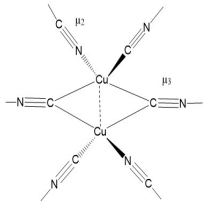

Figure 1

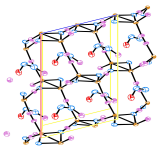

Figure 2