of Yb and Cu along c. Based on this result and the high resolution transmission electron microscopy images a 3-dimensional model of the superstructure was constructed in space group C2 [1]. Yb was distributed on 336 (4c) sites, 7 (2b) sites and 7 (2a) sites, while Cu was distributed on 1519 (4c) sites. Three different types of Yb co-ordination occur in the structure with their relative abundances 2:1:1 which is consistent with observed Mössbauer spectra. The Yb sites near the shear planes show Yb - Yb distances of the order of 3.6 Å which are presumably related to the formation of shear planes, and might be of relevance for the interpretation of the magnetic properties. The composition and calculated density of the model are consistent with their observed values. The calculated and observed X-ray structure factors agreed to R = 12 %. The structure of a related compound YbCu₅.₅ can be predicted as having the same topology of plane defects as YbCu₅.₅ but with a higher density of occurrence.


PS08.01.06 THE STRUCTURE OF COPPER(II) WITH 2-HYDROXYETHYL (PROPYL) IMINE - 2-HYDROXY-1-BENZALDEHYDE. Yu.M. Chumakov, T.J. Malinowski, Institute of Applied Physics, Kishinev, 277028, Moldova, V.I. Tsapkov, N.M. Samus, Moldavian State University, Kishinev, Moldova

The various coordination compounds obtained by the interaction of Cu(NO₃)₂·3H₂O with 2-hydroxethyl (propyl) imine - 2-hydroxy-1-benzaldehyde in function of pH of the medium and the nature of the proton acceptor reagent possess an antiseptic activity, which depends not only on the composition, but of the structure of the complex as well. In order to clarify this dependence the following complex compounds were synthesized and next analyzed by X-ray methods:

Cu[HL]NO₃[I][Cu(3-pic)(HL)]NO₃[II], Cu[4-pic](HL)NO₃[III], CuL[IV], CuL'[V], Cu(Py)(HL)NO₃[VI], were H₂L = 2HOC₆H₄CH₂OHCH₂OH, H₂L' = 2HOC₆H₄CH₂CH₂OH.

It was determined, that the coordination polyhedron around the central atom in the compounds I - III is an extended tetragonal pyramid meanwhile the complex are polymers. The compound II is an dimer. The nitrate group serves as bridge-ligand, but in dimers this function fulfills the oxygen atom of the benzaldehyde group, the nitrate group is threedentate in II and bidentate in III. In IV the copper atom is coordinated fully by the deprotonated molecule H₂L through the oxygen atoms of phenol and alcohol and by nitrogen of the imine. The tetramer as cubane complex is formed in the complex compound. The surroundings of the central ion in V is a distorted square with oxygen atoms of phenol and alcohol and by nitrogen of the imine. The tetramer as cubane complex is formed in the complex compound. The surroundings of the central ion in VI is a distorted square formed by oxygen atoms of the phenol and alcohol and of the nitrogen of the azometin H₂L'. The fourth molecule H₂L through the oxygen atoms of phenol and alcohol coordinates the copper atom two atoms like bridge-ligand, but in dimers this function fulfills the oxygen atom of the phenol.

PS08.01.08 CONTRIBUTION TO THE STEREOCHEMISTRY OF MONOVALENT THALLIUM TO OXYGEN ATOMS. H. Effenberger, Institut für Mineralogie und Kristallographie, Universität Wien, Althanstraße 14, A-1090 Wien, Austria

For Tl(I) atoms two principally different kinds of coordination spheres formed by oxygen atoms are known: (i) The Tl(I) atom is strongly covalently bound to a small number of neighbours with short Tl(I) - O bonds. In these cases usually two to four ligands with 2.50 Å < Tl(I) - O < 2.80 Å have been found to be arranged at one side of the Tl(I) atom. Additional ligands have definitely longer Tl(I) - O bond lengths starting by Tl(I) - O > 3.00 Å. These coordination figures are in accordance with expectations from the electron configuration of Tl(I) atoms with their lone-pair electrons. (ii) The Tl(I) atom is coordinated by a large number of O atoms with more or less equal Tl(I) - O bond lengths or at least without larger gap in the distribution of the distances. Regular polyhedra with up to 12 ligands are known. The Tl(I) - O bond lengths as a rule start with larger values as found for the type (i) coordinations. The type (ii) Tl(I) atoms sometimes replaces alkali or earth alkali atoms like K, Rb, Cs, and Ca or NH₄. It is to be mentioned that transitions between these two principally different kinds of coordination figures are known. A similar crystal chemical behaviour shows e.g. Pb(I).

In connection with an investigation of the geometry of the coordination figures of the Tl(I) atoms three Tl(I) arsenates have been synthesized hydrothermally and their crystal structures were determined by single crystal X-ray diffraction methods: Tl₃(AsO₄)(AsO₃) [a = 8.517(3), c = 5.233(2) Å, space group P6₃/m, T₃(i)Cu(I)As₂O₅ [a = 6.000(3), b = 5.343(2), c = 8.616(3) Å, β = 98.05(3)°, space group P2₁], and Tl₃Cu₂(As₂O₅)₃As₄O₁₈ [a = 6.407(2), b = 11.245(5), c = 10.173(4) Å, β = 98.64(2)°, space group P2₁/c]. All these compounds represent type (i) examples. In Tl₃(AsO₄) the Tl(I)-O bond lengths are 2.527, 2.542 and 2.562 Å, in Tl₃CuAsO₅ they are 2.487, 2.565 and 2.778 Å for Tl(I) and 2.509, 2.743, 2.749 and 2.847 Å for Tl(II), and in Tl₃Cu₂(As₂O₅)₃As₄O₁₈ they are 2.565 and 2.640 Å, next Tl(I)-O distances are ≥ 3.0 Å.