RIETVELD STUDIES OF THE COPPER-IRON SUBSTITUTION IN SYNTHETIC GOETHITE

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Secondary iron oxyhydroxides are widespread in soils, sediments and waters, occurring as very fine particles with large surface areas. These minerals can interact strongly with various ionic species and consequently, influence on the mobility of trace elements. For example, following adsorption, metallic ions may be incorporated in mineral structures. Among the Fe oxyhydroxides, goethite (alpha-FeOOH) is one of the more abundant phases and this mineral has a great potential for isomorphic substitution of Fe by other metals. The aim of the present study was, using Rietveld refinement from X-ray powder diffraction data, to establish the crystal structure of goethite in synthetic samples with copper (alpha-CuxFe1-xOOH). The preliminary results indicate that all solids with 0x0.042 are monophasic and crystallize in the orthorhombic system, space group Pnma. The values obtained for the lattice parameters or atomic coordinates show that the substitution of Fe3+ by Cu2+ does not obey the Vegard rule, i.e., no correlation was found between the copper concentration and lattice parameters, but an increase in the cell volume with copper content is observed. Also, with the x increase a deformation on the metal octahedra occurs, due to the Jahn-Teller effect.