Poster Presentation

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Comparative study of two oxalate isomers with different dimensionalities

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We report here two bimetallic oxalate isomers with the same chemical formula [RbCr(C2O4)2(H2O)2], which have been synthesized respectively by a slow evaporation method at room temperature (compound I) [1], and under hydrothermal conditions (compound II) [2] with the same starting salts. Their structures show a several discrepancies, due probably to the synthetic conditions. Indeed, the compound I crystallizes in space group C2/m with the Cr, Rb atoms and one oxygen from water molecule lying on special positions. Moreover, the unique oxalate ligand forms a bridge between metal centers. The Cr atom is coordinated to 2 bidentate-chelating oxalates and 2 aqua ligands in a trans-conformation and any water molecule has been found around the 8-coordinated Rb atom, leading to a layered structure consists of alternating Rb and Cr polyhedra connected via the unique organic ligand. Whereas, the compound II crystallizes in space group P21/n, with all atoms located on general positions. Furthermore, two independent oxalato ligands exhibit different configurations, which one is pentadentate and the other is hexadentate with two different chelating modes. The very slightly distorted Cr octahedra consists of 2 bidentate-chelating oxalato ligands and 2 water molecules in a cis-conformation, while the alkali metal is surrounded by seven O atoms from oxalate groups, completed with two H2O molecules which are bridging the Cr and Rb polyhedra by one common edge. This results in the formation of three different chains of alternating edge- and vertex-shared polyhedra through oxalates groups and aqua ligands, running along the three space directions to build a three dimensional framework. These two compounds can be considered as supramolecular isomers [3].

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