WATER IN THE ALLUAUDITE TYPE STRUCTURE: SYNTHESIS, CRYSTAL STRUCTURE AND MAGNETIC PROPERTIES OF $Co_3(AsO_4)_{0.5}(HAsO_4)_2(H_2AsO_4)_{0.5}(H_2O)_{0.5}$

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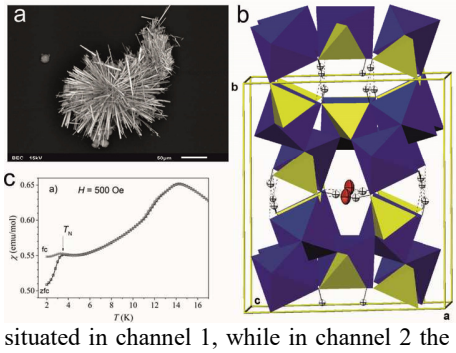
Single crystals of the new compound tri-Co(II)hemi-(arsenate(V))di-[hydrogen arsenate(V)]hemi-[di-hydrogenarsenate(V)]hemihydrate, $Co_3(AsO_4)_{0.5}(HAsO_4)_2(H_2AsO_4)_{0.5}\cdot\cdot(H_2O)_{0.5}$ (denoted CoAs-alluaudite) were grown under hydrothermal conditions. CoAs-alluaudite represents a new member of alluaudite-like protonated arsenates [space group $C2/c$, a = 11.698 (5), b = 12.571 (3), c = 6.7705 (14) Å, β = 113.25 (3) °, V = 914.8 (5) Å^3, Z = 4]. In the unit cell of CoAs-alluaudite, the one of the two Co, one of the two As and one of the seven O atoms lie at 4*e* special positions, with site symmetries 2. The crystal structure consists of the infinite edge-shared CoO_6 octahedra chains, running along the [1 0 $\bar{1}$] direction. The curved chains are interconnected by $[(As1O_4)_{0.5}(H_2As1O_4)_{0.5}]^{2-}$ and $[HAs2O_4]^{2-}$ tetrahedra forming a heteropolyhedral 3D open framework with two types of parallel channels. Both 1 and 2 channels are running along the *c*-axis and are located at positions (1/2, 0, *z*) and (0, 0, *z*), respectively. The H2 and H4 hydrogen atoms of O2H2 and O4H4 hydroxyl groups are situated in channel 1, while in channel 2 the uncoordinated water molecule H_2O7 at half-occupied 4*e* special positions and hydrogen atoms of O6H6 hydroxyl group were found. Infrared and single-crystal Raman spectra were measured and evaluated in order to obtain further information on the anion groups and especially on the short hydrogen bonds. The OH stretching frequency is in good agreement with the observed O···O distances.



The results of the magnetic investigations confirm the quasi one dimensional structure of divalent cobalt ions. They are antiferromagnetically coupled with the intrachain interaction parameter of $J \approx -8$ cm^{-1} and interchain parameter of $J' \approx -2$ cm^{-1} that become effective below the Néel temperature of 3.4 K.