MINERAL-LIKE ARSENATES: CRYSTAL STRUCTURE OF $Sr_2Mg(AsO_4)_2 \cdot 2H_2O$ WITH KRÖHNKITE-TYPE CHAINS

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In order to understand the role of arsenic in the environment, one has to investigate structura features and stabilities of naturally occurring arsenic compounds. In addition, a study o mineral-related synthetic phases should be very helpful because they can appear as a result o human activities. $Sr_2Mg(AsO_4)_2 \cdot 2H_2O$ was synthesised during an on-going research on natu ral and synthetic arsenates, with a focus on their structural and spectroscopic classification.
The crystal structure of the novel, hydrothermally synthesised $Sr_2Mg(AsO_4)_2 \cdot 2H_2O$ wa refined from single-crystal X-ray diffraction data (Mo$K\alpha$, 298 K, $2\theta_{max} = 70°$), starting fron the atomic coordinates of the isotypic mineral gaitite, $CaZn_2(AsO_4)_2 \cdot 2H_2O$ (KELLER et al. 2004). The compound is triclinic, space group $P\bar{1}$, with a = 6.0863(12), b = 7 1542(14) c = 5.6655(11) Å, α = 96.61(3)°, β = 109 15(3)°, γ = 108.39(3)°, V = 214.46(7) Å^3, Z = 1. Th refinement yielded for 1869 'observed reflections' with $F_o^2 \geq 4\sigma(F_o^2)$ $R_1(F)$ of 0.0250. Th mean bond distances are <As–O> = 1.688 Å, <Mg–(O,H_2O)> = 2.105 Å and <Sr–(O,H_2O)> = 2.638 Å. The positions of all H atoms were found in a difference-Fourier map and iso tropically refined.
$Sr_2Mg(AsO_4)_2 \cdot 2H_2O$ represents the first Sr compound based on kröhnkite-type chains. Thi infinite tetrahedral-octahedral chain has a composition of $[M(XO_4)_2(H_2O)_2]$, and is the mai structural unit in a large family of compounds with the general formula $A_nM(XO_4)_2(H_2O)$ [A = Na^+, K^+, Rb^+, Cs^+, Tl^+, NH_4^+, H^+ or Ca^{2+} (n = 1, 2), M = Mg^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+} Cu^{2+}, Zn^{2+}, Cd^{2+}, Al^{3+}, Fe^{3+}, Sc^{3+}, In^{3+} Tl^{3-}, X = P^{5+}, As^{5+}, S^{6+}, Se^{6+}, Cr^{6+}, Mo^{6+}, W^{6+}]. Thes compounds are assigned to seven types (triclinic A-C, E, G types and monoclinic D and I types), which differ in their linkage and stacking of the layers (FLECK & KOLITSCH, 2002 KOLITSCH & FLECK, 2006). $Sr_2Mg(AsO_4)_2 \cdot 2H_2O$ belongs to structure type A in this classi fication. Its crystal structure contains $[Mg(AsO_4)_2(H_2O)_2]$ chains oriented along [001] composed of $MgO_4(H_2O)_2$ octahedra alternating with each two AsO_4 tetrahedra sharin corners. These chains are connected through Sr–O bonds and one of two hydrogen bonds O5–H1···O4^i (i = -x+1, -y+1, -z+1) = 2.645(3) Å, into layers parallel to (010), which ar further linked by the Sr–O3 = 2.539(2) Å bond and the second hydrogen bond, O5–H1···O4 2.649(3) Å, into the three-dimensional structure. The [8]-coordinated Sr atoms occup interstices between the chains.

Financial support of the Austrian Science Foundation (FWF) (Grant V203-N19) is gratefully acknowledged.

FLECK, M., KOLITSCH, U. (2002): Z. Kristallogr., 217, 453-443.
KOLITSCH, U., FLECK, M. (2006): Eur. J. Mineral., 18, 471-482.
KELLER, P, LISSNER, F., SCHLEID, T. (2004): Eur. J. Mineral., 16, 353-359.