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Keywords: mineral, bimetallic sulfates, phase transition

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Structural analysis of new mineral phases

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Redikortsevite, NH_4MgCl_3 $x6H_2O$, from the burned dumps of the Chelabinsk coal basin in Russia, described by Chesnokov et al. (1988), has not been submitted to IMA for approval and it is not recognized as a valid mineral species. The occurrence of this phase has also been noticed on burning waste dumps of one of the Upper Silesia coal mines in Poland. Redikortsevite forms there aggregates and fine crystals suitable for structural study. We have determined its 3D structure and performed chemical and mineralogical analysis necessary for the approval process.

Alumohydrocalcite is hydrated calcium and aluminium carbonate. It is ascribed to have chemical formula $CaAl_2(CO_3)_2(OH)_4$ $x3H_2O$ and commonly forms compact fine-crystalline aggregates. This mineral still does not have reliable crystal structure although it has been known since 1926. The reason of such a situation is difficulty in finding single crystals of a good quality and adequate size. We have acquired a unique sample of this mineral from its classic occurrence site at Nowa Ruda, Sudetes Mts., Poland. It consists of spherulitic needle aggregates. Crystals are very well formed and large enough for X--ray structural investigations. They reach length even up to decimal parts of millimeter and are suitable for synchrotron sources rather than laboratory ones. For this mineral, powder diffraction and chemical analysis have been performed for the sake of its identification.

The chevkinite group of minerals are found as accessory phases in a wide variety of parageneses, including igneous rocks ranging from gabbros to peralkaline granites, fenites, ore deposits, granulite facies gneisses and metacarbonates [1]. The composition of the majority of occurrences closely approaches the ideal formula $A_4BC_2D_2Si_4O_{22}$, where A = REE, Ca, Sr, Th; B = Fe^{2+};
C = Ti, Al, Fe^{2+}, Fe^{3+}, Mn, Mg, Zr, Nb; and D = Ti, but there is a wide range of compositionally different species. The geochemical importance of chevkinite group is that they are strong REE-concentrators; total REE_2O_3 contents are up to 50 wt%. They can be the dominant REE-bearing phase in any given rock. The REE are being increasingly used in a host of green technologies, such as the production of novel wind turbines, low-energy light bulbs also mobile phones. Additionally neodymium, one of the most common REE, is a key part of neodymium-iron-boron magnets used in hyperefficient motors and generators. Published work has shown that compositional variations in the group are mirrored in the structure but there is still no consensus as to how. Further, several species within the group have not been structurally determined. We are attempting to define the complete composition-structure relationships in the group.

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The crystal structure of huemulite

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The crystal structures of natural (from the West Sunday Mine, Utah, USA) and synthetic huemulite, $Na_4Mg(V_{10}O_{28})\cdot24H_2O$, have been solved and refined to $R_1 = 0.0313$ (for 3535 unique $F_o > 4\sigma F$ reflections) and 0.0246 (for 3672 unique $F_o >_- 4\sigma F$ reflections), respectively. Huemulite is triclinic, space group $P\bar{1}$, with Z = 1; unit-cell dimensions of the natural sample are a 9.0453(2), b 11.3337(3), c 11.7372(8) Å, α 105.223(7), β 97.383(7), γ 100.790(7)°, V 1120.30(9) Å³, whereas those of the synthetic sample are a 9.0425(2), b 11.3303(2), c 11.7353 (8) Å, α 105.222 (7), β 97.377 (7), γ 100.791 (7)°, V 1119.47(8) Å³. The structure consists of decavanadate oxyanions $(V_{10}O_{28})^{6-}$ linked via an interstitial complex composed of isolated $[Mg(H_2O)_6]^{2+}$ octahedra and an $[Na_4(H_2O)_{14}]^{4+}$ cationic group (defining an infinite zig-zag chain). There are also four isolated H_2O groups, two of them positionally disordered. All except 4 H atoms have been located, showing a network of H-bonds that further links the interstitial complex and the structural unit, stabilizing the atomic arrangement. The Lewis acidity of the interstitial complex (0.18) is almost coincident with the upper limit of basicity of the structural unit (0.17), thus showing that the valence-matching principle is maintained in this structure.

It is probable that the X-ray pattern and the unit-cell dimensions informed in the original description of huemulite [1] were measured using a mixture that included fully hydrated and partially dehydrated material.

Huemulite is closely related to a synthetic family of general formula $Na_4M^{2+}(V_{10}O_{28})\cdot23H_2O$ (M=Ni,Mg) [2] [3], the main difference (in addition to having $\approx$ 23 H_2O molecules instead of $\approx$ 24) being that the latter compounds have a unit cell with doubled volume. Unit cell and atomic positions of huemulite are related to those of the synthetic family by the transformation matrix M = [1 0 0 / 0 1 1 / 0 $\bar{1}$ -1]. After the transformation, the space group of huemulite becomes $A\bar{1}$. Some of the symmetry restrictions (inversion centers, cell centering, etc.) present in huemulite are relaxed, with the consequence that fewer atoms are symmetry-related in the synthetic family.

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Structural Investigations of Synthetic Analogues of Murataite

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