

structures of 1, 2, 3, 4, 5, 7 it is tetragonal and pentagonal (deformed octahedra and pentagonal bipyramids, respectively), in the structure of 6 uranium atoms have UO_8 and UO_7 coordination, and in the structures of 8 and 9 three different uranyl ion coordinations – tetragonal, pentagonal and hexagonal are realized (actually, this is the first actinide compounds with the actinyl cation in three different coordinations). The configuration of the CCIs in these structures differ: dimers in 1 and 3, two types of trimers in 2, 4 and 5, pentamers in 8 and 9, in the structure of 6 circular hexamers are realized, and in the structure of 7 observes a one-dimensional array of two- and three-center cation-cation bonds. The configurations of CCIs realized in the structures of 5, 6, 7 and 8 have been observed for the first time. It should be mentioned that all compounds except 1 and 3 crystallized in new structure types.

Keywords: uranium compounds; crystallography inorganic; crystallochemistry

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The Tobermorite-Like Layer in Non-Tobermorite Minerals. Elena Bonaccorsi^a, Stefano Merlino^a. ^aUniversity of Pisa – Earth Science Department Via S. Maria 53, 56126 Pisa, Italy.

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The tobermorite-like layer (TLL) is a characteristic feature in all the structures of the natural and synthetic compounds of the tobermorite group [1]. In those structures eptahedra of calcium cations, characterized by ‘a pyramidal part on one side and a dome part on the other side joining the equatorial oxygen atoms’, form columns through edge sharing; the columns are connected each other, once again through edge sharing, and adjacent columns present the pyramidal apical ligands on opposite sides of the resulting infinite layers. These layers, decorated with wollastonite chains on both sides, build up the ‘complex layers’ which are the basic structural module in all the phases of the tobermorite group (Fig. 1).

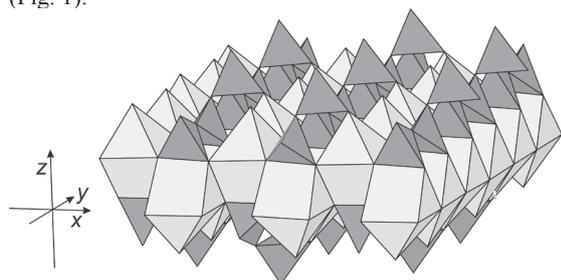


Fig. 1. The tobermorite-like layer decorated with wollastonite chains on both sides, as it appears in the structures of the natural and synthetic compounds of the tobermorite group.

TLL is a recurrent feature in several natural phases belonging to distinct mineral groups. In the structures of the compounds of the rinkite group the TLL is decorated on both sides by disilicate groups and is accompanied by an infinite ‘octahedral’ layer in building up the structural arrangement. Dovyrenite [2] and roumaite [3] are closely related to the minerals of the rinkite group and differ only

in the way of decoration of the TLL by the disilicate groups. Fukalite [4] too presents the TLL, decorated on both sides by four-repeat silicate chains and carbonate groups; tilleyite-type polyhedral layers are also present as distinct modules in building up the structural arrangement. The ubiquitous occurrence of TLL is related to its chemical and structural flexibility: the chemical and geometrical variations of the TLL in the different structures are described and discussed.

[1] Merlino S., Bonaccorsi E., Armbruster T. 1999: *American Mineralogist*, **84**, 1613–1621. [2] Kadiyski M., Armbruster T., Galuskin E.V., Pertsev N.N., Zadov A.E., Galuskina I.O., Wrzalik R., Dzierzanowski P., Kislov E.V. 2008: *American Mineralogist*, **93**, 456–462. [3] Biagioni C., Bonaccorsi E., Merlino S., Parodi G.C., Perchiazzi N., Chevrier V. 2008: *Plinius*, **34**, 211. [4] Merlino S., Bonaccorsi E., Grabezhev A.I., Zadov A.E., Pertsev N.N., Chukanov N.V. 2009: *American Mineralogist*, **94**, 323–333.

Keywords: layered silicates; crystal structures; mineralogical crystallography

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Byzantievite, the First Silicate-Borate-Phosphate Mineral. Elena Sokolova^a, Leonid Pautov^b, Atali Agakhanov^b, Frank Hawthorne^a. ^aDepartment of Geological Sciences, University of Manitoba, Winnipeg, Canada. ^bFersman Mineralogical Museum, Moscow, Russia.

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Byzantievite, ideally $Ba_2(Ca,REE,Y)_{22}(Ti,Nb)_{18}(SiO_4)_4[(PO_4)_2(SiO_4)]_4(BO_3)_9O_{22}[(OH),F]_{43}(H_2O)_{1.5}$, is the only mineral which contains three different oxyanions: (BO_3) , (SiO_4) and (PO_4) . They occur in the ratio 9:5:3. Byzantievite occurs in the moraine of the Dara-i-Pioz glacier, the Alai mountain ridge, Tien-Shan Mountains, northern Tajikistan. Byzantievite has no natural or synthetic analogues. The crystal structure of byzantievite, a 9.1202(2), c 102.145(5) Å, γ 120°, V 7357.9(5) Å³, sp. gr. *R3*, Z=3, D_{calc} 4.151 g/cm³, was solved by direct methods and refined to an R index of 13.14%. In the crystal structure, there are fifty cation sites. Twenty-three sites are fully occupied and twenty-seven sites are characterized by partial occupancy: six sites are more than 50% occupied and twenty-one sites are less than 50% occupied. In the crystal structure of byzantievite, there are two distinct parts that alternate along the c axis. Part one is characterized mainly by fully occupied cation sites and part two, mainly by partially occupied cation sites. Part one has a local inversion centre whereas part two does not. Hence the crystal structure of byzantievite lacks an inversion centre. For better understanding of this framework structure, we describe it as sheets of polyhedra stacked along [001]. Sheet a is composed of [12]-coordinated Ba atoms. Ti-dominant octahedra and B-triangles share common vertices to form sheet b. [8]-coordinated (Ca,REE, Y) polyhedra and B triangles share common vertices and edges to form sheet c. Sheet d is composed of [10]-coordinated (Ca,REE, Y) polyhedra and P tetrahedra. Sheet e is formed by [8]-coordinated (Ca,REE, Y) polyhedra, Si tetrahedra and B

triangles. Sheet f is composed of [9]-coordinated (Ca,REE, Y) polyhedra, Si tetrahedra and B triangles. In sheet g, [6]-coordinated sites are 67% occupied by Ti and Nb, and B triangles are only 17% occupied by B. In sheet h, [6]-coordinated sites are only 17% occupied by Ti, they are coordinated by OH and H₂O groups. Two identical h sheets are connected via common vertices of 17% occupied Ti octahedra which are H₂O groups. In sheet k, the [8]-coordinated sites are 22% occupied by Ba. The structure is a framework of cation polyhedra which can be considered an intercalation of three domains: one fully ordered with full occupancy of cation sites, and two partly ordered with cation-site occupancies of 67% and 17%, respectively. To acknowledge the extreme chemical and structural complexity of this mineral, we chose the name byzantievite. "Byzantine" means "intricately involved". For 12 centuries (374-1453), the Byzantine Empire was home to many different peoples and religions. The structure of the Empire was extremely complex but the state functioned very efficiently, and shaped Europe and modern civilization.

Keywords: byzantievite; framework; new mineral

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A Few Applications of the Superspace Approach in Mineralogy. Alla Arakcheeva. *Laboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.*

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It is fair to claim that the development of crystallography was initiated by mineralogy. First the crystal forms and later crystal structure determinations did primarily instigated the mathematical description of minerals. Crystal chemistry is essentially based on the large amount of structure determinations of natural minerals. It is not surprising that precisely the minerals natrite, Na₂CO₃ [1] and calaverite [2] have played a fundamental role in the development of the superspace theory. Currently, the superspace concept is successfully applied for the determination and description of a many incommensurately modulated crystal structures (IMCS) including minerals. For example, investigations of minerals like fresnoite, melilite, laszurite, akermanite, sartorite, labradorite, srebrodolskite, tridymite, quartz (between α and β modifications) could only be meaningful with the superspace symmetry approach. The IMCSs of minerals give the possibility to study details of their crystal chemistry, which can be used for a better understanding of their genesis. For instance, the determination of IMCSs in the calaverite-sylvanite group, Au_{1-x}Ag_xTe₂, [2, 3] reveals different degrees of valence fluctuations on the Au-position, which are due to different degree of the Ag ordering on the Au position. The IMCSs of two different occurrences of natrites allow to distinguish specific characteristics of Na and CO₃, although their average structures are identical. In material science, mineral names are used to characterize of structure types. With the superspace approach, the structure type (ST) concept can be generalised in (3+1)D symmetry space [4] (3+1)D ST can be used not only to predict 3D structures but also to identify them [4]. In addition to the

pioneering scheelite (3+1)D ST [4], the calaverite (3+1)D ST [3] is able to characterize calaverite, sylvanite, kostovite and krennerite minerals as well as NbTe₂, TaTe₂, VTe₂, synthetic compounds based on the unique *C2/m*($\alpha 0\gamma$)(0s) superspace group with identical basic structures. The (3+1) D ST concept permits also a unified symmetry approach for group-subgroup considerations in phase transitions [5]. The superspace approach born from the study of mineralogical samples now is an effective tool, which can be applied to the needs of mineralogy. The precise characterization of isomorphic substitution is greatly facilitated with IMCSs determination. Investigation of IMCSs allows to predict series of 3D structures and, sometimes, polymorphic modifications [6]. The extension of the ST concept in (3+1) D space appears to be an effective way to identify structure-relation properties.

[1] Brouns, E., Visser, J.W. & de Wolff, P.M., *Acta Cryst.*, **1964**, 17, 614; Van Aalst, W., Van den Hollander, J., Peterse, W.J.A.M. & De Wolff, P.M., *Acta Cryst.*, **1976**, B32, 47; De Wolff, P.M., *Acta Cryst.*, **1974**, A30, 777. [2] Goldschmidt, V., Palache, C., Peacock, M., *N. Jahrbuch, f. Mineralogie* **1931**, 63(A), 1; Janner, A., Dam, B., *Acta Cryst.* **1989**, A45, 115; Schutte, W.J., De Boer, J.L., *Acta Cryst.* **1988**, B44, 486. [3] Bindi, L., Arakcheeva, A., Chapuis, G. *Amer. Min.*, **2009** (accepted article). [4] Arakcheeva, A., Chapuis, G., *Acta Cryst.*, **2008**, B64, 12. [5] Stokes, H.T., Campbell, B.J., Hatch, D.M., *Acta Cryst.*, A63, 365. [6] Arakcheeva, A., Chapuis, G. *Acta Cryst.*, B62, 52.

Keywords: mineralogy and crystallography; incommensurately modulated structures; classification of crystal structures

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Cr_xRe_{1-x}O₂ Oxides with Different Rutile-like Structures: Changes in the Electronic Configuration and Resulting Physical Properties.

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Rutile type crystal structures and their derivatives are based on the same topology: straight chains of edge-sharing MO₆ octahedra for the cations M are connected via corner-sharing to four surrounding chains [1]. Rutile-derivatives show ordering of cations, anions or distortions of coordination polyhedra.

Several complex oxides of Cr³⁺ with rutile, trirutile or rutile-like structure exist, because the ionic radius of Cr³⁺ (0.62 Å) is close to the one of Ti⁴⁺ (0.61 Å) for octahedral oxygen coordination. Ternary oxides in the system Cr – Re – O are less intensively investigated, although these systems offer an additional degree of freedom due to the ability of the Re ion to adopt formal oxidation states between +4 and +7 in complex oxides with different resulting properties. Both end members, CrO₂ [2] and the monoclinic modification of ReO₂ [3], have a rutile-like structure.

In our work [4], mixed chromium-rhenium oxides, Cr_xRe_{1-x}O₂ with 0.31 ≤ x ≤ 0.66, have been synthesized for the first time by high-pressure high-temperature synthesis and