## FA2-MS01-P01

Layered Silicates: Polysomatic Macaulayiteburckhardtite Series. Olga V. Yakubovich ${ }^{\text {a }}$, Werner Massa ${ }^{\text {b }}$, Nikita V. Chukanovc. ${ }^{\text {a }}$ Department of Geology, Moscow State Lomonosov University, Russia. ${ }^{b}$ Department of Chemistry, Philipps-University of Marburg, Germany. 'Institute of Problems of Chemical Physics, Chernogolovka, Russia. E-mail: yakubol@geol.msu.ru

The macaulayite-burckhardtite family [1] of layered silicates is discussed along in terms of the modular concept. The characterization of a new mineral britvinite $\left[\mathrm{Pb}_{7}(\mathrm{OH})_{3} \mathrm{~F}\left(\mathrm{BO}_{3}\right)_{2}\left(\mathrm{CO}_{3}\right)\right]\left[\mathrm{Mg}_{4.5}(\mathrm{OH})_{3}\left(\mathrm{Si}_{5} \mathrm{O}_{14}\right)\right][2,3]$ allowed considering this mineral group as a polysomatic series with a TOT-"pyrophyllite" block as one end-member. Along $c$ axis of the unit cells these three-layered blocks alternate with lamellar modules of different size and composition, such as oxide, oxide-carbonate, oxide-carbonate-sulfate, ect. The group involves among britvinite the minerals macaulayite, lourencewalsite, burckhardtite, kegelite, surite, ferrisurite, and niksergievite. In the absence of data of precision structure investigations, the preliminary inferences regarding their structures were made using the results of chemical, spectroscopic, and X-ray powder diffraction analyses and, in a number of cases, microdiffraction experiments.
Tetrahedral fragments of the britvinite crystal structure built from 12 -membered rings are topologically identical to tetrahedral nets in zeophyllite $\mathrm{Ca}_{13}(\mathrm{~F}, \mathrm{OH})_{10}\left[\mathrm{Si}_{5} \mathrm{O}_{14}\right]_{2} 6 \mathrm{H}_{2} \mathrm{O}$ [4, 5] and synthetic $\mathrm{Rb}_{6} \mathrm{Si}_{10} \mathrm{O}_{23}$ [6] structures. These tetrahedral $\left(\mathrm{Si}_{5} \mathrm{O}_{14}\right)_{\infty \infty \infty}$ layers differ only by the direction of apical vertices of $\mathrm{SiO}_{4}$ tetrahedra, and can be presented as $(U U U \ldots)_{\infty}$ in britvinite, (UUUDUUUD ... $)_{\infty \infty}$ in zeophyllite, and (UDUDUD...) $)_{\infty \infty}$ in $\mathrm{Rb}_{6} \mathrm{Si}_{10} \mathrm{O}_{23}$. In the crystal structures of orthorhombic and hexagonal modifications of $\mathrm{Rb}_{6} \mathrm{Si}_{10} \mathrm{O}_{23}$, neighboring tetrahedral layers share oxygen vertices with formation of a tetrahedral 3D framework $\left(\mathrm{Si}_{10} \mathrm{O}_{23}\right)_{\text {moxs }}$.
Two types of blocks alternate along the $c$ axis in the britvinite crystal structure. Blocks of the first type are built from brucite-like layers of edge-sharing octahedra bounded on both sides by networks of Si tetrahedra in three-layer sandwiches of $\left\{\mathrm{Mg}_{4.5}(\mathrm{OH})_{3}\left[\left(\mathrm{Si}, \mathrm{Al}_{5} \mathrm{O}_{14}\right)\right]\right\}_{\infty \times \infty}$ composition. Blocks of the second type are complex defect sevenlayer packs described by the formula $\left[\mathrm{Pb}_{7.1}(\mathrm{OH})_{2.7} \mathrm{~F}_{\left(\mathrm{CO}_{3}\right)}\right)$ $\left.\left(\mathrm{BO}_{3}\right)_{1.7}\left(\mathrm{SiO}_{4}\right)_{0.3}\right]_{\infty}$. Observed diffuse streaks along the $c^{*}$ direction of the reciprocal lattice of britvinite were interpreted as diffuse scattering from lead atoms associated with one-dimensional disorder. The translational $\mathrm{Si}, \mathrm{O}$ layers parallel to the $a b$ plane and containing ordered vacancies in Si positions, are displaced with respect to the neighboring Pb layer. Thus, the "vacant" tetrahedra and, hence, the Pb atoms appear to be displaced in the second and third superposed equivalent layers (stacking disorder).
[1] Strunz H.I., Nickel E.N. Strunz Mineralogical Tables. E. Schweizerbart'sche Verlagsbuch. Stuttgart. 2001. [2] Chukanov N.V., Yakubovich O.V., Pekov I.V., Belakovsky D.I., Massa W. Geology Ore Deposits, 2008, 50, 713. [3] Yakubovich O.V., Massa W., Chukanov N.V. Cryst. Reports, 2008, 53, 206. [4] Merlino S., Acta Cryst., 1972, B28, 2726. [5]. Mikenda W., Pertlik F., Povondra P., Ulrych J., Mineral. Petrol., 1997, 61, 199. [6]. Lapshin A.E.,

Borisova N.V., Ushakov V.M., Shepelev Yu.F., Russ. J. Inorg. Chem., 2006, 51, 438.

Keywords: layered silicates; britvinite crystal structure; polysomatic series

## FA2-MS01-P02

Fettelite, $\quad\left[\mathrm{Ag}_{6} \mathbf{A s}_{2} \mathbf{S}_{7}\right]\left[\mathrm{Ag}_{10} \mathbf{H g A s}_{2} \mathbf{S}_{8}\right]: \quad$ Structure, Twinning, and Revised Chemical Formula. Silvio Menchetti ${ }^{\text {a }}$, Luca Bindi ${ }^{\text {b }}$, Frank N. Keutsch ${ }^{\text {c }}$, Carl A. Francis ${ }^{\text {d }}{ }^{a}$ Dipartimento di Scienze della Terra, Univ. Firenze, Italy. ${ }^{b}$ Natural History Museum of Florence, Italy. ${ }^{\text {c Department of Chemistry, Univ. Wisconsin- }}$ Madison, USA. ${ }^{\text {d}}$ Harvard Mineralogical Museum, Cambridge, USA.
E-mail: crystal@unifi.it
The crystal structure of the rare mineral fettelite [1] was solved using intensity data collected from a twinned crystal from Chañarcillo, Copiapó Province, Chile. The study revealed that, in spite of the strong hexagonal pseudosymmetry, the structure is monoclinic (space group C2) with $a=26.0388(10), b=15.0651(8), c=15.5361(8)$ $\AA, \beta=90.48(1)^{\circ}$ and $V=6094.2(5) \AA^{3}$. The refinement of an anisotropic model led to an $R$ index of 0.0656 for 7143 observed reflections $[I>2 \sigma(I)]$ and 0.0759 for all 17447 independent reflections [2]. Fettelite is intimately twinned with six twin domains. The structure consists of the stacking of two module layers along [001]: an $A$ module layer with composition $\left[\mathrm{Ag}_{6} \mathrm{As}_{2} \mathrm{~S}_{7}\right]^{-2}$ and a $B$ module layer with composition $\left[\mathrm{Ag}_{10} \mathrm{HgAs}_{2} \mathrm{~S}_{8}\right]^{2+}$. The As atoms form isolated $\mathrm{AsS}_{3}$ pyramids typical of sulfosalts, Hg links two sulfur atoms in a linear coordination, and Ag occupies sites with coordination ranging from quasi linear to almost tetrahedral. The $A$ module layer found for fettelite is identical to that described for the minerals belonging to the pearceite-polybasite group. On the basis of information gained from this characterization the crystal chemical formula was revised according to the structural results, yielding $\left[\mathrm{Ag}_{6} \mathrm{As}_{2} \mathrm{~S}_{7}\right]\left[\mathrm{Ag}_{10} \mathrm{HgAs}_{2} \mathrm{~S}_{8}\right](Z=8)$.
[1] Wang N., Paniagua A., Neues Jahr. Mineral. Monat., 1996, 313. [2] Bindi L., Keutsch F., Francis C., Menchetti S., Am. Mineral., $\mathbf{2 0 0 9}, 94$, in press.

Keywords: sulfosalts; twinning; mineralogical crystallography

## FA2-MS01-P03

Ordering of the Al Cation Distribution in the Octahedral Sheets Related to the Ordering of Al in the Tetrahedral Sheets of Phlogopite Investigated by 2D CPMAS NMR and Monte Carlo Simulations. Ramona Langner ${ }^{\text {a }}$, Michael Fechtelkord ${ }^{\text {a }}$, Erika Palin ${ }^{\text {b }}$, Alberto Garcia ${ }^{\text {c }}$, Javier López-Solano ${ }^{\text {d }}$. ${ }^{a}$ Institut fuer Geologie, Mineralogie und Geophysik, Ruhr-Universitaet Bochum, Germany. ${ }^{b}$ Department of Earth Sciences, University of Cambridge, UK. ${ }^{c}$ ICMAB-CSIC, Institut de Ciencia de Materials de

