There are minor differences between the chemical compositions of baratovite and berezanskite and their blocks in the crystal structure of faizievite. Baratovite, $KLi_3Ca_7Ti_2(Si_6O_{18})_2(OH)_2$, and the baratovite block in faizievite, $K_2(Ca_6Na)Li_6Ti_4(Si_6O_{18})_2F_2$, are related by the substitution: $^{VI}Ca^{2+} + (OH)^-_2 \leftrightarrow {}^{VI}Na^+ + F^-_2$. Berezanskite, $K^{IX}\square L_3Ti_2(Si_{12}O_{30})$, and the berezanskite block in faizievite, $KNaLi_3Ti_2(Si_{12}O_{30})$, are related by the substitution: $^{IX}\square \leftrightarrow {}^{IX}Na^+$. Therefore assembley of faizievite from baratovite and berezanskite components is accompanied by the following substitution:
$^{VI}Ca^{2+} + {}^{IX}\square + (OH)^-_2 \leftrightarrow {}^{VI}Na^+ + {}^{IX}Na^+ + F^-_2$.
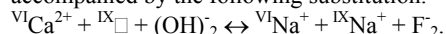
[1] Pautov, L.A. & Agakhanov, A.A. *Zap. Vser. Mineral. O-va.* 1997, 126(4), 75.
[2] Sandomirskii, P.A., Simonov, M.A., Belov, N.V. *Dokl. Akad. Nauk SSSR*, 1976, 231, 615.

MS41 P23

Crystal structures of new pyrovanadates $A_2MnV_2O_7$ (A = K, Rb) <u>Hamdi Ben Yahia,</u> Etienne Gaudin, Jacques Darriet, *Institut de Chimie de la Matière Condensée de Bordeaux, Université Bordeaux 1, 87 Avenue du Docteur Schweitzer, 33608 Pessac Cedex, France.*
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Keywords: Melilite layered structure, Crystal structure determination, Single crystal diffraction

The compounds $A_2MnV_2O_7$ (A = K, Rb) with structures related to the melilite-type [1] have been synthesised. The crystal structures of $K_2MnV_2O_7$, $KRbMnV_2O_7$ and $Rb_2MnV_2O_7$ were determined using single crystal samples. The compound $K_2MnV_2O_7$ has tetragonal unit cell parameters a = 8.6091 Å, c = 5.5375 Å and crystalize with $P\text{-}42_1m$ space group, Z = 2 whereas $Rb_2MnV_2O_7$ and $KRbMnV_2O_7$ crystalise in $P4_2/mnm$ space group, Z = 4 with unit cell parameters a = 8.5304 Å, c = 11.4659 Å and a = 8.5766 Å, c = 11.8094 Å respectively. The structures contain layers build up by MnO_4 tetrahedra and V_2O_7 pyrovanadate units. The linkage of tetrahedra forms five-membered rings which form sheets parallel to (001). The eight coordinated A alkali cations are positioned between the sheets and form distorted square antiprisms in $K_2MnV_2O_7$ and distorted square prisms in $Rb_2MnV_2O_7$ and $RbKMnV_2O_7$.

[1] Warren B.E., *Z. Kristallogr.* 1930, 74, 131.

MS41 P24

Analysis of structural ordering of mineral solids from microscopic images <u>Yevgeny A. Golubev</u> *Institute of Geology, Russian Academy of Sciences, Syktyvkar, Russia.*
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Keywords: AFM-STM studies of minerals and glasses, supramolecular structures, statistical distribution

We solved a problem of studying of supermolecular structures ordering of natural X-ray amorphous substances. We was shown earlier that the most part of these substances have nanodispersed structure [1]. The most effective method of studying of nanostructurized substances is direct observation of their structure by microscopy. In case of a nonregular arrangement of structural units there is a question on a degree of their ordering. The statistical methods are necessary for

studying ordering, allowing to determine local structural characteristics of system. In this work the modernized method *of n-symmetric points* [1, 2] was used. This method based on statistical approximation of dependences of spatial distribution of points (particles), enabled to determine a randomness of points arrangement. At their regularity distribution this method enables to receive the appropriate statistical appraisal, for example, to measure of scale of particles aggregation (on two, on three etc).
We carry out research of supermolecular structures ordering of natural X-ray amorphous substances by SEM and AFM. Among the investigated substances only two have revealed the disorder supermolecular constitution. In the others tendencies to aggregation from two to seven particles in aggregate were found [2].

[1]. Golubev Ye. A. Journal of Crystal Growth, 2005, 275, e2357.
[2]. Golubev Ye. A. Supermolecular structures of natural X-ray amorphous substances Yekaterinburg: Nauka Press, 2006.

MS41 P25

Electron diffraction analysis of amorphous geological materials V.K.Kis[a], M. Pósfai[b], J.L. Lábár[a], I Dódony[c]
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Keywords: disordered structures; electron diffraction; mineralogy

Poorly crystalline and amorphous materials occur in a wide range of geological environments. They include aluminosilicate glasses and opals in rocks, highly disordered Fe hydroxides and oxy-hydroxides in soils, and carbons such as soot in the atmosphere or shungite in the lithosphere.
A knowledge of the structure of poorly crystalline materials is useful for deducing formation/precipitation conditions and helps in understanding their physico-chemical behaviour such as adsorption properties, stability and reactivity.
Amorphous structures lack long-range order but can be described by the nearest neighbour interatomic distances. Since a Fourier transformation of diffraction data gives the frequency distribution of interatomic distances, information on the local structure can be inferred from diffraction data. Electron diffraction (ED) has some advantages over X-ray and neutron beam methods in structural studies. The high spatial selectivity of ED allows one to discriminate between the scattering contributions of the individual components of a heterogeneous material. The strong scattering power of electrons makes a short exposure time possible and results in good statistics in the signal. Light elements (such as carbon or oxygen) are also well measurable.
We used electron diffraction measurements to investigate the local structure of volcanic glasses (obsidian and pumice) and atmospheric soot. In the case of volcanic glasses amorphous, partly ordered, and nanocrystalline regions were distinguished and analysed separately. The deconvoluted atomic distances obtained from experimental diffraction patterns through total pair-distribution functions are consistent with distances for ideal SiO_4 tetrahedra. Partly ordered structures in pumices