$y = FeL_\beta/L_\alpha$, $C = (Fe^{2+} + Fe^{3+})$ and $x = Fe^{2+}/C$.
Then for magnetite (for trend 3) $x = 2. 13y-0. 51$,
  for garnets $x = 4. 17y-2. 08$.
The concentrations of Fe^{2+} and Fe^{3+} are calculated using the equations: $Fe^{2+} = x \cdot C$; $Fe^{3+} = (1-x) \cdot C$. We have studied the intensities FeL_β/L_α and the compositions of magnetites in local volume from various differentiates of the Talnakh intrusion of gabbro-dolerite with different oxidation states (Noril'sk, North Siberia). It was found that Fe^{2+}/Fe^{3+} ratio of magnetites is dependent on rock oxidation potential and therefore it can serve as the criterion of physicochemical environment of magma crystallization.

[1] Laputina I. P. Proc. Y11 Europ. Congr. Electron Microscopy and IX Intern. Conf. on X-Ray Opt. and Microanal. , Haaga, 1980, V. 3, p. 154-155.

PS-08.04.31
THE CRYSTAL STRUCTURE OF JAFFEITE AND RELATED COMPOUNDS.

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The crystal structure of jaffeite, $Ca_6[Si_2O_7] \cdot (OH)_6$, from Kombat mine, Namibia (Sarp. H. , Peacor D. R. Amer. Mineral. , 1989, 74, 1203-1206) has been determined by X-ray methods (hexagonal, P3, lattice constants: a 10. 035, c 7. 499Å, $Z =$ 2. 871 reflections, R_{anizo} 0. 030). Jaffeite and its synthetic analogue are isotypic with fluoborite $B_3[Mg_9(F, OH)_9O_9]$, jeremejevite $B_2[B_3Al_6](OH)_3O_{15}]$ and painite $CaZrB \cdot [Al_9O_{18}]$. All these structures contain octahedral frameworks, formed by double bands, in which octahedra share edges. At the contacts of these bands there are trigonal and hexagonal channels. The trigonal channels are filled by pyrogroups $[Si_2O_7]$ (jaffeite), by trigonal Zr-prisms and B-triangles (painite) or by $[BO_3]$-triangles (fluoborite, jeremejevite). The type of the fillers (Si-O-Si, Zr with B or two B-atoms) determine the similarity of a (b)-cell parameters and the difference of c-parameter in the considered structures.

PS-08.04.32 ### CRYSTAL STRUCTURE OF $AlCa_2$ $(SO_4)_2F_2Cl \cdot 4H_2O$.

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The crystal structure of aluminum dicalcium disulphate fluoride dichloride tetrahydrate, $AlCa_2(SO_4)_2FCl \cdot 4H_2O$ has been determined. Space group I 4/m, a = 6. 870 (1), c = 13. 342 (2) Å, $Z = 2, D_x = 2. 353g/cm^3$, The 447 unique reflections were obtained with Syntex P2$_1$ diffractometer with Mo radiation for 0. 1x0. 1x0. 05mm colorless plate square crystal. The structure has been solved by direct methods and refined by full-matrix leastsquares to R-factor 0. 046 ($R_w = 0. 048$). Hydrogen atoms have been located in difference synthesis.

In the crystal structure of $AlCa_2(SO_4)_2F_2Cl \cdot 4H_2O$ the chains of polyhedra are arranged along [001]. These chains consist of pairs of CaO_4ClF polyhedra alternat with single AlO_4F_2 polyhedra which are rolated along [001] with a difference of 24°. The chains are combined by SO_4-tetrahedra so that all four sulphate oxygen atoms take part in coordinating Ca to form with Cl and F atoms distorted octahedra, which are two nonequal perfect tetragonal pyramids with common base. The stredched one has Cl atom on top, the flattened one an F atom. The Al coordination sphere consists of two F atoms and four oxygen atoms of water moleculecules as flattened perfect tetragonal dipyramide. The Al coordination polyhedron has not direct contacts with SO_4-tetrahedra but interatomic distances analysis performs that in spite of the long distance between oxygen atoms (2. 815Å), a distance from water hydrogen atom to tetrahedron oxygen atom is shortened (H···O = 2. 03 (5) Å) and so these atoms have the specific interaction by hydrogen bond to penetrate crystal structure (Fig.).

Bond distances (Å and angles (deg.) in structure: Ca polyhedron: Ca-Cl = 2. 689 (3), Ca-F = 2. 233 (6), Ca-O$_1$ = 2. 366 (3), ClCaF = 180. 0 (1), ClCaO$_1$ = 84. 9 (1), FCaO$_1$ = 95. 0 (1), O$_1$CaO$_1$' = 89. 6 (1), O$_1$CaO$_1$'' = 169. 9 (1).
Al polyhedron: Al-F = 1. 750 (5), Al-O$_2$ = 1. 918 (6), FAlF = 180. 0 (2), FAlO$_2$ = 90. 0 (2), O$_2$AlO$_2$' = 180. 0 (2), O$_2$AlO$_2$'' = 90. 0 (2).
S tetrahedron: S-O$_1$ = 1. 474 (4), O$_1$SO$_1$' = 109. 1 (2), O$_1$SO$_1$'' = 109. 7 (2).

PS-08.04.33 ### PRINCIPLES OF CRYSTAL CHEMISTRY OF COMPOUNDS CONTAINING TETRAHEDRA $[OT_4]$.

By S. K. Filatov, T. F. Semenova', St. -Petersburg University, Russia.

Revealed are laws of compounds (oxi-salts, oxides) in which the strongest structure fragments are tetrahedra $[OT_4]$, $[OCu_4]$ in particular. Here O is "monatomic" oxygen not present in acid residuals SO_4, SeO_3, Cl etc. , hydroxyl groups OH, water molecules H_2O. Such oxygen ions are the most highly charged negative particles, O^{-2} and that is why in gaseous phase, liquids and crystal structures they collect cations around them.

It is known that classic tetrahedra $[TO_4]$ (valency of central atom 7, 6, 5, 4, 3) are polymerized under atmospheric conditions only through their vertices. At the same time tetrahedra $[OT_4]$ (valency of the central atom 2) may be polarized both through the vertices (up to 4 tetrahedra in a vertex) and through the common edge. This sharply increases the diversity of formed polyions $[OCu_x]$ (S. K. Filatov, T. F. Semenova, Doklady Ac. Sc. USSR, 1992, Vol. 322, No3, pp. 536-539).

By now there are the following known types of polyions from tetrahedra $[OCu_4]$: isolated tetrahedra $[OCu_4]^{6+}$ (e. g. , ponomarevite $K_4Cu_4OCl_{10}$); couples of tetrahedra interconnected through the common edge, $[OCu_3]_2^{2+}$ (fedotovite $K_2Cu_3O(SO_4)_3$; chains of tetrahedra interconnected through the vertices, $[OCu_3]_\infty^{4+}$ (kamchatkite $KCu_3OCl(SO_4)_2$); chains of tetrahedra interconnected through the edges, $[OCu_2]_\infty^{2+}$ (piypit $K_4Cu_4O_2(SO_4)$ MeCl); chains of tetrahedra interconnected by turns through the

vertices and through the edges, $[OCu_{2.5}]^{3+}_{\infty}$ $(Cu_5O_2 (PO_4)_2)$; layers of six-fold rings formed by tetrahedra connected through the vertices with variable up and down orientation of free vertices, $[OCu_{1.5}Pb]^{3+}_{\infty \infty}$ $(Pb_2Cu_3O_2 (NO_3)_2 (SeO_3)_2)$; layers of fedotovite couples connected through the common vertices, $[OCu_2]^{2+}_{\infty \infty}$ (dolerophanite $Cu_2O (SO_4)$); frameworks $[OCu]_{\infty \infty \infty}$ (tenorite CuO), $[OCu_2]^0_{\infty \infty \infty}$ (cuprite Cu_2O) and frameworks of cuprite type in Cu_2O (SeO_3).

The average length of the bond O-Cu in the tetrahedron $[OCu_4]$ increases from 1.916 Å for free vertices to 1.940 Å for vertices common to two tetrahedra, and 1.96 for vertices common to four terrahedra (tenorite). Angles of bonds Cu-O-Cu take values mainly in the interval of 95-125°.

Tetrahedra $[OCu_4]$, polyions and compounds containing these tetrahedra may be formed from volcanous gases, self-igniting dumps of coal basins, blast furnaces and oxygen converters, and from the liquid phase in hydrothermal and other processes. Such complexes can preserve information on the structure of crystallization environment.

PS-08.04.34
LATTICE MISFIT IN MICAS AND THE GROWTH BENDING PROBLEM.

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The origin of micas with sphere bending of basal plane is part of the general problem of growth curvature of crystals. Complex investigation of phengite-muscovite from Urals amazonstone pegmatites has been performed to find out the connection between mica bending and chemical deformation of crystal lattice.

Goniometer research has shown sharp oscillations of crookedness in growth direction of crystals, with a trend diverging from the law of inheritance of crookedness. Geometry of bending and degree of deformation are different in various growth sectors for faces of various simple forms. This is the evidence of growth origin of bending and also of changebility of bending factor with time.

Variations of cell dimensions within the volume of the crystal have been determined by the X-ray powder diffraction method. They have been compared with local changes of chemical composition obtained by microprobe analysis. Linear correlation of lattice parameters (a and b) with iron content and of d_{001} with rubidium content has been found. Some increase of the parameter and d_{001} in growth sector (110) in comparison with those (001) sector has been revealed. Cation composition and lattice parameters of investigated crystals vary strongly within the crystal. The most significant variations have been observed for b parameter and estimated to be 1% of the mean value.

Data received prove the existing hypotheses to be insufficient. High polytype homogeneity ($2M_1$) of crystals excludes bending because of coherence syntactic coalescence of polytypes. Random character of cell dimensions variations excludes the existence of constant moment on growth front. However existing differences in lattice parameters are sufficient for formation of mosaic structure. Mosaic structure of (110) growth sector confirms this proposal. A new mechanism of the bending of crystals is being suggested. The bending of crystals is the consequence of geometrical selection of systematically misorientated blocks, derived by lattice misfit strains.

PS-08.04.35 ESTIMATION OF HYDROTALCITE IN SERPENTINITES BY X-RAY DIFFRACTION AND IR SPECTROSCOPY.

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The amount of hydrotaloite $Mg_6Al_2(OH)_{16}CO_3 4H_2O$ (HT) in serpentinite is of importance since it is responsible for many properties of this material, as well as being acid absorbent and catalyst carrier of praotical use in cement and metal corrosion technology, for studies of different geological processes. The determination of HT in natural mixtures by XRD is beset with problems of X-ray amorphous serpentine, of preffered orientation and disorder in minerals. These reasons prevent to use the X-ray method alone to estimate HT content in mixtures, because often more than one crystal type—usually several serpentine and other minerals—is present (Moroz T., Arkhipenko D., Geol. Geophys., 1991, 2, 58). The development of a simple and convenient IR spectroscopic method for quantitative determination of HT in serpentinite is based on measurements of the relationship between intensities of υ_3 vibrations of CO_3 ions (at 1375 cm^{-1}) and υ Si-O(Si), Si-O(Mg) vibrations (at 980-1060cm^{-1}), the former being absent in serpentine, the latter in HT. Calibration is required by another established method (DTA, miorochemistry) and the accuracy of the calibration is $\pm 10\%$. The intensity and position of carbonate-related absorption defines the amount of interlayer carbonate and the local environments of the anions, and gives information about the cation order-disorder in octahedral sheets. The method appears to be applicable to crystallochemical estimation of natural HT from different deposits in mixture with chlorite and talo, for checking on the separation of fine fraction and determination of structural regularities of hydrotalcite after T, P-treatment.

PS-08.04.36 STRUCTURAL PECULIARITIES OF PHASE TRANSITION ANATASE - RUTILE.

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In nature there are 3 polymorphic modifications of TiO_2: anatase - D_{4h}^{19}, z=4, brookite - D_{2h}^{15}, z=8, rutile D_{4h}^{14}, z=2. It is known that anatase and brookite on heating transform to rutile. Methods of X-ray diffraction and vibration spectroscopy have been used. X-ray anomalous intensities ("AnI") of different hkl - reflections depending on temperature and heating conditions have been observed. The differences have been registered in IR and Raman-laser spectra as well. Lab IR - study of sorption of oleic acid on anatase, brookite and rutile structures showed essential differences. On the other hand X-ray analyses of samples of anatase and rutile from agold deposit registered "AnI" also; "markings" of phase transition: bipyramidal anatase forms were substituted by rutile. Samples of rutile with "AnI" from differ-