

## 08-Inorganic and Mineralogical Crystallography

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$y = FeL_{\beta}/L_{\alpha}$ ,  $C = (Fe^{2+} + Fe^{3+})$  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  $FeL_{\beta}/L_{\alpha}$  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 X 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:  $a = 10.035$ ,  $c = 7.499 \text{ \AA}$ ,  $Z = 2$ , 871 reflections,  $R_{int} = 0.030$ ). Jaffeite and its synthetic analogue are isotopic with fluorborite  $B_3[Mg_9(F, OH)_9O_9]$ , jeremejevit  $B_2[B_2Al_6](OH)_3O_{15}]$  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 pyrogro groups  $[Si_2O_7]$  (jaffeite), by trigonal Zr-prisms and B-triangles (painite) or by  $[BO_3]$ -triangles (fluorborite, jeremejevit). 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  $AlCa_2(SO_4)_2F_2Cl \cdot 4H_2O$ . By G. L. Starova\*, V. S. Fundamenskiy, S. K. Filatov, G. L. Matusevich, L. P. Vergasova. Department of Crystallography, Sankt Petersburg State University, Russia.

The crystal structure of aluminum dicalcium disulphate fluoride dichloride tetrahydrate,  $AlCa_2(SO_4)_2F_2Cl \cdot 4H_2O$  has been determined. Space group I 4/m,  $a = 6.870(1)$ ,  $c = 13.342(2) \text{ \AA}$ ,  $Z = 2$ ,  $D_x = 2.353 \text{ g/cm}^3$ . The 447 unique reflections were obtained with Syntex P21 diffractometer with Mo radiation for  $0.1 \times 0.1 \times 0.05 \text{ mm}$  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 lo-

cated 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 related along  $[001]$  with a difference of  $24^\circ$ . The chains are combined by  $SO_4$ -tetrahedra so that all four sulphate oxygen atoms take part in coordinating Ca atoms to form with Cl and F atoms distorted octahedra, which are two nonequal perfect tetragonal pyramids with common base. The stretched 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 molecules 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 ( $2.815 \text{ \AA}$ ), a distance from water hydrogen atom to tetrahedron oxygen atom is shortened ( $H \cdots O = 2.03(5) \text{ \AA}$ ) and so these atoms have the specific interaction by hydrogen bond to penetrate crystal structure (Fig.).

Bond distances ( $\text{\AA}$ ) and angles (deg.) in structure: Ca polyhedron: Ca-Cl = 2.689 (3), Ca-F = 2.233 (6), Ca-O<sub>1</sub> = 2.366 (3), ClCaF = 180.0 (1), ClCaO<sub>1</sub> = 84.9 (1), FCaO<sub>1</sub> = 95.0 (1), O<sub>1</sub>CaO<sub>1</sub>' = 89.6 (1), O<sub>1</sub>CaO<sub>1</sub>'' = 169.9 (1). Al polyhedron: Al-F = 1.750 (5), Al-O<sub>2</sub> = 1.918 (6), FAlF = 180.0 (2), FAlO<sub>2</sub> = 90.0 (2), O<sub>2</sub>AlO<sub>2</sub>' = 180.0 (2), O<sub>2</sub>AlO<sub>2</sub>'' = 90.0 (2). S tetrahedron: S-O<sub>1</sub> = 1.474 (4), O<sub>1</sub>SO<sub>1</sub>' = 109.1 (2), O<sub>1</sub>SO<sub>1</sub>'' = 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  $[OT_4]$ ,  $[OCu_x]$  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  $[OCu_x]$ : isolated tetrahedra  $[OCu_4]^{6+}$  (e. g., ponomarevite  $K_4Cu_4OCl_{10}$ ); couples of tetrahedra interconnected through the common edge,  $[OCu_3]^{5+}$  (fedotovite  $K_2Cu_3O(SO_4)_3$ ); chains of tetrahedra interconnected through the vertices,  $[OCu_3]^{4+}$  (kamchatkite  $KCu_3OCl(SO_4)_2$ ); chains of tetrahedra interconnected through the edges,  $[OCu_2]^{3+}$  (piypit  $K_4Cu_2O_2(SO_4)MeCl$ ); chains of tetrahedra interconnected by turns through the