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The Ti-rich biotite from graphite-bearing metapelitic xenoliths (El Joyazo – Spain) have been recently studied trough a multitechnical approach [1]. The study, combining several techniques, showed TiO_2 content ranging from 4.5 to 4.9 wt% and a constant X_{Fe} = 0.67. According to the results of their investigations, Cesare *et al*. [1], suggest that titanium (as Ti^{4+}) is logged only in octahedral site. The aim of the present work is the investigation both the oxidation state and the site partition of titanium accepting the main crystal chemical conclusion achieved by [1]. The following Ti-coordination polyhedra have been considered during XPS analysis: 4-fold coordination (tetrahedral), 5+1 coordination (distorted octahedral), 6-fold coordination (regular octahedral). In order to obtain the best fitting, the BE of the Ti^{4+} for the octahedral and tetrahedral coordination have been determined following the procedure in [2]. While the BE for Ti^{4+} in distorted octahedron (5+1) has been obtained by means of *ab initio* calculations [3]. The result of XPS investigation shows that Ti^{4+} populates both tetrahedral and octahedral sites. Taking in account the structural formula proposed by [1], we note that the entrance of Ti^{4+} in the tetrahedral site and of Al^{3+} in octahedral site, in the same amount, results in a both better balance of the substitution mechanisms and in a better m. a. n.'s agreement between EPMA and SCXRD data.

[1] Cesare B., Cruciali G., Russo U., *Am. Mineral.*, 2003, **88**, 583-595. [2] Malitesta C., Losito I., Scordari F., Schingaro E., *Eur. J. Mineral.*, 1995, **7**, 847–858. [3] Saunders V.R. *et al.*, *CRYSTAL'03 User Manual*, Turin, University of Torino, 1999.

Keywords: Ti-bearing micas, XPS analysis, Ti speciation

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Mg, Al, Si, Ca -Bearing Magnetite from Korshunovskoe, East Siberia

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The crystal chemistry of magnetite crystals from Korshunovskoe iron ore deposit were investigated by means of single-crystal X-ray diffraction and electron microprobe analyses. The crystals were picked from two rock samples and show significant Mg, Al, Si and Ca content The cell parameters are close to 8.392 Å, slightly smaller than for pure magnetite, and the oxygen positional parameters are close to 0.2550. After refinement, weak residual peaks were systematically founded in position 48f; possibly an indication of interstitial atoms [1]. Introducing an atom in the suggested position led to significant improvement in the refinement disagreement factors [2]. Refined site occupancies led to an estimate of about 25 electrons both in the T and M sites, consistent with the substitution in both sites of some elements lighter than iron. However the number of electrons calculated from the microprobe analyses is significantly lower, therefore some of the detected cations could not be part of the magnetite structure, however no other phases were detected from the powder diffraction profile.

[1] Fleet M.E., *Acta Cryst*., 1982, **B38**, 1718. [2] Hamilton W.C., *Acta Cryst*., 1965, **18**, 502.

Keywords: magnetite, structure analysis, interstitial atoms

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Analysis of Structure Factors of 2D-connected Crystal Structures

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The solution of complex inorganic structures from powder diffraction data is much easier when dominant scatterers are present. Due to the small X-ray scattering contrast between Si and O, solution of complex zeolitic materials is still difficult. One characteristic of the latter is their 3D connectivity and the known tetrahedral coordination that means that once the positions of the Si are located, the positions of the O atoms can be interpolated. In other words, the positions of the O atoms are not independent from the Si positions. The ideal situation for solving crystal structures from powder data at moderate resolution (d>2Å) by direct methods would be to have at one's disposal structure factor moduli with the contributions of the O atoms removed [1], [2].

In order to better analyse this possibility, the modulus C and the phase angle δ of group structure factor of one triangular O polyhedron around a central Si atom have been plotted as a function of its orientation. The respective variation coefficients of C are 9.1 and 21.5% at 2 and at 1.85 Å resolution, respectively, while the corresponding standard deviations of δ are 27º and 12º. These values are used to estimate the accuracy of the structure factors of an hypothetical planar 2D connected model built of such triangular polyhedra after removal of the average O contribution.

[1] Rius J., *Acta Cryst.*, 1993, **A49**, 406. [2] Rius J., *Z. Kristallogr*., 2004, **219**, 826.

Keywords: powder structure solution, complex compounds crystal structure, inorganic materials

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The Spinels Unit Cell Parameter as Diamond Potentiality Indicator

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The Russia (Yakut and Archangel kimberlite provinces), South Africa,North America and Australia spinels grains (about 500) content from different types deep rocks was discovered. The spinels are characterised by two types of substitutions:1)$Cr^{(3+)}$-$Al^{(3+)}$, 2)$Cr^{(3+)}$–$Fe^{(3+)}$+$Ti^{(4+)}$.

The clear lineal dependance between unit cell parameter **(a_0)** and oxides contents was not observed. The obtained data are testified the limitations of using the diagram based on the Yakut and Archangel regions spinels X-ray data.The lineal dependance can be observed within the samples with $Cr^{(3+)}$–$Al^{(3+)}$ or $Cr^{(3+)}$–$Fe^{(3+)}$ isomorphism.The realisation both substitutions schemes and also enough amount of titanium (more than 2 mas.%) in spinel structure and the wide substitutions between $Mg^{(2+)}$–$Fe^{(2+)}$ disturb the lineal dependance between oxide contents and a_0 **:** decreasing a_0 is held by decreasing Al_2O_3, and increasing a_0 depends not only from chrome (III) oxide, but from Cr_2O_3,Fe_2O_3 and TiO_2,MgO and FeO togerther influence. Therefore during first steps searching spinels upon X-ray data one can get highferrous and titanious varietes.

The two lines have been identified between a_0 and IR-spectra absorbence maximum within spinels from kimberlites which indicates on a crystallyzation consequence and a fluid-magmatic differentiation on the first mantle magmas.

This approach also can be used as a guide by Geological Enterprises to search spinels as mineral-indicators on diamondferrous rocks.

Keywords: spinels, unit cell parameter, IR-spectra absorbence maximum

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Variations in the Morphologies and Magnetic Properties of Magnetite Crystals in Bacteria

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