PS08.02 13 CHEMICAL AND STRUCTURAL VARIATIONS IN SERPENTINES FROM SOME METAULTRAMAFITES OF THE ROMANIAN CARPATHIANS (ROMANIA). Lucia Robu, Gabriela Stelea, I.N. Robu, Geological Institute of Romania, 1, Caransebes str., 78344-Bucuresti-32, Romania

Serpentine mineral samples come from some metaultramafic bodies included in the geological formations of the Romanian Carpathians.

For the most part of the samples mesh-texture are characteristic. Its one is determined due to the substituted processes of the olivene or/and pyroxene by chrysolile and/or lizardite in the marginal zones, and antigorite in the central ones. Sometimes, some small antigorite flasks are spread in the serpentine mass.

Crystallochemical data have been calculated according to $M_6N_4O_{10}(OH)_8$, general formula, whereM=Mg, Fe^{2+}, Ni, Fe^{3+}, sometimes Cr and N=Si, Al.

However, Si and Al contents show some evident substituted processes in the tetrahedral levels, between Si and Al. A lack of silica in these levels, in the calculated formula suggests a completion of these ones by Fe^{3+} cations.

Mg, Ni, Fe^{2+}, Fe^{3+} cations were identified as filling of the octahedral chains. The exchanges between Mg and other above mentioned cations are insignificantly, so that their sum varies among 0.267-0.617. Sometimes Al cations are presented in these structural levels.

IR absorption spectra confirm these substitutions processes, registering absorption bands at the characteristic frequencies (cm^{-1}).

However the registered bands about 610 cm^{-1} varies directly proportional to the Mg substitution by Fe,Ni, Cr, at the octahedral levels. Its intensity increases when Mg content is increasing. There is no possibility to evidence the proportion in which took place this substitution, but some possible combination would be suppose, MgMgMg, NiMgMg, NiFeMg, FeFeMg, FeMgMg, sometimes CrNiMg or CrFeMg.

Some of IR spectra present at the 663cm^{-1} frequency a very low intensity peak, which could be assigned to NiNiNi combination.

These high inhomogeneous and discontinuous substitutional exchanges in the octahedral level have determined these variations of the IR absorption data.

At OH-stretching region, about the 3700 cm^{-1} domain the allures of the curves are similar to these ones characteristics for low Ni content.

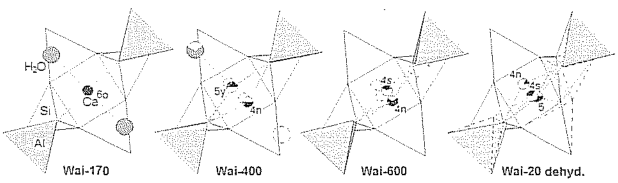
PS08.02 14 HIGH TEMPERATURE POWDER DIFFRACTION OF POLLUCITE UP TO 1073K. J. Schneider, H. L. Meyerheim, Institut fuer Kristallographie, Universitaet Muenchen, Theresienstrasse 41, D-80333 Muenchen, Germany

Framework silicates such as pollucite ($CsAlSi_2O_6.nH_2O$), leucite ($KAlSi_2O_6$) or analcite ($NaAlSi_2O_6.H_2O$) are characterized by four- and six-membered rings of corner linked $(Si,Al)O_4$ tetrahedra. In the cubic polymorphs this leads to formation of non-intersecting channels parallel to {100}- and {111}-directions, housing Cs- and Na-cations in the case of pollucite.

Powder diffraction of a sample from Bikita, Simbabwe (K. Rank, Bergakademie, TU Freiberg) was performed on a STOE diffractometer (MoKα1 radiation) and a STOE stove using a rotating sample capillary. Rietveld analysis yields a distinct contraction of cell dimensions in the range between 473K and 873K, which may be ascribed to irreversible loss of crystal water. The structure model of R. M. Beger (Z.Kristallogr.129(1968)280-302, space group Ia3d), which takes into account a significant amount of analcite, could be confirmed by refining the occupancies of the Cs,O(16b) and Na(24c) positions. Special emphasis was put onto the refinement of the temperature factors, which reach rather high values, i.e. at T=673K: B(Cs)=5A2, B(Na)=10A2. While B(Cs) shows a linear temperature dependence, B(Na) displays a change of slope at about 470K. Complementary single crystal measurements permitting anharmonic temperature factor analysis will be presented.

PS08.02.15 EVOLUTION OF CALCIUM-COORDINATION IN WAIRAKITE DURING HIGH TEMPERATURE TRANSFORMATIONS. Seryotkin Yu.V.[1], Joswig W.[2], Bakakin V.V.[3], Fursenko B.A.[1], Belitsky I.A.[1]. [1]Institute of Mineralogy and Petrography, Novosibirsk, 630090, Russia; [2]Institute of Kristallography, Frankfurt University, Germany; [3]Institute of Inorganic Chemistry, Novosibirsk, 630090, Russia.

Single crystal X-ray structure data are obtained for wairakite (Wairakei, New Zealand) - $Ca_{0.95}Na_{0.06}[Al_{1.96}Si_{4.04}O_{12}]*2H_2O$ at temperatures 20°C (I), 170°C (II), 210°C (III), 400°C (IV), 600°C (V), and again at 20°C (I_{dh} - dehydrated at 600°C and quenched). I - monoclinic, 13.666, 13.623, 13.531Å, β = 90.50°, *I2/a*. Al-fractions in 6 various Si,Al-tetrahedra correlate with Ca(Na) positions and are (%): 2, 3, 8, 13, 84, 89. Above 140°C I transforms to tetragonal phase II (*I41/acd*) - 13.712, 13.681 Å, $\Delta V \approx +2\%$. No water loss was observed below 200°C. III - 13.713, 13.687 Å. Na sites were localized in II and III. IV - is partially dehydrated (to 0.62 H_2O per formula unit) - 13.662, 13.555 Å. V is fully dehydrated - 13.645, 13.515Å. Phase I_{dh} has monoclinic superstructure - 27.257, 27.253, 13.432Å, β =90.20°. Structure data for I_{dh} are presented in a subcell with 13.629, 13.627, 13.435Å, β=90.21°, *I2/a*. Ca coordination changes as follows (Fig.): in I, II, III - octahedral [6o] $\rightarrow O_4(H_2O)_2$, (avr Ca-O = 2.39 Å); in IV - semioctahedral [5y] $\rightarrow O_4(H_2O)$ (2.36 Å) and pyramidal [4n] $\rightarrow O^4$ (2.40 Å) - statistically with the ratio 0.48/0.47); in V - [4n] (2.37 Å) and square-coplanar [4s] (2.31 Å) with the ratio 0.65/0.31; in I_{dh} - five-fold [5] $\rightarrow O_5$ (2.40 Å), [4n] (2.38 Å) and [4s] (2.33Å) with the ratio 0.52/0.27/0.19.



PS08.02.16 THE STRUCTURAL FEATURES OF CLAY MINERALS FROM THE SUPERDEEP WELL TSG-6 OF THE WEST SIBERIAN PLATE. E.P. Solotchina, T.A. Korneva and P.A. Solotchin, United Institute of Geology, Geophysics and Mineralogy, Siberian Branch RAS, Novosibirsk, Russia

The composition as well as the structural and crystallochemical features of clay minerals of Triassic deposits lying at a depth of 6000-6500 m penetrated by the unique Tyumen superdeep well have been studied. The basic method was X-ray diffraction analysis. Optical and electron microscopy as well as thermal analysis were used in addition.

The widespread development of 7 Å berthierine as mineral with the serpentine-like structure and the composition identical to iron-rich chlorite has been established. Two polytype modifications of berthierine: orthogonal A and monoclinic B (denoted by B. Zvyagin) of different genesis have been revealed. Berthierine is the most abundant mineral of tuffs making up as much as 85 % of rock in association with kaolinite. Two modifications of mixed-layer minerals as illite/smectites with d_{001}=10.5-11Å and d_{001}=24.5 Å in initial state are dominant in argillites and in a cement of siltstones. Berthierine, chlorite, kaolinite and mica are present in such rocks as an impurity. Illite/smectites with interplanar space 24.5 Å have been revealed in more deep horizons. These minerals contain appreciable amount of adsorbed water ((7.2 %) and interlayer water ((1%) on evidence derived from thermogravimetric curves. When the specimens were saturated with ethylene glycol d_{001} was enhanced to 26.8Å and an integral series of intense basal reflections up to ninth order was observed in the X-ray diffraction pattern. Decoding the structures of mixed-layer minerals has been performed. The content of illite and smectite