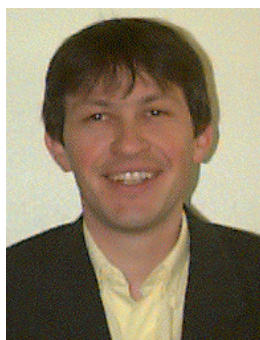


Colloquium Cukrovarnická

ve středu dne 18. ledna 2012 v 15:00 hod.
ve Fyzikálním ústavu Cukrovarnická v seminární
místnosti (budova A, 1. patro)

The determination of multiple cation location and ordering: example on natural and heat treated columbites



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The AB_2O_6 type materials have attracted much interest from a wide community of scientists including mineralogists, chemists and physicists. Indeed, these mineral are important economically as source of tantalum, in addition they are widely studied from fundamental point of view since they present interesting physical properties (magnetic and electric ones in particular) which have motivated numerous investigations among the last two decades. The minerals are composed of at least 4 different cations (Fe, Mn, Nb, Ta...) that can be located on either A or B sites. We propose a new approach to determine unambiguously the location of four cations within the crystal structure of a natural AB_2O_6 columbite type compounds and their derivatives, when it is submitted to order-disorder transitions caused by heat treatments. This method is based on the successive use of electron microprobe analysis to determine the cation concentration, Mössbauer spectroscopy to identify the Fe occupation, followed by a crystal structure determination of the samples combining Rietveld refinements of both neutron and X-ray diffraction. This approach is tested successfully to investigate (Fe, Mn, Nb, Ta) natural mineral as well as oxides obtained by heat treatment of the initial AB_2O_6 columbite type compound.