Structure and *vs*. vibrational behavior of spodumene from Conţu (Cindrel Mountains, South Carpathians, Romania)

[1]Ştefan Marincea, [1]Delia-Georgeta Dumitraş, [1]Cristina Sava Ghineţ, [1]George Dincă, [2]Fabrice Dal Bo, [2]Frédéric Hatert

1 – Geological Institute of Romania, 1 Caransebeş Str., RO-012271 Bucharest, Romania.

2 - Laboratoire de Minéralogie, Université de Liège, Sart-Tilman, Bâtiment B 18, B-4000 Liège, Belgium

Spodumene, known for his important role as Li source, occurs at main mineral in the pegmatite from Conţu, of albite-spodumene type, located on the homonym valley, at N 45°33'39" – E 23°52'19". The main associated minerals are albite, microcline, quartz, and muscovite, with an important number of accessories (e.g., beryl, purpurite - heterosite, amblygonite - montebrasite, fluorapatite, triphylite - lithiophylite, maricite, gatehouseite, monazite, schorl, spessartine, cassiterite, columbite - tantalite, uraninite). The average chemical composition, obtained on the basis of 21 electron-microprobe point analyses, with Li deduced for stoichiometry, is (in wt.% oxides): SiO_2 = 64.47, Al_2O_3 = 28.00, Fe_2O_3 = 0.59, Li_2O = 8.05, Total =101.11. The chemical-structural formula, calculated on the basis of 6 oxygen atoms *p.f.u.*, is: $Li_{0.995}(Al_{0.995}Fe^{3+}_{0.013})(Si_{1.981}Al_{0.019})O_6$. The mineral can be satisfactorily refined as monoclinic, space group *C*2/*c* (with R = 0.0244), and have as cell parameters: a = 9.4670(4) Å, b = 8.3967(3) Å, c = 5.2198(3) Å, β = 110.15(4)°. As expected, the SiO_4 tetrahedron is far to describe a punctual T_d symmetry. The Si-O distances obtained by refinement are Si-O_1 = 1.640(1) Å, Si-O_2 = 1.586(1) Å, Si-O_3 = 1.621(1) Å, Si-O_4 = 1.629(1) Å. All the bands that can be assigned to Si-O-Si vibrations in the FTIR spectrum seems triple degenerate (antisymmetric stretchings at 1163, 1085, 1072 cm^{-1}, symmetric stretchings at 919, 860 and 797 cm^{-1}, in-plane bendings at 695, 641 and 593 cm^{-1}) corresponding to the three dispersed Si-O values given before, whereas O-Si-O are simple degenerate, reflecting the presence of a sole tetrahedron in the chain repeat unit (antisymmetric stretching at 919 cm^{-1}, symmetric stretching at 779 cm^{-1}, in-plane bending at 518 cm^{-1}, out-of-plane bending at 450 cm^{-1}). In the Raman spectrum the trend remains the same: the Si-O-Si antisymmetric stretching bands were recorded at 1092, 1050 and 1017 cm^{-1}, the symmetric stretching at 841, 793 and 706 cm^{-1} whereas the in-plane bending at 596, 523, and 481 cm^{-1}. The out-of-plane O-Si-O bending was recorded at 446 cm^{-1}. Bands expressing lattice vibrations (Al-O and Li-O) were recorded at 396, 357, 299, 249, 114 and 78 cm^{-1}.