Spectroscopic studies, theoretical models and structural characterization. II. Synthesis and X-ray powder diffraction of the elpasolites Cs2NaSmCl6

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In this research work, we report the synthesis and structural characterization of the stoichiometric elpasolite Cs2NaSmCl6. The synthesis was performed under a solid state reaction in nitrogen atmosphere from the chemicals CsCL, NaCl and SmCl3 weighted stoichiometrically. The best possible crystallization temperature was obtained using thermal studies of the type DTA/TGA (the thermal treatment was allowed to proceed for 2.5 hours at 755°C, showing a temperature gradient of 10°C/minute). The structural characterization by powder X-ray diffraction (XDR) indicates that this elpasolite belongs to the Fm3m(script O signh 5) space group and the optimized structural parameters are as follows: a0 = 10.8342 Å, V = 1271.72 Å3, Z = 4, M = 651.88, Dx = 3.406 and Dexp = 3.41 ± 0.01. The profile refinement, using the Rietveld method, allowed us to fit the experimental and the calculated intensities of a total of 32 lines. The above result indicates that the condition Rexp < 2Rwp is fulfilled, and th