

# Spectroscopic studies, theoretical models and structural characterization. I. The elpasolites $\text{Cs}_2\text{NaLnCl}_6$ , where $\text{Ln}^{3+} = \text{Er}^{3+}, \text{Yb}^{3+}$

Poblete, V.

Acevedo, R.

Tanner, P. A.

The stoichiometric elpasolites of the type  $\text{Cs}_2\text{NaLnCl}_6$  are known to belong to the space group  $\text{Fm}\bar{3}\text{m}$  (No. 225). The structural data of these elpasolites is both scarce and rather limited and therefore a thorough experimental study is needed. Over the last few years, our research group has been engaged in a project to undertake: the synthesis, the structural and spectroscopic characterization for these materials. We aim to gain understanding about the most likely intensity mechanisms associated with the one and the two photon spectroscopies. These theoretical studies are indeed, very complex, since they involve transitions of the kind  $f \rightarrow d$  and/or  $f \rightarrow g$  at the central metal as well as ligand subsystem excitations, among terminal states of different parity. The above described mechanism is currently being used, though its apparent conceptual simplicity, nevertheless we recognize the intrinsic limitations of the model calculation. We could, in principle relax many of these approxima