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Effect of the temperature in optical parameters in the reflectance spectrum of the composition $Li_2Co_{(1-x)}Ni_xTi_3O_8$ doped with nickel to 8%

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Abstract - In this work we evaluated the influence of the temperature in the reflectance spectra of the compound $Li_2CoTi_3O_8$ doped with nickel to 8% and we observed the behavior of the force of the oscillator and of the relative polarizabilities. We observed an increase of these properties in the strip from 500 to 700 °C

Spinel-type oxides ($Me^{2+}Me^{3+}O_4$) represent one of the most studied classes of materials in solid-state science, because of their relevant magnetic, refractory, semiconducting, and coloring properties. They are stable even under drastic thermal and redox industrial treatments. The incorporation of transition metal (TM) ions into stable diamagnetic spinels is a successful process to obtain materials with peculiar physical properties and, sometimes, very intense colors. The coloring properties of spinels obtained by this approach are mainly determined by the crystal field surrounding the TM ion, i.e. by its d–d and/or charge transfer transitions. A large number of cations can be accommodated in the spinel structure.[1] Moreover; these cations can occupy two types of sites, T, tetrahedral, or O, octahedral. All distribution ratios are allowed in spinels, from the *normal* type (Me^{3+} in the O sites) to the *inverse* type (Me^{2+} in one half of the O sites), depending on chemical composition and temperature. The possible presence of several TM cations in different coordination accounts for the variety of colors that can be obtained.

In this context, the main goal of the present study was to synthesize pigments from polymeric precursors using the method proposed by Pechini. In particular, doped $Li_2Co(M)Ti_3O_8$ spinels (M= Co) were addressed.

In this work we studied the effect of the temperature in composed of the type $Li_2CoTi_3O_8$ doped with nickel to 8%, starting from the reflectance spectra, in the temperatures of 500, 600, 700 and 1000 °C. We obtained for Simpson's rule, the baricenter of the transitions of the warm composition in the respective temperatures and we calculated through the program SIMP2FOS the oscillator strenght relative and for the program POLAZ-F, the static and dynamic relative polarizabilities.

Table 01 - Baricenter of the frequency, oscillator strength relative, and static and dynamic polarizabilities relative of the $Li_2CoTi_3O_8$ doped with nickel to 8% in different temperatures.

Temperature °C	Baricenter of Transitions cm^{-1}	Relative Oscillator Strength ($x10^{-4}$)	Relative Polarizabilities		
			α_{sta} $x10^{-27}(cm^3)$	α_{max} $x10^{-20}$ (cm^3)	$\alpha_{out\ phas}$ $x10^{-19}$ (cm^3)
500	19.489,7	1,382	2,600	5,639	1,128
600	19.526,4	1,910	3,580	7,749	1,550
700	19.603,1	2,421	4,502	9,708	1,942
1000	19.633,1	1,557	2,887	6,215	1,243

α_{sta} - polarizability static; α_{max} - polarizability dynamic maximum; $\alpha_{out\ phas}$ - polarizability dynamic maximum out-of-phase

We observed starting from the data of the table 01, that the baricenter of the transitions was moved and the oscillator strength and the relative polarizabilities were also influenced by the heating of the

compound and they had your values magnified in the strip that is going from 500 to 700 ^{o}C. A decrease in the values of those properties, except for the baricenter that continued increasing, it was verified to 1000 ^{o}C, that can it is related with some structural change of the composition, or modification in your composition caused by the action of a larger heating and consequent action oxidative by the atmosphere in the compound, combined with an inevitable structural alteration. To 700 ^{o}C, in this group of experiments, the largest contribution was observed for the reflectance of this compound, that it can be attributed at this time, to an ideal crystalline accommodation, so that the atoms in the material, transfer photons through the levels of energy with better efficiency, what makes possible a larger medium scattering of light around of 510,1 nm.

[1] M. S. C. Câmara,; M. F. C. Gurgel,; S. R . Lazaro,.; A . Beltran,.; E. R Leite,.; T. M . BOSCHI,.;, P. S . Pizani.; E . Longo, Room Temperatura Photoluminescência Of The $Li_2znti_3o_8$ Spinel: Experimental And Theoretical Study. INTERNATIONAL Journal Of Quantum Chemistry, V. 3, P. 580-587,(2005).

[2] F. J. S. Lima, V. S. M, Lopes,,D. R Silva,, A. S . Dantas,. D. M. A . E Moura,.- T.Quim.,06(2009), 7-10