Ligand Field States and Vibrational Modes of Solid and Molten Elpasolite: $Cs_2NaHoCl_6$

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Electronic absorption and Raman spectra of solid and molten $Cs_2NaHoCl_6$ elpasolite have been measured in the temperature range 20 – 780 °C. The Raman spectra of the solid indicate that there is no phase transition above room temperature. It appears, that the internal vibrational modes of the solid are transferred into the melt, indicating that the $[HoCl_6]^{3-}$ "octahedra" are the predominant species. The $^5G_6 \leftarrow {}^5I_8$ and $^3H_6 \leftarrow {}^5I_8$ hypersensitive transitions of Ho(III) in elpasolite have been studied and analyzed in terms of the ligand field splittings of these states in the octahedral $[HoCl_6]^{3-}$ field. The temperature-induced changes in the spectra are attributed to the presence of "hot" bands arising from sets ("zones") of energy levels in the ground $^5I_8$ state. The continuous and smooth spectral changes observed upon melting indicate the presence of $[HoCl_6]^{3-}$ octahedra in both phases.

Key words: Molten Salts; Raman; Electronic Absorption; Ho(III); Hypersensitive Transition; Structure; Elpasolite.