Dopant Concentration Effect on NiO-doped Sodium Metaphosphate Glasses: A Combined X-Ray Absorption Fine Structure (XAFS) and UV/VIS/NIR Spectroscopic Investigation

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NiO-doped sodium metaphosphate glasses \((\text{NaPO}_3)_{1-x}(\text{NiO})_x (0.008 \leq x \leq 0.30)\) show a color shift from yellow to orange-brown with increasing NiO concentration. XANES and EXAFS spectra of these glasses suggest the presence of \([\text{Ni}^{II}\text{O}_6]\) groups as chromophores. EXAFS (Ni K-edge) analysis of the NiO-doped phosphate glasses including an evaluation of higher coordination shells leads to \(d_{av}(\text{Ni-O}) = 2.06(2)\ \text{Å}\). Evidence is provided for an increased connectivity of \([\text{Ni}^{II}\text{O}_6]\) chromophores at higher NiO concentration in the glasses. A decrease in the intensity of the main absorption edge with increasing nickel oxide concentration is observed. This systematic decrease is attributed to a change in the bonding characteristics between nickel(II) and the coordinating phosphate groups from mainly ionic to a small but significant contribution of covalent bonding. A similar effect is observed in the electronic absorption spectra of glasses showing a decrease of the Racah parameter \(B\) for the Ni\textsuperscript{2+} ions.

Key words: XANES; EXAFS; UV/VIS/NIR Spectroscopy; Sodium Metaphosphate Glasses; Metal-ligand Interaction.