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Optical Parameters and Dispersion Behavior of Potassium Magnesium Chloride Sulfate Single Crystals Doped with Co^{+2} Ions

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Abstract.

Single crystals of potassium magnesium chloride sulfate (KMCS) doped with cobalt ions are grown by slow cooling method. Powder XRD study confirms the monoclinic structure of the grown crystals. The functional group vibrations were checked through FTIR spectroscopy measurements. In optical studies, the absorbance behavior of the crystals and their optical energy gap are established by Tauc plot. The refractive index, the extinction coefficient and other optical constants were calculated for the grown crystals. The normal dispersion of the refractive index is analyzed according to single oscillator Sellmeier's model. The Urbach's rule was applied to analyze the localized states density in the forbidden gap.

Keywords: KMCS single crystals; Crystal growth; X-ray Powder diffraction; Optical properties; FTIR spectroscopy.

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1. Introduction.

Potassium magnesium chloride sulfate known as kainite with chemical formula $KMgClSO_4.3H_2O$ (abbreviated as KMCS) is a mineral known for its use as a fertilizer [1]. The crystal structure of kainite has been studied in detail by Robinson et al. [2]. The structure follows (C2/m) monoclinic symmetry with the lattice parameters a=1.972, b=1.625 and c= 0.953 nm, β=94.9° and it contains 16 molecules/unit cell (Z=16). Recently, Voigt's report on KMCS confirmed the structure with a small fractional variance in the water molecules (2.75 H_2O instead of $3H_2O$) [3].

Electron paramagnetic resonance (EPR) is a powerful tool for elucidating the effect of transition or rare earth metal ions doping on the electronic properties of any crystals. EPR spectra of kainite doped with some transition metal ions such as VO^{2+}, Mn^{2+} and Cu^{2+} were studied extensively [4–6]. Further EPR investigations on Cu^{2+} and Mn^{2+} in kainite predict the replacement of Mg^{2+} ion by the transition metal ion resulting in structure distortion. Many EPR studies were implemented on transition metal ions (Cr^{3+}, Cu^{2+}) doped in potassium zinc chloride sulfate trihydrate. They considered analogue of potassium magnesium chloride sulfate and reported that, at room temperature, the spectra demonstrates the magnetically inequivalence of the two Cr^{3+} and Cu^{2+} sites in the structure and the two sites enter the lattice substitution at Zn^{2+} sites [7,8].

The optoelectronic applications could be tested and examined from the optical parameters of a material [9]. The sufficient knowledge of optical parameters and constants for any crystal is vital to examine the material preference for optoelectronic applications [10-14].

For the best of our knowledge, studies on optical and spectroscopic properties of $KMgClSO_4.3H_2O$ single crystals are scare. Single crystals of KMCS weren't studied sufficiently and many optical parameters aren't reported. The dispersion behavior is an important factor in the analysis