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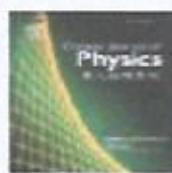
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Prospective theoretical investigations of optical, dielectric, mechanical and third-order NLO property in potassium tri-hydrogen di-succinate single crystal

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ABSTRACT

A prospective third-order nonlinear optical crystal potassium tri-hydrogen di-succinate (PTHS) ($\text{CaH}_3\text{O}_2\text{K}$) is grown by conventional slow evaporation technique maintained at 300 K. Single crystal XRD analysis (XRD) evidences the grown crystal pertains to centrosymmetric space group $P\bar{2}1/c$ with monoclinic crystal system and powder X-ray diffraction (PXRD) confirms the purity of the grown crystal. The existence of various functional groups was assessed by Fourier transform infrared (FTIR) spectral analysis and the optical absorption study authenticates to the transparency in the visible region. ICP-OES study substantiates the prevalence of alkali metal potassium. Interestingly, the Urbach energy of the grown crystal is found to be minimum proving the good crystalline nature of the yielded crystal. The various optical constants were calculated in detail. The optical band gap was used to determine the position of the valence band (E_v) and conduction band (E_c) and the Wemple-Di-Donati single oscillator method was used to find the different dispersive parameters. In dielectric, the various solid state parameters including dielectric polarisability were calculated with different formulas and the value was proved to be higher than that of KDP. To determine the mechanical stability, Vickers microhardness test was carried out and their indentation size effect was elucidated by using different models. The crystal exhibits negative photoconductivity. By using photo-acoustic study, the thermal diffusivity value is 1.25 times greater than standard KDP, signifying that the harvested crystal is remarkable material for nonlinear optical applications. In brief, the real and imaginary parts are reviewed by Z-scan technique and the susceptibility was compared with other single crystals.



PRINCIPAL

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