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SPECTROSCOPIC CHARACTERIZATION OF PURE AND METAL DOPED KDP SINGLE CRYSTALS

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ABSTRACT
Potassium dihydrogen phosphate (KDP) is an excellent inorganic non linear optical material with different device applications. In the present work, single crystals of pure and doped (silver nitrate and mercuric Chloride) KDP crystals have been grown from aqueous solution by slow evaporation technique. The grown crystals have been subjected to various characterization studies like FT-IR, UV-Vis and AAS. Fourier Transform Infrared Spectroscopic analysis confirms the various functional groups present in the grown crystals. From the FT-IR spectrum, it is concluded that both pure KDP and Silver nitrate doped KDP have same spectrum which implies that there is no incorporation of Silver in the KDP crystal which further confirmed by atomic absorption spectrum. But mercuric chloride doped KDP crystals show a slight difference from pure KDP.UV-Vis spectrum gives the optical transmittance of the grown crystals and it is found that silver nitrate doped crystals have low transmittance and Mercuric chloride doped increases the transmittance in visible region and the lower cut off wavelength is slightly shifted to higher wavelength for both the doped crystal from the pure KDP. The presence of metal dopants (silver and mercury) was confirmed by Atomic Absorption studies and it is found that there is no silver element present in the silver nitrate doped crystal but it modifies the growth and habitat of the pure KDP crystal and also silver nitrate decreases the transmittance of the pure KDP.

KEY WORDS
KDP, Silver nitrate, Mercuric Chloride, FT-IR, UV-Vis, AAS

1. INTRODUCTION
Great efforts have been made to the research and design of highly efficient non-linear optical (NLO) materials due to widespread applications such as high speed information processing, optical communication and optical data storage [1]. The rapid development of optical communication systems has led to the search for more efficient compounds for the processing of optical signals. In the last decade, however this effort has also brought its fruits in applied aspects of non linear optics. The aim is to develop materials presenting large non linearities and satisfying at the same time all the technologies requirements for applications such as wide transparency range, fast response and high damage threshold. But in addition to the processability, adaptability and interfacing with other materials improvements in non linear effects in devices, led the way to study of new non linear effects and the introduction of new concepts. ADP & KDP are two of the oldest crystals grown in large size for many applications and continues to be interesting materials both academically and industrially. Potassium dihydrogen phosphate (KDP) is an excellent inorganic nonlinear optical (NLO) material and has considerable interest amongst several

research workers because of its wide frequency, high efficiency of frequency conversion, high damage threshold against high power laser. With the aim of improving the SHG efficiency of KDP, researchers have attempted to modify KDP crystals either by doping different type of impurities or by changing the growth conditions [2-9]. The addition of some transition metals ions is expected to influence the growth kinetics, habit modification and large size single crystals. The presence of small amount of impurities plays an important role in the growth habit modification of the crystal and its properties [10]. An impurity can suppress, enhance or stop the growth of the crystal completely. The impurity effect may depend on the impurity concentration, super saturation, temperature, pH of the solution and this can be successfully explained for many NLO crystals [11]. Most of amino acids possess NLO property; therefore, it is of interest to dope them in KDP crystals. The effect of amino acid on the NLO efficiency of KDP crystals were already published [2-8]. Research on silver nano particles has been triggered by their potential application in optics, photography, catalysis, biological labeling, photonics, opto electronics and surface enhanced Raman Scattering detection [12-15]. Additionally, silver nano particles have a surface plasmon resonance absorption in the UV-Vis region. The formation of the metal nano particle dispersed in solid dielectric materials, which can result in novel optical properties, have been of increasing interest because of their potential applications in non linear optics. Metal-organic coordination compounds as NLO materials have attracted much more attention for their high NLO coefficients. In the present study, silver nitrate and mercuric chloride doped KDP crystals were grown by slow aqueous solvent evaporation technique. Spectroscopic studies have been studied and discussed in detail.

2. MATERIALS AND METHODS

AR grade samples of pottasium dihydrogen orthophosphate (KDP), silver nitrate and mercuric chloride were used. 300 ml saturated solution of KDP in distilled water is prepared at first and 100 ml saturated solution is poured in three different beakers and named as 1, 2 and 3. 0.2% of silver nitrate and mercuric chloride is added to beaker 2 and 3 respectively and stirred well for nearly 5 hours. The stirred solution is filtered and allowed to evaporate slowly. Within a week, transparent crystals were produced which are shown in **Fig 1-3**.

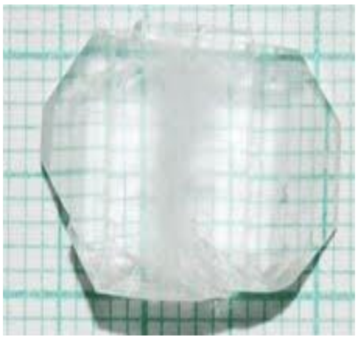

Fig1. KDP crystal

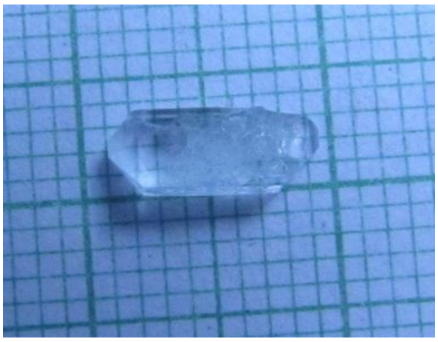

Fig.2 Mercuric chloride doped KDP

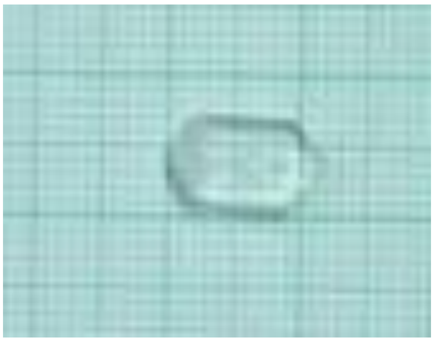

Fig.3 Silver nitrate doped KDP

2.1. Characterization

The grown crystals were subjected to Fourier Transform Infrared Spectroscopy, Atomic Absorption Spectroscopy and UV-Vis spectroscopy. A Perkin Elmer Spectrum one FT-IR spectrometer was employed to record the IR spectrum to analyze the functional groups present in the crystals. The sample for this measurement was finely grounded and mixed with KBr and the spectrum was recorded

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between the wave number ranges 400-4000cm^{-1}. The UV-Visible spectrum of the grown crystals was recorded between 200-1200 nm using CARY/5E/UV Spectrophotometer.

3. RESULTS AND DISCUSSION

3.1. Optical Transmission Spectral Analysis

A good optical transmittance is desirable property for NLO crystal since the absorptions, if any, in an NLO material near the fundamental or the second harmonic will lead to the loss of conversion efficiency in those wavelengths. Absorption spectra of NLO material play a major role in device fabrication. Wider the transparency window more will be the practical applicability of that material. The UV-Vis spectrum gives information about the structure of the molecule that the absorption of UV and visible light involves in the promotion of electrons in σ and π orbital from the ground state to higher energy state. The UV transmission spectrum of pure and doped KDP is shown in **Figure 4**. From the spectrum, it is clear that addition of mercuric chloride to pure KDP increases the transmittance and silver nitrate decreases the transmittance. Also it is found that silver nitrate dopant, the absorption edge slightly shifted to higher wavelength region from that of pure KDP and it is due to the excitation of surface Plasmon vibration [16]. And the cut off wavelength is found to be ~375 nm for all spectrums. Thus high transmittance % is observed from 375 nm clearly indicates that the crystal possess good optical transparency for SHG of Nd:YAG laser.

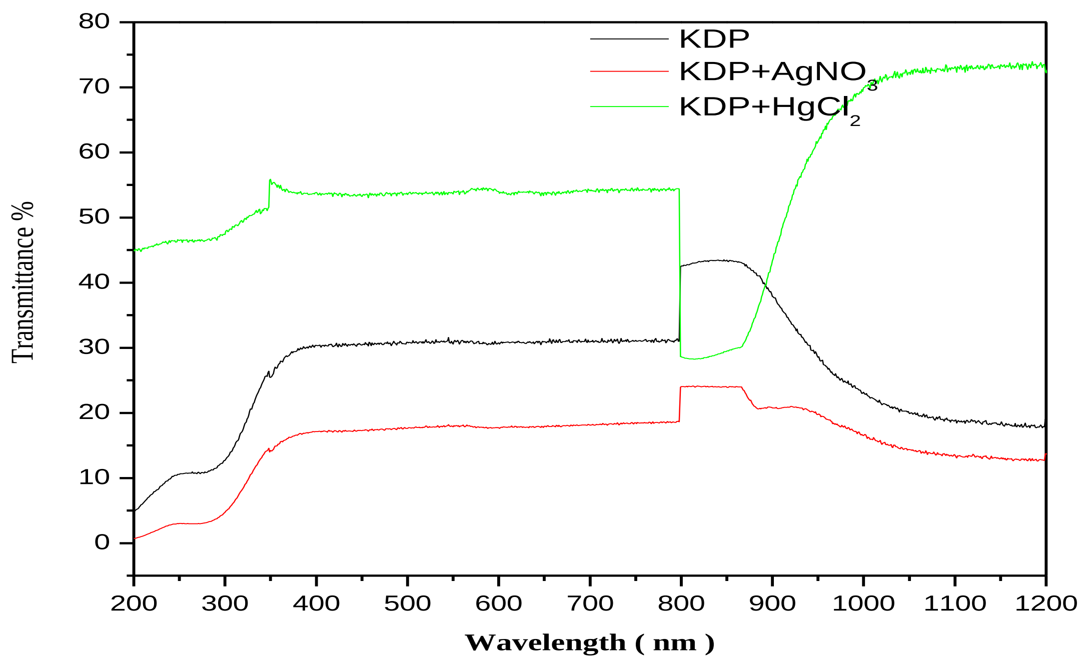

Fig.4 UV-Visible spectrum of pure and doped KDP single crystals

3.2. Fourier Transform Infrared Spectroscopic Analysis

The FTIR spectroscopy studies were used to analyze qualitatively the presence of functional groups in synthesized pure and doped KDP materials. Figure.5 shows the Fourier Transform Infrared Spectrum of the pure and doped KDP crystals. In the FT-IR spectra of pure KDP crystal, the observed absorption peaks correspond to the P-OH stretching, P-O-H bending,P=O stretching, P-O-H stretching and HO-P-OH bending [17]. In the mercuric chloride doped crystals, the same peaks have been observed with some additional peaks which confirm the presence of mercury. Also in the silver nitrate doped KDP spectrum it is concluded that most of the peak shifted to higher wave number side and otherwise disappears which confirm the absence of silver. The peak at 3613 cm^{-1} is due to O-H stretching. Strong peak appears at 495 cm^{-1} and 393 cm^{-1} are due to P-OH deformation for pure KDP. These peaks shifted to 514 and 421 cm^{-1} for silver nitrate doped KDP crystals and for mercuric (II) chloride, these peaks shifted to 505 and 403 cm^{-1} respectively. The broad band absorption at 3326 cm^{-1} is assigned to O-H stretching of KDP.

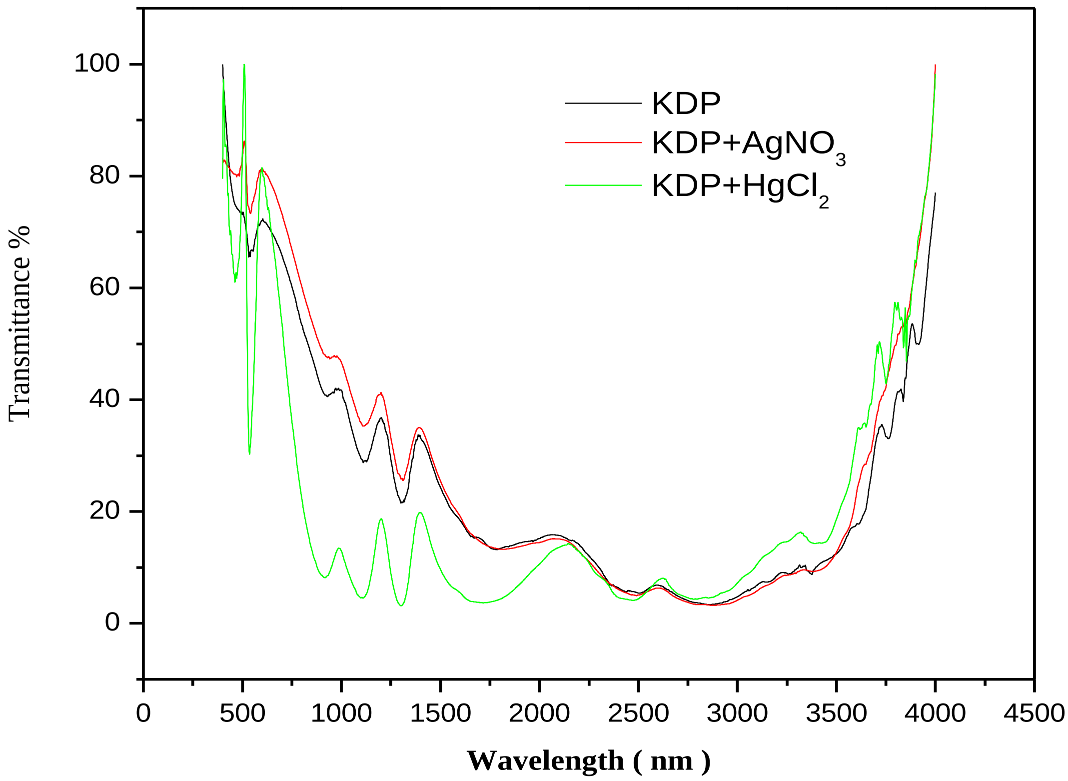

Fig.5 Fourier Transform Infrared Spectrum of pure and doped KDP single crystals

4. CONCLUSION

Single crystals of pure and doped (silver nitrate and mercuric chloride) KDP crystals have been grown from aqueous solution by slow evaporation technique. From the UV-Vis spectrum it is clear that silver nitrate doped crystals have low transmittance and mercuric (II) chloride doped increases the transmittance in visible region and the lower cut off wavelength is slightly shifted to higher wavelength for both the doped crystal from the pure KDP. Fourier Transform Infrared Spectroscopic analysis confirms the various functional groups present in the grown crystals. The presence of metal dopants (silver and mercury) was confirmed by atomic absorption studies and it is found that there is no silver element present in the silver nitrate doped crystal but it modifies the growth and habitat of the pure KDP crystal and also silver nitrate decreases the transmittance of the pure KDP. Strong peak appears at 495 cm^{-1} and 393 cm^{-1} are due to P-OH deformation for pure KDP. These peaks shifted to 514 and 421 cm^{-1} for silver nitrate doped KDP crystals and for mercuric (II) chloride, these peaks shifted to 505 and 403 cm^{-1} respectively. In the present work, an attempt has been made to enhance the KDP applications by using metal complexes in optics, biological labeling, photonic and Opto electronics.

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