Vibrational Spectroscopic Studies of KDP, Pure and Doped with NH4Cl(0.1m)

B.Sheeba, C. Rathika Thaya Kumari, K. Seevakan

Abstract: ***Monopotassium phosphate or potassium dihydrogen phosphate, KDP (KH2PO4) is a soluble salt which is used as a fertilizer, a food additive and fungicide. It is a source of phosphorus and potassium. It is also a buffering agent. This chapter presents in detail the vibrational analysis on the molecular structure of the compound named KDP doped with NH4Cl by using RAMAN as investigating tools.***

Keywords : ***RAMAN,KDP, vibrational analysis***

I. INTRODUCTION

Potassium dihydrogen phosphate (KDP) isomorphic crystals, deuterated KDP known as KD*P or DKDP (KD2PO4) are commonly used in ND-doped laser structures for frequency duplication, frequency tripling and frequency quadrupling, as well as for electro-optical modulators. Potassium dihydrogen phosphate is well known for their good piezoelectric and nonlinear optical properties [2, 3].

Nonlinear optics is a very helpful technology because it increases laser utility by expanding the amount of accessible wavelengths. Non-linear optics has appeared as one of the most appealing fields of present studies in perspective of its essential applications in the fields of optical modulation, optical switching, optical logic, frequency changing, high-speed data processing, and different auto electric applications [4-7

They probably drawn interest from many theoretical and experimental scientists due to their comparatively easy structure and very intriguing characteristics connected with a hydrogen bond scheme.. This includes a big isotope effect, a wide range of transparency, a high threshold for optical harm and comparatively low cost of production[8].]

Doping with some additives on pure KDP crystals is increasingly interesting due to the reality that dopants can alter their characteristics [9, 10].

In the present thesis, some KDP crystals doped with NH4Cl and NH4Br are prepared using solution method, and their FT-IR and Raman Spectra are studied. [2],[4],[6]

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II. MATERIALS & METHODS

The crystals for the present study (pure KDP, KDP doped with NH4Cl in three different concentrations (0.1 mol, 0.2 mol and 0.3 mol) are prepared using solution growth method and gel method.

In a beaker 100 ml of distilled water was taken. The saturated solution of KDP (33 gm) was prepared. After 5 days the seed crystals were found. From that good quality transparent crystals were collected. These were hung in the solution by a nylon thread. After 16 days the crystals were harvested and washed with triple distilled water. [8],[10] ,[12]

Ammonium chloride and was added as dopants with KDP. According to the molarity of ammonium chloride , they were taken in three different ratios and added with KDP.

In a beaker, 100 ml of distilled water was taken. A saturated solution of KDP
(33gms) was prepared. For 0.1 mol/l molarity of ammonium chloride, 1g of it was added to the saturated solution of KDP. After 10 days seed crystals were found, which were later harvested and washed with triply distilled water.
[31],[33],[35]

Similarly, for 0.2 mol/l molarity, 2g of ammonium chloride was added with the saturated solution of KDP, and for 0.3 mol/l, 3g of ammonium chloride was added with KDP.

III. RESULTS AND DSCUSSION

The Raman spectra of pure KDP, and KDP doped with NH4Cl, in different concentrations, were recorded.

Raman spectra of pure and doped KDP are shown in Figs 4.3 to 4.9. The Raman peaks, and their assignments to different modes are given in Table 4.2 .

For the KDP crystal belonging to D2d, factor group analysis for KDP was performed, forming space group I42d. A= 0.74532(3) nm and c= 0.69742 nm are the cell size. The primitive cell includes four units of formula[1,2]. Using the Bhagavantham and Venkatarayadu method of factor group analysis, the irreducible representations of the lattice vibration of the KDP crystal are as follows:

They can be designed for a wide

11 A1 + 11 A2 + 13 B1 + 13 B2 + 24 E.

For the D2d group the Raman and infrared active optical phonon modes at zero wave vector are:

11 A1 (Raman) + 13 B1 (Raman) + 12 B2 (Raman, IR) + 23 E (Raman, IR).

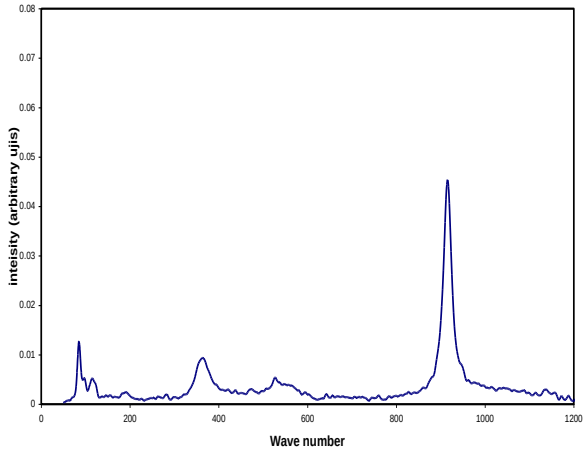

Fig 1 wave number

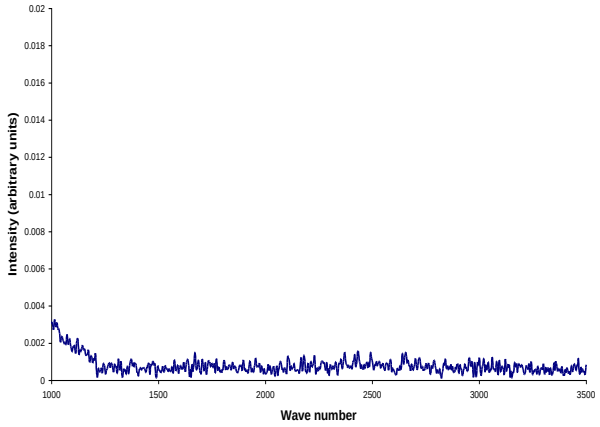

Fig 2:wave number

IV. CONCLUSIONS

In the case of Raman spectra of these samples, an increase in intensity of the Raman lines is observed in the case of KDP doped with 0.1 M NH4Br. Such an increase is not observed in other cases. In fact doping with higher concentration of both NH4Cl and NH4Br are reducing the intensities of both Raman and IR intensities. There is no considerable shift in the frequencies. A few shifts observed may be either chance of instrumental error[14],[16], [18]

It can be concluded that doping the KDP crystal with 0.1 M NH4Cl increases the bond strength. This is in agreement with the findings in [11].

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