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Characteristics, Optical, Structural, And Dielectric Studies on Pure and Dopeed L-Prolonium Trichloroacetate Single Crystals

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KEYWORDS

Powder XRD, Hardness, Metal dopants, Solution Method, Single crystal, FTIR.

ABSTRACT:

A slow evaporation approach was used to make single crystals of pure and metal substituted L-Prolonium trichloro acetate (LPTCA). Diffraction of X-rays in a single crystal (XRD), Particle X-ray diffract, UV-Vis.-NIR, and other techniques were used to examine the crystals. FTIR, and other studies. Image catalytic activity, electromagnetic and toughness, testing. Inductively Coupled Plasma (ICP) analysis was used to determine the dopant content in the crystals. The generated crystals of pure and metal substituted LPTCA adhere to the trigonal system, according to single crystal X-ray diffraction measurements. Ni2+ and Co2+ doping had a minor effect on the lattice constants of LPTCA without affecting the crystal's basic structure. Vickers' micro hardness test was used to assess the mechanical behaviour of pure and doped crystals. Features of doped and undoped crystals in terms of light transmission, dielectric, and photoluminescence were investigated.

I INTRODUCTION

Because of their potential applications in telecommunications, computers, and optical data processing .Semi organic materials based on amino acids and their complexes have been studied for a range of applications during the last few decades. Amino acid molecules have been combined with synthetic or natural salts in recent years to improve physical and chemical properties, as well as laser injury thresholds, temperature, and optical characteristics. Numerous studies show that doping crystals with modest levels of contaminants improves their optical and electrical properties.

Furthermore, impurity selection aids in the improvement of crystal properties. Metal ions, especially transition metal ions, when it comes to changing the characteristics of amino acid-based crystals, have shown to be the most versatile. Trivalent dopants are found in the interstitial area of crystal structures and have good optical characteristics. The semi-organic single crystal L-prolinium trichloroacetate has structural, mechanical, and optical properties. However, there hasn't been a comprehensive investigation into the fabrication of metallic ions doped LPTCA single crystals yet.

II RELATED WORK:

The slow evaporation solution technique (SEST) was used to generate single crystals of pure and L-Proline (LP) C5H9NO2 doped di-potassium hydrogen phosphate (ADP) (NH4) H2PO4 at room temperature [1]. Experimental data and predicted wavelength counts for L-proline (LP) and Zn (L-proline) 2 are examined [4-5]. Chemical and biological sciences. Vibrating FT-IR, Raman and NMR MAS, and Raman and NMR MAS [7-9]. At different operational circumstances [40–

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120 bars], The influence of different water percentages on the hydrate phase shift of methane [CH4], as well as the hydrate inhibitory intensity of AA L-proline, is investigated [10].

As people live longer, the wear and tear to joints caused by increasing physical activity increases. The creation of representatives and nontoxic lubrication materials has a significant social and economic influence in this area [11-12]. In the past, researchers have been looking for new materials with distinctive nonlinear optical (NLO) capabilities in the metallic, artificial, and semi organic classes [13].

Optical materials have become more popular as a result of their wide range of applications in transistors, superconductivity, and optoelectronics, including high-speed data transmission, frequency conversion, optoelectronic devices, and high optical disc data storage, among others [14]. L-Proline-stabilized copper Nano clusters with outstanding water solubility, high photo durability, and salt chloride tolerance were manufactured using a simple, green, and low-cost approach [15].

III PROPOSED METHOD

3.1 Synthesis and Crystal growth

The general public has access to it. L-proline and trichloroacetic acid were the two main components of the LPTCA complex. L-proline and trichloroacetic acid were dissolved in distilled water in a stoichiometry to form an aqueous solution of LPTCA. At a temperature of 25°C, pure LPTCA crystals were created using a gradual evaporation approach.

$$C5H9NO2 + Cl3CCOOH \rightarrow C5H10NO2 + C2Cl3O2- \quad (1)$$

It has been discovered that Co_2^+ dopants promote faster development than Ni_2^+ dopants.

3.2 L-proline doped with metal ions was synthesised as single crystals

A temperature-controlled magnetic stirrer was used to thoroughly agitate the reactants for 6 hours, yielding a homogenous solution. Then, as in the previous situation, the identical approach was followed. Whatmann filter paper was used to filter the final solution. Following that, the filtered solution was maintained in crystal growth jars and slowly evaporated at room temperature. Figure 1 Single crystals of pure and metal ion doped L-proline were photographed.

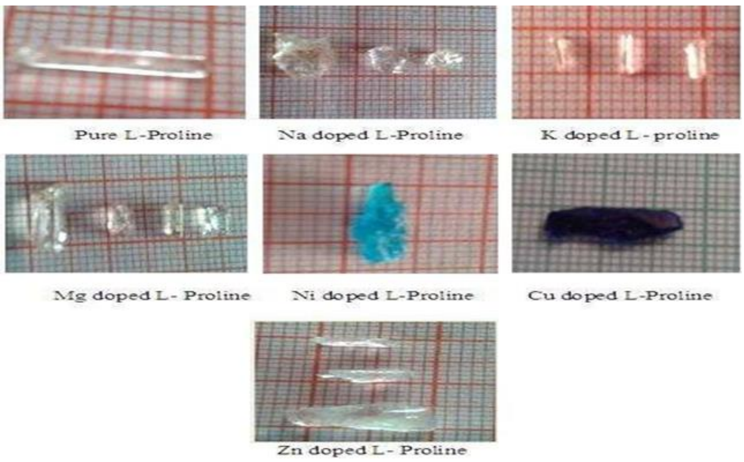

Fig. 1: Photographs of single L-Proline crystals that have been produced to a high-quality level.

3.3 XRD was used to examine single crystals of pure and metal ion doped LPTCA

Ni2+ and Co2+ doped LPTCA crystals have slightly different lattice characteristics than pure crystals. This could be due to doped production in the LPTCA crystal. The findings are consistent with what has already been published.

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3.4 Etching studies of single crystals of L-proline doped with metal ions

Chemical etching is a straightforward and elegant method for revealing crystal flaws and crystal development mechanisms. On the crystal surface, It can produce growth stresses, etching spiral, rectangular etch pits, and other features. Etching studies were carried out for 10-30 seconds on the surface of as produced single crystals of L-proline. For the etch duration of 10s, only a few dispersed etching holes and transient strains were evident. The size of the etch pits grew larger when the etching period was increased to 30s, and some development strains extended along an axis.

3.5 Powder XRD study of LPTCA with and without metal ions

Using the XPERT-PRO X-ray diffract metre and CuK_g (λ=1.5406) radiation, Powder X-ray diffract was used to investigate pure and metal ion doped LPTCA crystals. Scans were performed at a rate of 2 degrees each minute for two temperatures varies from 10 to 80 °.

3.6 Studies on Inductively Coupled Plasma

10 mg of Ni^{2+} and Co^{2+} doped LPTCA powder was diluted in 10 ml distilled water and subjected to inductively coupled plasma elemental analysis to determine the exact wt. presence of metal alloying elements involved in the LPTCA crystals. The weight percentages of Ni2+ and Co2+ can be calculated using the equation.

$$Weight\ (\%) = ppm(mg/l)\ x\ volume\ in\ mL\ x\ dilution\ factor\ x\ 10-4/weight\ of\ samples\ in\ grown \quad (2)$$

The amount of alloying elements crushed into the host crystal lattice, according to these data, is negligible in compared to the quantity of dopants in the original sample.

3.7 Energy of the optical band gap

The connection was used to calculate optical absorption coefficients (3) for wavelengths between 190 and 1100 nm.

$$\alpha = \frac{(2.303)\log 1/T}{t} \quad (3)$$

The crystal thickness is T and the transmittance is t.

The gap between the bands was computed.

$$ahn = A\,(hv - Eg)1/2$$

(4)

The formula was used to calculate the hardness value.

3.8 Hardness

Where h stands for Planck's constants, L stands for light speed, a stands for continuous, and E_g stands for energy band energies, and all of these numbers are given. Co_2^+ doped LPTCA crystals have a substantially greater band gap than pure or Ni_2^+ doped LPTCA crystal.

$$Hv = 1.8544P\,/d\,2\,(kg.mm-2) \quad (5)$$

VI EXPERIMENTAL RESULT

4.1. L-proline single crystals with metal ion doped and pure solubility

The absorbance of single crystals of pure and metal ion doped L-proline was examined at six different temperatures: 15,20,38,47, and 40°C. Initially, super-saturated solution was made at 20°C in a 100 mL airtight container inside a 0.01°C precise constant temperature bath.

Table 1: Pure and doped with metal ions L-proline single crystals

Temp (oc)	Conc(g/100m)	Pure proline	Na doped proline	K doped proline	Mg doped proline	Ni doped proline	Cu doped proline	Gn doped proline
10	15	28	26	29	35	45	54	58
20	20	27	29	25	42	48	52	51
30	38	32	34	33	37	43	54	53
40	47	25	32	38	42	39	55	56

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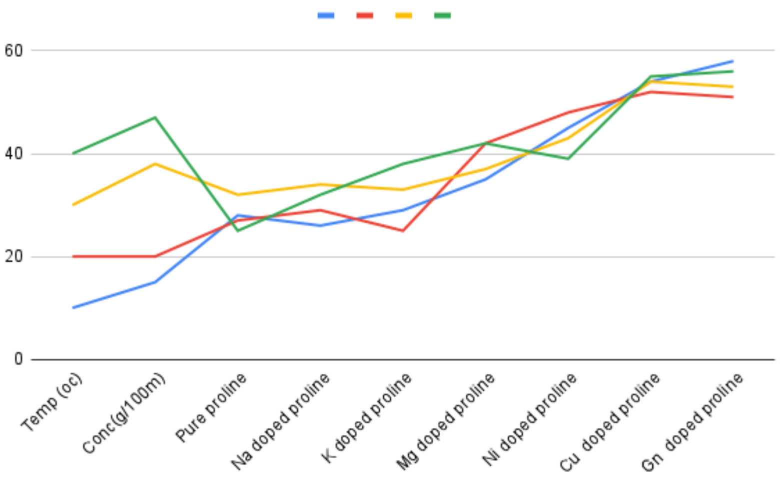

Fig. 2: Single crystal L-proline solubility curves with pure and metal ion doped solubility

4.2 SEM–EDAX analysis

Metal ions in the sub lattices may cause the material to become dipolar by increasing the carrier concentration. The ratio of atoms included in the generated crystal is shown in Table 2. and EDAX spectrum analysis clearly shows the presence of zinc and chloride in L-proline.

Table 2: EDAX spectrum study of DCBPZ crystal composition.

Element	**DCBPZ**	**EDAX**
Co^{2+}	38.08	32.05
Ni^{2+}	42.78	46.47

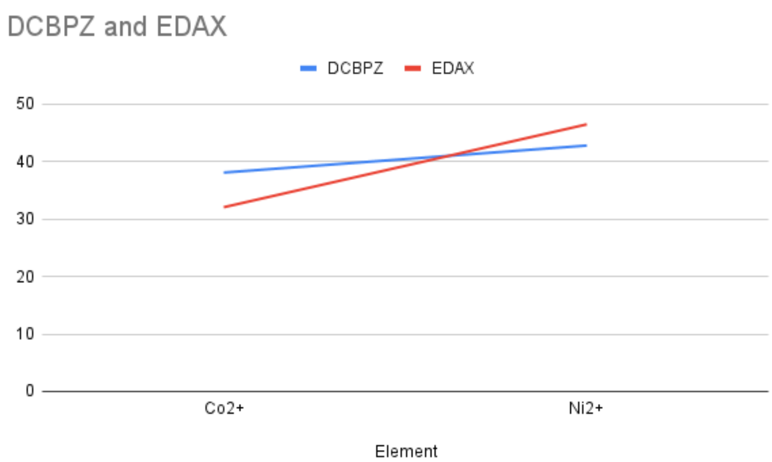

Figure 3: EDAX spectrum compositional study of DCBPZ crystal

SEM–EDAX examinations were used to discuss microstructure and compositional analysis. The surface characteristics and growth mechanism were studied using atomic force microscopy.

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V CONCLUSION

LPTCA crystals containing pure Co_2^+ and Ni_2^+ metal ions were created via a protracted evaporation technique. a single crystal and a powder XRD testing was used to confirm the crystal system of the produced crystals. Absorption bands in the crystals were discovered via FTIR spectrum analysis. The slimmer silhouette frequency in LPTCA crystals did not change much as a result of ion absorption, according to Spectral data. Furthermore, Co_2^+ dipoles improve the crystal's visual properties, resulting in greater transmittance than pure LPTCA crystals. The electrical and optical features of Co2+ doped LPTCA crystals are clearly superior to those of pure and Ni2+ doped LPTCA single crystals, as demonstrated by the findings of this study.

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