# Mechanically potent Organo-strontium crystal as optical filters in the Ultraviolet region

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## Abstract

Organometallic complex crystals are evolving as a mechanically potent and chemically flexible for optical filters. Here we crystallised Alanine cadmium chloride (ACC) and strontium admixed Alanine cadmium chloride amino metallic crystals by a simple technique at normal atmospheric pressure and temperature. Density measurements of the grown crystals were carried out using the simple flotation technique. On the particular face of (101) plane high mechanical properties achieved for the strontium admixed crystal. Optical properties are analysed by means of the spectroscopic techniques, the higher transmittance in the region 250 -1800 nm. This property and calculated optical parameters favours the material is possible for optical filters in ultra violet region.

## Keywords

L-Alanine Cadmium Chloride; Microhardness; Refractive index; Strontium.

## Introduction

Single crystals of organometallic compounds have been assessed as a feasible material for an optical and mechanical properties therefore actively researched in the recent years [1, 2]. Organo-strontium is an organometallic compound that contains at least one or more linkage between the strontium carbon bonds. The main application of strontium compound considered as a high beta emitter which prevents X-ray emission [3, 4]. In the medical field also strontium plays an important role such as prevents teeth sensitivity, main composition in bones and dentals [5]. L-Alanine is the simplest and neutral amino acid which exists as zwitterions; it possesses high transparency with favourable mechanical and optical properties crystallized in orthorhombic crystal structure with space group $P_{21}$ and the cell parameters are a = 6·032 Å, b = 12·343 Å, c = 5·784 Å; α = β = γ = 90 [6]. The incorporation of L-Alanine Cadmium chloride and strontium have been developed as a potential organic crystals as organic waveguides in the visible region. As some of the organometallic compounds that stands before as a organic wave guides, their optical, physical and mechanical properties are accessible and tuneable [1].

The single crystal namely L-Alanine Cadmium Chloride was first crystallized by the team of Kathleen et al. [7] and its physico chemical properties are studied by different research groups due to its wide optical applications [8, 9]. The wide varying properties of the compound have been altered and reported by adding different metallic compounds as impurities [10-13]. This review proves that no such report based on the strontium added parent compound. So an attempt is made to prepare and analyse its properties. We have recently reported the growth and spectroscopic properties of strontium doped L-Alanine cadmium chloride crystal [14]. The studies have been focussed on the crystallization of ACC and strontium ions added ACC and analyse its mechanical and optical properties.

**Experimental methods**

Organometallic crystals such as Alanine cadmium chloride (ACC) and strontium admixed ACC crystals have been crystallized by means of solvent evaporation crystal growth technique. In the synthesis process an equal molar ratio of amino acid L-Alanine and metal cadmium chloride was completely dissolved with water solvent for about five hours using the temperature controlled magnetic stirrer. During the mixing process, the temperature of the homogeneous mixture was maintained $40^{\circ}$ C to prevent further decomposition. As a result dried samples were obtained, which was completely dissolved with water solvent to make a saturated solution. The solution was standby for solvent evaporation, after a month good quality transparent single crystals are obtained.

Strontium admixed ACC crystals are grown by mixing L-Alanine, cadmium chloride and strontium chloride with the water solvent. During the synthesis process, along with the L-Alanine and cadmium chloride (1:1), one mole percentage of strontium chloride was added as a dopant and completely dissolved for about five hours using the temperature controlled magnetic stirrer. During the mixing process, the temperature of the homogeneous mixture was maintained $40^{\circ}$ C to prevent further decomposition. As a result dried samples were obtained, which was completely dissolved with water solvent to make a saturated solution. The solution was standby for solvent evaporation, after a month good quality transparent single crystals are obtained

**Result and Discussion**

The densities of the prepared organometallic crystals were accurately determined by the principle of floatation. In practise flotation method is considered generally as a sensitive method to determination the densities of the prepared crystals. It was found that the density of ACC and strontium admixed crystal is 2.139 g/cc and 2.165 g/cc respectively. Because of the addition of one molar percentage of strontium, the density of strontium added crystal increases slightly.

The study on the mechanical behaviour of the crystal helps to identify the nature of the materials. The most important property analysed in the present study is hardness. Hardness is determined by means of the indentation measurements. The prepared ACC and strontium admixed ACC crystals were subjected to Leitz microhardness tester with the applied load of 0.025 to 0.100 kg. Indentation was carried out along the face (101) plane for 10 s. For each and every applied load P, several indentations are performed and its average diagonal length (d) is calculated. The micro hardness number ($H_v$) using the relation [15];

$$H_v = \frac{1.8544\ P}{d^2}\ \text{kg mm}^{-2} \qquad (1)$$

Micro hardness plot with respect to the applied load is traced in the figure 1.

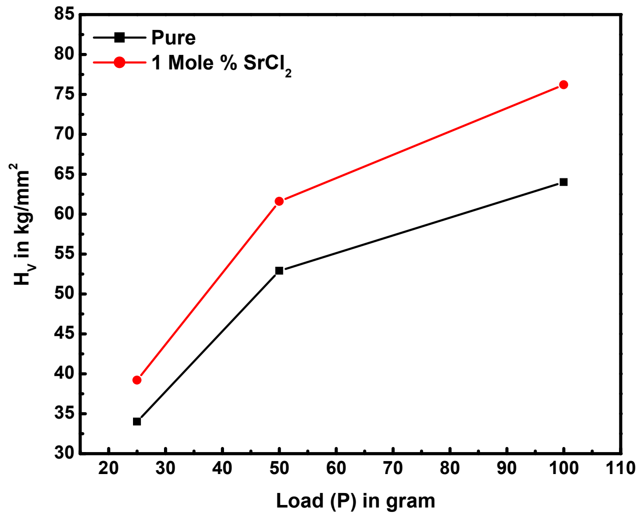


**Fig. 1: Plot of Hardness number with the applied load.**

From the plot of hardness and the applied load, it was known that for both the crystals the hardness number increases gradually with the applied load and the hardness number is greater for the strontium added crystal compared to the ACC crystal. The increase in hardness value is due to the incorporation of $Sr^{2+}$ ions into the host lattice of ACC crystal. From the Mayer's formula [16], the work hardening coefficients of the grown crystals are obtained from the slope of the plot log d and log P.

$$P = kd^n \tag{2}$$

Where k is the proportionality constant. The corresponding plot of log d with respect to log P for the ACC and $SrCl_2$ added ACC crystals are given in figures 2 and the work hardening coefficient (n) is estimated using the method of least square fit. For the ACC and $SrCl_2$ added ACC crystals the estimated work hardening coefficients are 3.54661 and 3.70638 respectively. Moreover the calculated work hardening coefficients are greater than the limit 1.6 [17], Therefore it was concluded that both the prepared crystals comes under the category of soft materials. Thus the addition of strontium ions improves the mechanical properties of the amino acid crystals. Moreover the enhanced hardness value of organo-strontium can be utilised in the medical field such as artificial bone and dental cement manufacturing [18].

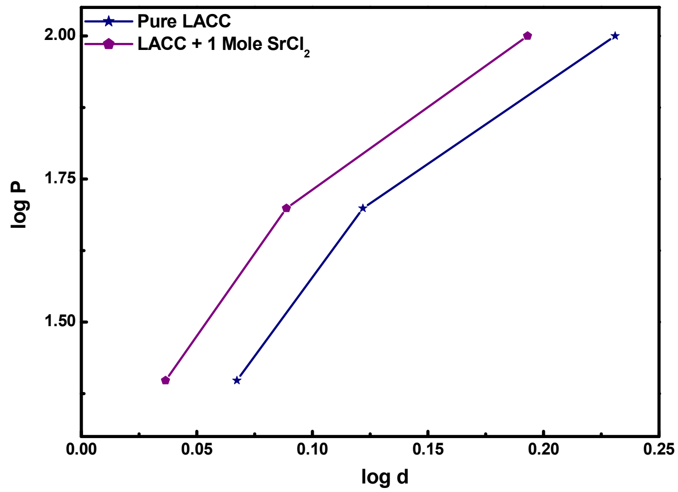


**Fig. 2: Plot of log d and log P.**

The Ultra Violet (UV) absorbance spectrum of ACC and $Sr^{2+}$ ions added ACC crystals were recorded using the UV- VIS spectrophotometer was depicted in the figure 3 and 4. From the UV absorbance spectrum, no absorptions obtained in the complete UV-Visible range, that is due to the presence of L-Alanine an amino acids present in both the crystals. In the case of L-Alanine, the transitions due to the conjugated bonds are absent, which in turn leads to much wider transparency in the entire visible and ultra violet spectral regions. Both the crystals ACC and $Sr^{2+}$ ions added ACC experiences the lower cut of wavelength value around 250 nm.

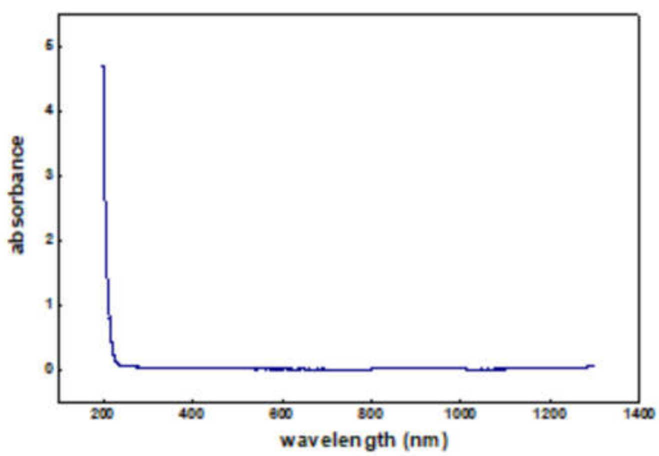


**Fig. 3: UV absorbance spectrum for ACC crystal.**

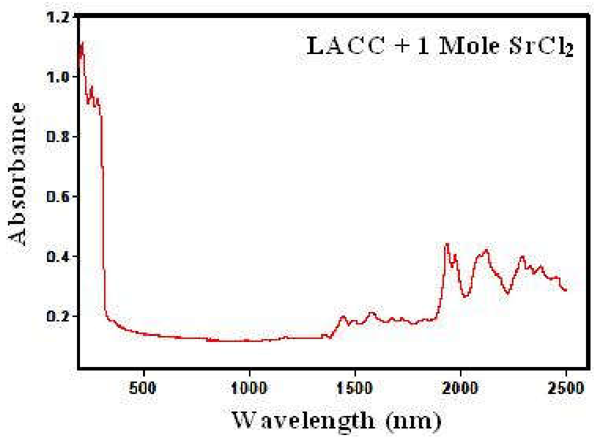


**Fig. 4: UV absorbance spectrum for strontium doped ACC crystal.**

The optical energy ($E_g$) gap observed in the absorption spectra of the grown crystals is determined using the relation;

$$E_g = \frac{hc}{\lambda} \tag{3}$$

Where, h is plank's constant, c is velocity of light and λ is lower cut of wave length. The optical bang gap of ACC and strontium admixed ACC crystal is found to be 5.26 and 4.85 eV respectively. Furthermore the calculated values elucidates that the grown crystals can be used as an insulators. Above this, the position of the valance ($E_{(CB)}$) and conduction band ($E_{(VB)}$) of the grown crystal is determined using the relations as follows;

$$E_{(CB)} = \chi - E^c - 0.5Eg \tag{4}$$

$$E_{(VB)} = E_{(CB)} + Eg \tag{5}$$

χ represents absolute electro negativity of the prepared compound and $E^c$ denotes the energy of the valence electrons based on the hydrogen scale (4.5 eV). In order to fetch the information about the optical property of the crystal, the optical absorption coefficient (α) is evaluated using the following relation [19];

$$\alpha = \frac{2.303 \times \log\frac{1}{T}}{t} \tag{6}$$

Where, T is transmittance and t is thickness of the prepared crystal. In fact, the optical parameters such as refractive index (n) and extinction coefficient (k) are evaluated from the transmittance data are depicted in table 1. Extinction coefficient of the crystal gives information about the light loss due the scattering effect and absorption. It denotes the quantity of the absorption loss when electromagnetic waves propagated through the prepared crystal [20];

$$K = \frac{\lambda\alpha}{4\pi} \tag{7}$$

The reflectance (R) and Refractive index (n) was evaluated from the relation [21, 22];

$$R = \frac{\exp(-\alpha t) + \sqrt{\exp(-\alpha t)T - \exp(-3\alpha t)T + \exp}(-2\alpha t)T^2}{\exp(-\alpha t) + \exp(-2\alpha t)T} \tag{8}$$

$$n = \frac{-(R+1) + 2\sqrt{R}}{R-1} \tag{9}$$

The optical conductivity and complex dielectric constant is calculated from refractive index and the extinction coefficient using the following relation,

$$\sigma_{opt} = \frac{\alpha n c}{4\pi} \tag{10}$$

$$\varepsilon = (n - K) + 2nK \tag{11}$$

**Table 1 Calculated optical parameters.**

| **Optical parameters** | **ACC** | **$Sr^{2+}$ ions doped ACC** |
|---|---|---|
| Cut off Wavelength(nm) | 236 | 256 |
| Band gap (eV) | 5.26 | 4.85 |
| Absolute electro negativity ($\chi$) | 6.7571 | 6.566 |
| $E_{(CB)}$ (eV) | -0. 3729 | -0. 3598 |
| $E_{(VB)}$ (eV) | 4.8871 | 4.4918 |
| Extinction coefficient | $0.2104 \times 10^{-6}$ | $0.8194 \times 10^{-6}$ |
| Reflectance | 1.0222 | 1.1611 |
| Refractive index | 4. 5 | 3.7 |
| Optical Conductivity | $1.2 \times 10^{9}$ | $3.55 \times 10^{9}$ |
| Complex dielectric constant | 4.499 | 3.699 |

Optical band gap is an important optical phenomenon which gives the information about the conduction process and the position of the band edges due to the application of light energy. Due to the addition of the strontium ions in the amino acid the band gap decreases. Therefore strontium improves the optical conductivity of the crystal. This was proved in the optical conductivity calculated value. Furthermore the strontium admixed ACC crystal can be efficiently used as a display in optical devices; it also prevents the X-ray radiation emissions [3]. Absolute electro negativity of the material is directly related with the bonded atoms present in the crystal. Because of the influence of the strontium atom, covalent and ionic bonds arises which tends to decreases the bond strength. Reflectance of the crystal depends on the cutoff wavelength of the prepared crystal, the reflectance value enhances in the case of strontium added crystal. The decreasing refractive index suggests that, the Ultraviolet light can propagate quickly through the strontium added crystal than

ACC crystal. The optical transition between the electronic ground state $5s_2$ $^1S_0$ and the meta-stable 5s $5p^3$ $P_0$ to the excited state is considered as a principal candidates for the optical transition.

Thus strontium is capable to tune the optical behaviour of the amino acid crystal which is highly recommended for optical device fabrications. Moreover after strontium addition, the optical conductivity of the crystal increases with decrease in dielectric constant this property can be utilised as an antireflection coating mainly in the solar cells.

**Conclusion**

Organometallic complex crystals are productively crystallised as Alanine cadmium chloride (ACC) and strontium admixed Alanine cadmium chloride by a simple technique called slow evaporation at normal atmospheric pressure and temperature. Density measurements confirms that the addition of strontium ions in the lattice of ACC lattice using the simple flotation method. On the particular face of (101) plane high mechanical properties achieved for the strontium admixed crystal, moreover both the crystals are identified as a soft category. Optical properties are analysed and higher transmittance achieved in the region 250 -1800 nm. This property favours that the material is suitable for optical filters in ultra violet region. The theoretically calculated optical parameters suggested that the strontium can be able to tune the optical property of host compound.

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