IJARSCT

International Journal of Advanced Research in Science, Communication and Technology

International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal

ISSN: 2581-9429

Volume 6, Issue 2, June 2026

Impact Factor: 8.2

Comparative Study of Electronic and Optical Properties of Pure and Modified Copper Tartrate Crystals

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Abstract: *The present paper reports a comparative study on optical and electrical properties of pure and sodium modified copper tartrate single crystals. Single crystal growth of these materials followed by their characteristics has already been published somewhere else. Having achieved the growth of pure and sodium modified copper tartrate single crystals and established their basic characteristics, it is thought worthwhile to have an understanding of various factors on which optical and electrical properties depend and how these two are related to each other. The electrical properties are studied by measuring electrical conductivity in the temperature range from 80 to 300 K. The optical properties are studied by recording the absorption spectra of these crystals at room temperature in the wavelength range of 200 nm to 800 nm. The study reveals that both electrical and optical properties are not independent rather dependent on each other. The relation between the two has been explained on the basis of experimental and theoretical results*

Keywords: Single Crystal, Optical Properties, Electronic Properties, Substitution , Doping

I. INTRODUCTION

Organic metallic compounds have a great impact on information technology and non linear optical applications [1] . ‘Single crystals are the backbone of revolution in modern technology. Tartaric acid is serving as a base for the development of new class of materials due to the presence of two hydroxyl and two carbonyl groups that readily permits the incorporation monovalent, divalent and trivalent metal ions [2] . Single crystals of tartrate compounds are of great interest due to their excellent optoelectronic properties [3] . These properties explore the possibility of tartrate compounds to be exploited for various device applications such as piezoelectric, dielectric ferroelectric [4 - 6] . They are also used in non linear optical devices (NLO) such as crystal oscillators based on optical second harmonic generation, optical transmission characteristics and controlled laser emission [7] . Presently great attention has been devoted to the growth and characterization of pure and doped tartrate crystals with an aim to identify new materials for device applications This has attracted the attention of several workers to grow single crystals of tartrate compounds and study their properties [8 - 11] . Investigating the effect of dopant on the properties of single crystal is of great importance from technological point of view [12] . The present paper reports a comparative study of optical and electrical properties of pure and sodium modified copper tartrate single crystals

II. EXPERIMENTAL

Optical absorption spectra of the grown crystals were recorded at room temperature in the wavelength range of 200 to 800 nm using Varian Cary 5000 UV-VIS-NIR spectrometer covering the entire ultraviolet and visible regions . Electrical resistivity measurements were performed using standard four probe technique in the temperature range of 80-300 K using a closed cell refrigerator (CTI 8200). All the resistivity measurements were carried out in the warm up cycle

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III. RESULTS AND DISCUSSION

Metal tartrate compounds are sparingly soluble in water and decompose before melting so gel method provides an excellent technique to grow these materials Single crystal growth of pure and modified copper tartrate using gel method have already been published [13 - 15] . Having achieved the growth of pure and sodium modified copper tartrate single crystals and established their basic characteristics, it is thought worthwhile to have an understanding of various factors on which optical and electrical properties depend and how these two are related to each other . The stoichiometric composition of pure crystals so obtained is $CuC_4H_4O_6.3H_2O$ whereas that of modified ones is $(Cu)_{0.77}(Na)_{0.23}C_4H_4O_6.3H_2O$ and $(Cu)_{0.65}(Na)_{0.35}C_4H_4O_6.H_2O$

IV. COMPARATIVE STUDY

Electronic properties describe how an electron in a material behaves in presence of electric field including its energy and momentum. Electronic band structure describe the possible energy states for electron in a material which is essential to understand electrical conductivity, the ability of material to conduct electric current and dielectric property of a material which determines its response to its electric external field. Optical properties describe how a material interacts with light or electromagnetic radiations such as absorption, reflection and transmission. These sets of properties are interconnected and influence each other. For example for a material to be transparent to visible light its band gap must be larger than the energy of visible photons so that no photon is absorbed by the electron of the material. The width of optical band gap also determines the colour of light emitted by a material. The optical properties of a material such as absorption spectrum are critical for its efficiency in converting sunlight into electricity. The ability to tune both electronic and optical properties allow for the development of specialized sensors for specific wave length. Electronic properties like band structure influence optical properties like the reflective index which are critical for application like LEDs, solar cell and optical sensors

Optical behaviour of pure and modified copper tartrate single crystals was studied by recording absorption spectra in the wavelength range of 200 to 800 nm that covers the entire ultraviolet and visible region. The plots of absorbance against wavelength for all the three compositions (pure and modified) are shown in fig.1. From the figure it is clear that transmittance is more than 80 % for both pure and modified copper tartrate crystals for a particular range of wavelengths. The value of this range is 422-556 nm for pure crystals of composition $CuC_4H_4O_6.3H_2O$ and 441-560 nm and 459-553 nm for substituted crystals bearing composition $(Cu)_{0.77}(Na)_{0.23}C_4H_4O_6.3H_2O$ and $(Cu)_{0.65}(Na)_{0.35}C_4H_4O_6.H_2O$ respectively

The optical band gap of pure and modified copper tartrate are calculated from the absorption wavelength using the formula

$$E = \frac{hc}{\lambda}\ in\ eV$$

$$E = \frac{1240}{\lambda}\ in\ eV$$

The values of the optical energy band gap so calculated are shown in table 1 . From the table it is clear that the value of energy gap is higher for pure copper tartrate crystals as compared to modified copper tartrate and this gap decreases with the increase in impurity . This indicates that on modifying pure crystals by Na^+ ions there is a shift in the value of wavelengths absorbed by these crystals which is responsible for the change in band gap of pure crystal

The electrical resistivity as a function of temperature for both pure copper tartrate single crystals bearing composition $CuC_4H_4O_6.3H_2O$ whereas that of modified ones is $(Cu)_{0.77}(Na)_{0.23}C_4H_4O_6.3H_2O$ and $(Cu)_{0.65}(Na)_{0.35}C_4H_4O_6.H_2O$ is shown in fig 2 . The temperature dependent electrical conductivity measurements were carried out in the temperature range of 80-300 K. The variation of resistivity with temperature shows exponential behavior for all the samples

The electrical behavipur of pure copper tartrate on modification by Na ions can be explained on the basis of Variable Range Hopping model . Using this model electrical parameters like carrier density, hopping distance and hopping

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energy are calculated . The values of these parameters are shown in the table 2 . From the table it is clear that hopping energy W and the hopping distance R are lesser in case of sodium modified copper tartrate crystals. This observation indicates that the electronic property in the system is driven by the induced disorder effect due to the presence of foreign ions in the parent material . This can be explained on the basis that substituting Na ions in the pure copper tartrate crystal leads to an increase in the carrier density. This increase in carrier density in the system decreases in the energy gap. Actually, this substitution provides statistical randomness and leads to decrease in the band gap due to inhomogeneities caused by the substitution. In other words, this situation gives rise to novel mechanism for hopping transport. As a result the value of resistivity decreases on modification of copper tartrate crystals by Na^+ ion

From table 1 and table 2 it is clear that both the values of optical energy gap and electronic energy gap are higher for pure crystals as compared to modified copper tartrate crystals . This change in the value of band gap is on account of addition of Na^+ ion in the pure copper tartrate crystals . Pertinent to mention here that the values of optical band and electronic band gaps are slightly different but they are proportional to each other which means that the two are inter connected

V. CONCLUSION

1. Width of optical band gap of pure crystals is more than that of modified copper tartrate crystals
2. Width of electronic band gap of pure crystals is more than that of modified copper tartrate crystals
3. Value of optical band gaps and electronic band gaps are slightly different but they are proportional to each other which means that the two are inter connected
4. Excellent optical and electronic properties of copper tartrate in pure and modified form explore the possibility of these materials to be used in industry for device application

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Table 1 Value of wavelength absorb and energy gap for pure and modified copper tartrate crystals

Crytal Type	Colour	Wavelength	Energy Gap
Pure copper tartrate			
$CuC_4H_4O_6.3H_2O$	Bluish green	422-556	2.938
Modified copper tartrate			
$(Cu)_{0.77}(Na)_{0.23}C_4H_4O_6.3H_2O$	Light green	441-560	2.811
$(Cu)_{0.65}(Na)_{0.35}C_4H_4O_6.H_2O$	Dark green	459-553	2.701

Table 2 Value of resistivity and electrical parameters of pure and modified copper tartrate crystals

Crystal	ρ (Ω cm)	$N(E_f)x10^{19}$ (eV^{-1} cm^{-3})	R_h (nm)	E_h (eV)
Pure copper tartrate				
$CuC_4H_4O_6.3H_2O$	$4.9x10^{-2}$	1.22	0.096	0.200
Modified copper tartrate				
$(Cu)_{0.77}(Na)_{0.23}C_4H_4O_6.3H_2O$	$1.8x10^{-2}$	1.35	0.068	0.173
$(Cu)_{0.65}(Na)_{0.35}C_4H_4O_6.H_2O$	$0.6x10^{-}$	1.98	0.051	0.162

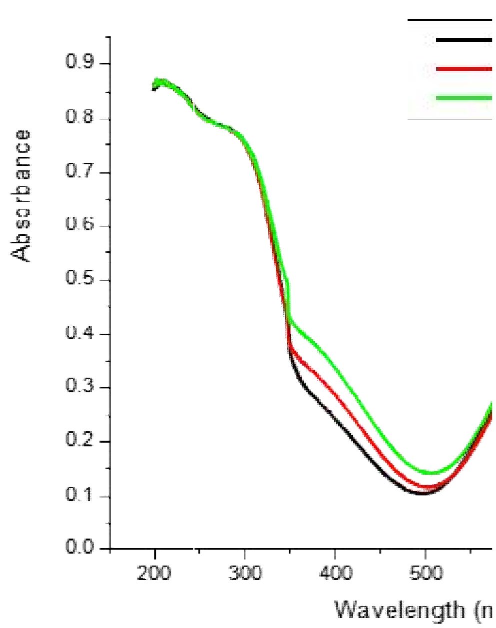

Fig 1 Absorbance as a function of wavelength

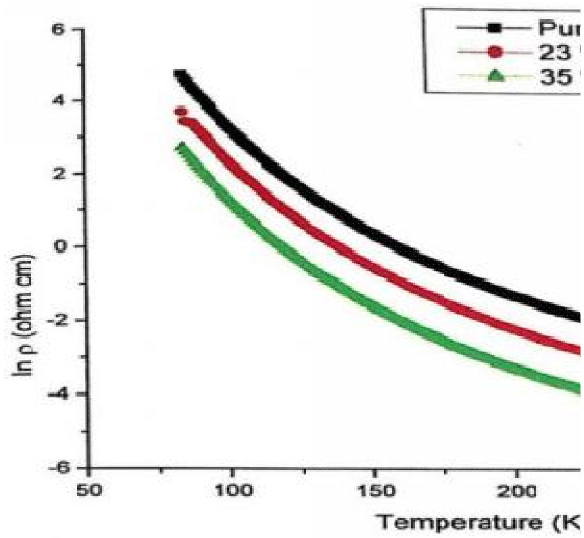

Fig 2 Resistivity as a function of temperature