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# STUDY ON THE DIELECTRIC PROPERTIES OF A NEW POLYMORPH OF STRONTIUM D,L- MALATE

**Lekshmi P.Nair[1], Divya R.[1], B.R.Bijini[1], M.Deepa[2*], K.RajendraBabu[1]**

[1]*Post Graduate Department of Physics, M.G. College, Thiruvananthapuram.*

[2]*Department of Physics, All Saints' College, Thiruvananthapuram.*

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**Abstract:**

A new polymorph of strontium D, L-malate (DSM) is grown by the conventional gel method and the crystal belongs to triclinic system, P1 space group with cell dimensions $a$ = 6.3815 (3) Å, $b$ =7.7753 (3) Å, $c$ =9.0309(4) Å, $\alpha$ =73.528(2)°, $\beta$ = 75.608 (2)°, $\gamma$ = 86.901(2)°. The UV-Visible spectrum of DSM is taken between 200nm and 1200nm. The refractive index (n) of DSM is obtained from the reflectance data for the first time. The frequency dependent dielectric property of the complex is studied at room temperature using a Hioki 3532 LCR Hitester meter. Using the results of Single crystal XRD, UV-Visible spectrum and the value of dielectric constant at higher frequencies, the crystal parameters like the Plasma energy, Penn Gap, Fermi energy and polarisability of DSM are calculated and tabulated.

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## 1. INTRODUCTION:

Metal organic frameworks (MOFs) or Porous Coordination Polymers (PCP) are advanced class of porous materials with immense applications[1]. The need for new polymorphs of alkaline earth MOFs are also increasing because of their variety in co-ordination behavior and tailor made properties. We studied and reported the growth, structural, spectral and thermal studies of a new polymorph of strontium malate, distrontium D, L-dimalate pentahydrate (DSM )[2]. DSM is a porous polymeric biologically active MOF. Dielectric properties are correlated with the electro-optic properties of the crystal. The wide band gap of the grown porous material prompted us to study its dielectric behavior. Here the frequency dependent dielectric property of DSM at room temperature is analysed and reported for the first time. Fundamental parameters like Plasma energy, Penn gap, Fermi energy, Polarisability of the grown crystal are calculated.

## 2. EXPERIMENTAL:

### 2.1. CRYSTALLISATION METHOD:

Good quality single crystals of DSM were obtained by single gel diffusion technique. Crystals were grown in borosilicate glass tubes of length 20cm and diameter 2.5cm. Silica gel of specific gravity 1.03 to 1.06g/cc prepared by dissolving sodium metasilicate (SMS) in double distilled water was acidified using 1M racemic malic acid to get the pH in the range 3 to 7. About 20 ml of above solution was taken in each test tube, sealed and kept undisturbed for gellation. Over the set gel, aqueous solution of strontium

chloride (0.5M – 1.5M) was added as the top reagent without damaging the gel system. The experimental set up was kept undisturbed for crystallization.

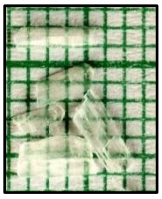

**Fig. 1 Photo of grown DSM**

### 2.2. CHARACTERISATION:

Absorption spectrum of the powdered sample was studied using Varian Cary 5000 UV-Vis-NIR spectrometer in the range 200-1200nm.The frequency dependent dielectric property of DSM was studied at room temperature using a Hioki 3532 LCR Hitester meter.

## 3. RESULTS AND DISCUSSION:

### 3.1. CRYSTAL GROWTH:

Good quality single crystals suitable for single crystal XRD studies were grown in gel medium of pH 6.5 and density 1.04g/cc with 1M D,L-malic acid and 1M strontium chloride. The characteristic shape of the crystal is shown in Fig. 1.

### 3.2. UV- VIS SPECTRAL STUDIES:

UV-Visible absorption spectrum of distrontium D, L-dimalate pentahydrate crystals was carried out in the range 200 nm and 1200nm and is given in fig. 2. The material is found to have indirect forbidden transitions as the band gap of distrontium D, L-dimalate pentahydrate is estimated by plotting $(\alpha h\nu)^{(1/3)}$ versus $(h\nu)$ as in fig. 3. The band gap of the material is obtained by extrapolating the linear portion of the curve to zero absorption and the value is estimated as 5.39eV. Large band gap of DSM indicates the wide transparency of the crystal [2].

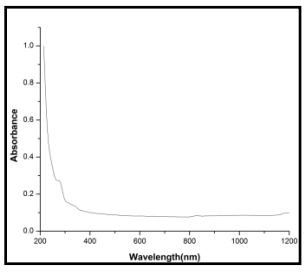


**Fig. 2 Absorption spectrum of DSM**

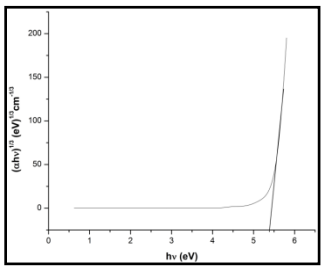


**Fig. 3 Plot of alphaenergy versus energy**

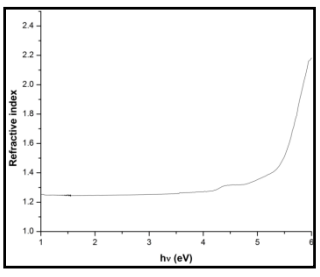


**Fig. 4 Plot of energy versus refractive index**

From the reflectance data, the refractive index can be obtained from the relation:

$$n = \left[-(R+1) \pm \sqrt{-3R^2 + 10R - 3}\right]/2(R - 1 \ldots\ldots\ldots(1)$$ [3]

Fig. 4 shows the energy dependence of n in the range 1 to 6eV. The refractive index increases with increasing energy. The refractive index of DSM is obtained as 1.46 at 5.39 eV.

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From the Single crystal XRD data, the empirical formula is $C_8H_{18}O_{15}Sr_2$, the molecular weight of the grown sample is 529.46g, the density of the grown crystal, ρ=2.113g/cc and the total number of valence electrons, Z [2].

The valence electron plasma energy is given by,

$\hbar\omega_p = 28.8\sqrt{[(Z\rho)/M]}$ …… …….(2)

The Fermi energy $E_F = 0.2948\ (\hbar\omega_p)^{4/3}$ …(3)

### 3.3 DIELECTRIC STUDIES:

The dielectric study of distrontium D, L-dimalate pentahydrate was carried out at room temperature using HIOKI 3532-50 LCR HI Tester apparatus utilizing the parallel plate capacitor method. The variation of dielectric constant, dielectric loss, impedance and ac conductivity as a function of frequency at room temperature is plotted in fig. 5-a,b,c,d. The dielectric constant and dielectric loss decreases with the increase in frequency. The dipoles can easily switch alignment with the changing field at low frequencies. As the frequency increases, the dipoles can orient less. Thus they reduce their contribution to the polarization field and hence the observed reduction in dielectric constant and dielectric loss. The very low value of dielectric constant at higher frequencies is important for the fabrication of materials for ferroelectric, photonic and electro-optic devices [4]. The dielectric impedance also shows a decrease with the increase in frequency.

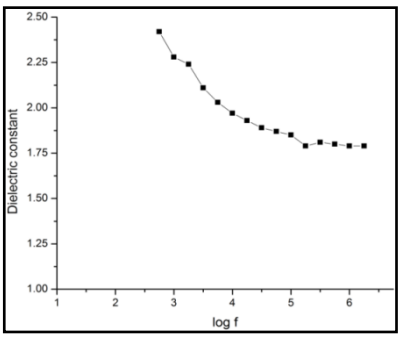



**Fig. 5.a Dielectric constant Vs log frequency**

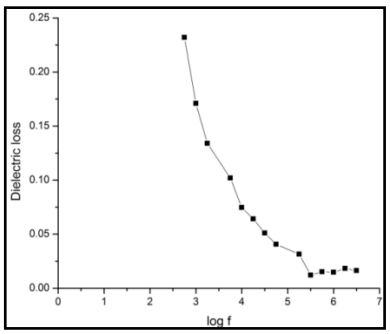
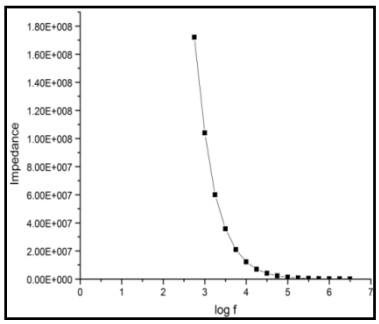



**Fig. 5.b Dielectric loss Vs log frequency**



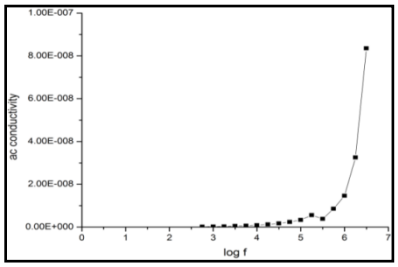



**Fig. 5. c Impedance Vs log frequency**

**Fig. 5. d ac conductivity Vs log frequency**

The ac conductivity of distrontium D, L-dimalate pentahydrate increases with increase in frequency. Using the dielectric constant at higher frequency and the SXRD data, some theoretical parameters of the complex can be calculated. The calculated parameters are given in table 1.

The Penn gap is given by $E_P = \frac{\hbar\omega p}{\sqrt{\epsilon_\infty - 1}}$ .....(4)

The electronic polarisability α is obtained using the relation,

$$\propto = \left[\frac{(\hbar\omega p)^2 S_0}{(\hbar\omega p)^2 S_0 + 3E_p^2}\right] \times \frac{M}{\rho} \times 0.396 \times 10^{-24} cm^3 \ldots(5)$$

where, $S_0 = 1 - \left(\frac{E_p}{4E_F}\right) + \frac{1}{3}\left(\frac{E_p}{4E_F}\right)^2$ .....(6)

The value of ∝ obtained from equation (5) closely matches with that obtained using Claussius – Mossotti relation, $\alpha = \frac{3}{4}\frac{M}{\pi N_a \rho}\left(\frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 2}\right)$ .....(7)[5]

**Table 1 Calculated theoretical parameters of distrontium D, L-dimalate pentahydrate**

| Parameters | Values |
|---|---|
| Plasma energy ($\hbar\omega_p$) | 21.8 eV |
| Penn gap ($E_P$) | 24.5 eV |
| Fermi energy ($E_F$) | 17.9 eV |
| Polarisability ($cm^3$)<br>a)Penn analysis<br>b)Claussius- Mossotti Equation<br>c)From band gap | <br>$3.52 \times 10^{-23}$<br>$3.40 \times 10^{-23}$<br>$4.23 \times 10^{-23}$ |

## 4 Conclusion

Single crystals of a new non-centrosymmetric polymorph of distrontium D, L-dimalate pentahydrate with chemical formula $Sr_2(C_4H_4O_5)_2.5H_2O$ is grown successfully by conventional gel method. Good quality single crystals belonging to the triclinic system with P1 space group are grown from the gel medium of pH 6.5 and density 1.04g/cc. Higher band gap reflects the rigidity and stability of the crystal structure. Wide band gap materials have applications in band gap engineering. Wide transparency of distrontium D, L-dimalate pentahydrate in the entire visible range makes it a suitable candidate for optoelectronic application. Dielectric measurements show that the dielectric loss, dielectric constant and impedance of distrontium D, L-dimalate pentahydrate decreases with the increasing frequency. The least value of dielectric constant 1.78 is obtained for DSM at higher frequency. The

porous structure of distrontium D, L-dimalate pentahydrate with wide band gap and low dielectric constant can make it a suitable candidate for Inter Layer Dielectrics (ILD). Fundamental parameters like plasma energy, penn gap, fermi energy and electronic polarisability of the crystal have been calculated.

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