Spectral, Optical and Electrical Characterization Of 1-(2-Hydroxyethyl)-2-Methyl-5-Nitroimidazole (Metronidazole) Single Crystal

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Abstract: Single crystal of 1-2-(hydroxyethyl)-2-methyl-5-nitroimidazole (Metronidazole) is a well-known antibacterial drug, was grown by slow evaporation method. The spectral and optical characterization of the crystal was determined using UV-Visible spectroscopy and photoluminescence study. The crystal show very good transparency of 95% in the entire visible region. The optical band gap energy E_g was calculated from the tauc's plot as 2.44 eV. On screening the material for photoluminescence, four emission peaks are observed at 360 nm (3.44 eV), UV radiation; sharp peak at 380 nm (3.26 eV), visible violet; 490 nm (2.53 eV), visible blue and sharp peak at 525 nm (2.36 eV) due to the emission of green light. This study confirms that the drug metronidazole shows excellent optical properties.

Key Words: —T*ransmittance, optical constants, electrical parameters, emission.*

I. Introduction

1-(2-hydroxyethyl) 2-methyl-5-nitroimidazole, known as metronidazole is used in the treatment of anaerobic protozoan and bacterial infections [1-9]. Most of the research on metronidazole is concentrated on its biological activities since metronidazole is an anti-parasitic and antibacterial drug [10]. The mechanical, thermal and optical absorption characterization of metronidazole has been reported earlier [11, 12].

In this research work, we have discussed the optical, electrical and photoluminescence property of 1-(2-hydroxyethyl) 2-methyl-5-nitroimidazole, known as metronidazole.

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Since no studies are reported on the optical transmission, optical constant and photoluminescence property of this well-known drug, aroused by the curiosity we have reported the optical transmission and photoluminescence spectrum of the title compound in this research work.

1.1 Experimental

Metronidazole [ALDRICH] 1.7115 mg was dissolved in 25 ml hot ethanol and allowed the solution to evaporate slowly.

Pale yellow block shaped crystals were obtained after a month on slow evaporation of the solvent. Fig 1 shows the grown crystals. Fig 2 shows the chemical diagram of the title compound.

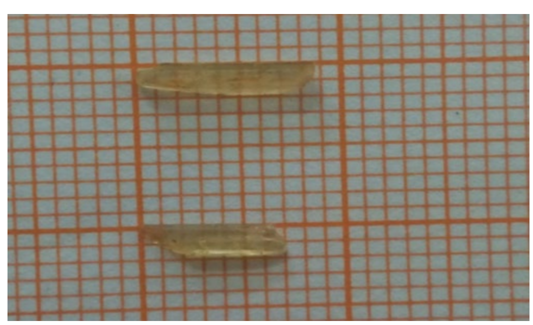

Fig.1. Crystals of Metronidazole

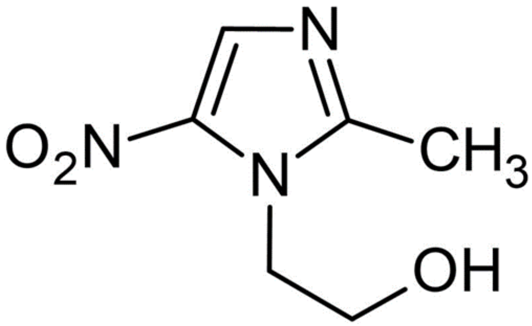

Fig.2. Chemical Diagram of Metronidazole

II. Result And Discussion

2.1 Optical Transmission Studies

The optical properties of the material are useful as they give valuable information about the electronic band structures, localized states and types of optical transitions [13]. The optical property of metronidazole was characterized by using UV-DRS-Spectrophotometer in the range of 190 nm – 1100 nm. For optical applications, especially for SHG, the crystal should be highly transparent in the considerable region of the UV-Vis wavelength [14, 15]. Fig 3 shows the optical transmission spectrum of metronidazole. The transparency is around 95% within the range of 425 nm to 800nm. The good transmission property of the crystal in the visible region indicates its suitability for second harmonic generation [16, 17]. The UV absorption edge of the crystal was observed around 490 nm. The optical transmission spectrum is shown in the Fig 3.

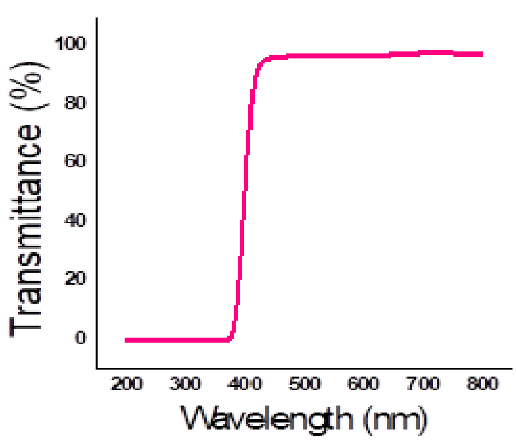

Fig.3. Optical Transmission Spectrum of Metronidazole

2.2 Absorbance Spectra of Metronidazole

From the optical absorbance spectrum as shown in the Fig 4, the cut-off wavelength is observed at 380 nm and the crystal show poor absorbance in the wavelength range of 400 nm – 800 nm. The absorbance band arises due to the promotion of an electron from the highest occupied orbital to the lowest unoccupied molecular orbital confirms the formation of charge transfer of the molecular complex [18]. Fig 4 represents the optical absorbance spectrum. As it is clear from the spectrum that metronidazole crystal is transparent throughout the entire visible region, the crystal is highly suitable for optoelectronic device fabrications [19].

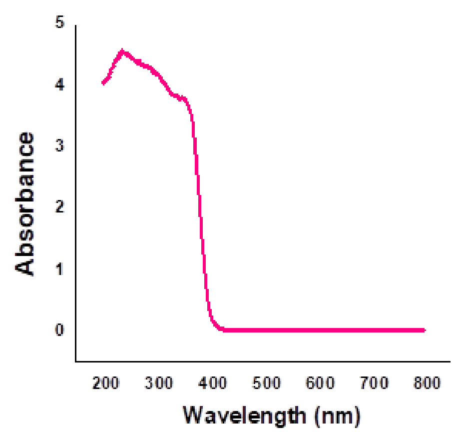

Fig.4. Optical Absorption Spectrum of Metronidazole

2.3 Optical Band Gap Energy (E_g) Calculation

The dependence of optical absorption coefficient with the photon helps to study the band structure and the type of transmission of electrons [20].

The optical absorption coefficient (α) was calculated from the transmittance using the following relation,

$$\propto = \frac{2.3036 \log(\frac{1}{T})}{d}$$

Where, T is the transmittance and d are the thickness of the crystal.

In the high photon energy region, the energy dependence of absorption coefficient suggests the occurrence of direct band gap. As a direct band gap semiconductor, the crystal under study has absorption coefficient (α) obeying the following relation for high photon energies (hυ).

The band gap energy (E_g) was calculated from the following relation [21],

$(\alpha h\upsilon)^2 = A\,(h\upsilon - E_g)$

Where, E_g is the optical band gap of the crystal, A is a constant, h is the Plank's constant, and υ is the frequency of the incident photons. Fig 5 shows the band gap energy obtained from tauc's plot. The band gap energy of grown metronidazole was found to be 2.44 eV.

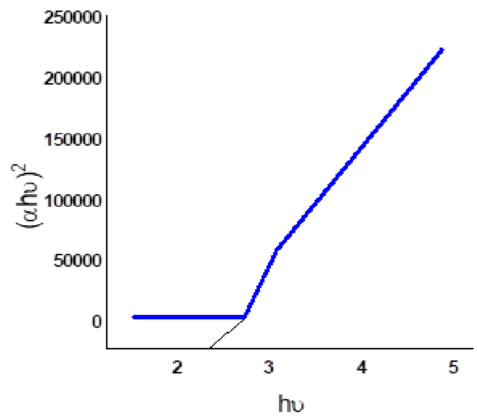

Fig.5. Plot of hυ versus $(\alpha h\upsilon)^2$

2.4 Determination of Optical Constants

The refractive index can be determined from the reflectance (R) data using the relation as mentioned below [22]

$$R = \frac{(n-1)^2}{(n+1)^2}$$

and the transmittance (T) is given by [23]

$$T = \frac{(1-R)^2 \exp(-\alpha t)}{1 - R^2 \exp(-2\alpha t)}$$

Extinction coefficient (K) is a measure of light loss due to scattering and absorption per unit volume.

The extinction coefficient can be obtained from the following relation,

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

The plot of wavelength versus extinction coefficient is shown in Fig 6. The calculated value of extinction coefficient (k) is 1.5781 x 10^{-6}.

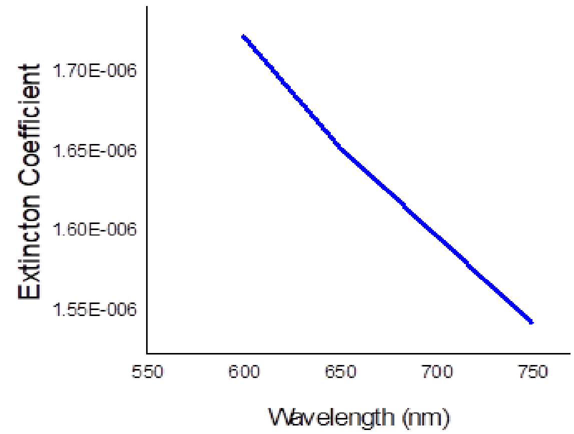

Fig.6. Plot of wavelength versus extinction coefficient of Metronidazole

The reflectance in terms of the absorption coefficient can be derived from the below equation. The plot of wavelength versus reflectance is shown in Fig 7. The calculated value of reflectance (R) is 0.1552.

$$R = \frac{1 \pm \sqrt{(1 - exp(-\alpha t) + \exp(\alpha t)}}{1 + \exp(-\alpha t)}$$

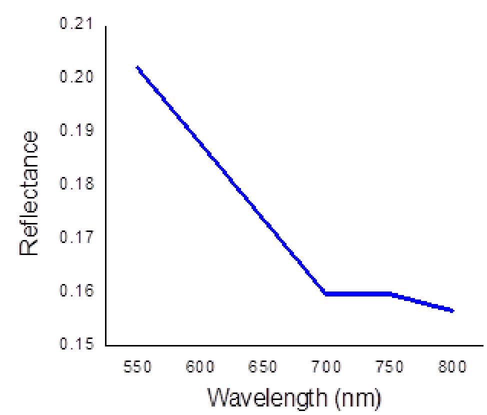

Fig.7. Plot of Wavelength versus Reflectance of Metronidazole

The refractive index n can be derived as

$$n = \frac{-(R+1) \pm \sqrt{-3R^2 + 10R - 3}}{2(R-1)}$$

The calculated refractive index (n) value using the above equation for the grown metronidazole crystal is 2.3022. The plot of wavelength versus refractive index is shown in Fig 8.

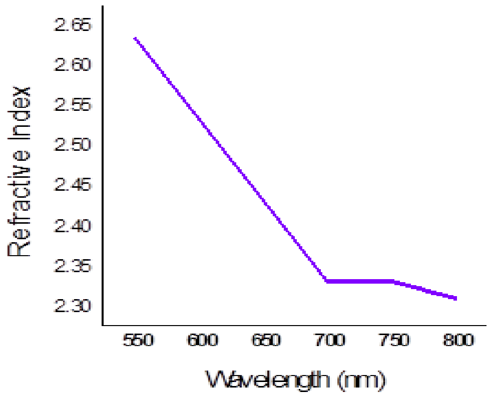

Fig.8. Plot of Wavelength versus Refractive Index of Metronidazole

2.5 Optical Conductivity

The optical response of a material is studied in terms of the optical conductivity. Optical conductivity is one of the powerful tools for studying the electronic states in materials. It has dimensions of frequency which are valid only in a Gaussian system of units. The optical conductivity (σ_{op}) has been determined from the relation,

$$\boldsymbol{\sigma_{op}=\alpha nc/4\pi}$$

Where c is the velocity of light, **α** is the optical absorption coefficient and n is the refractive index. The variation of optical conductivity with wavelength is shown in Fig 6. Optical conductivity has higher values in the UV region of the order of $1\times10^8 S^{-1}$. The higher value of optical conductivity (10^9-10^{12}) shows very good photo response of the crystal [24]. Here in our case the optical conductivity is higher in the order of $10^8 S^{-1}$, indicates metronidazole exhibits almost very good optical response.

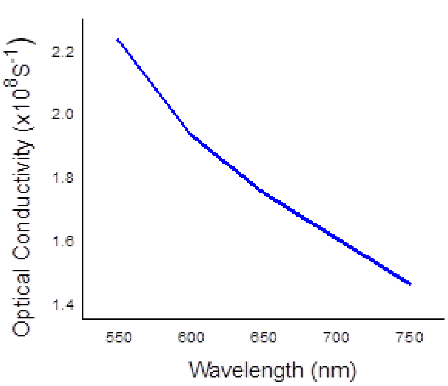

Fig.9. Plot of Wavelength versus Optical Conductivity Metronidazole

2.6 Electrical Conductivity

The value of electrical conductivity of a material is related with the optical conductivity value of the crystal using the following equation

$$\boldsymbol{\sigma_e=2\lambda\sigma_{op}/\alpha}$$

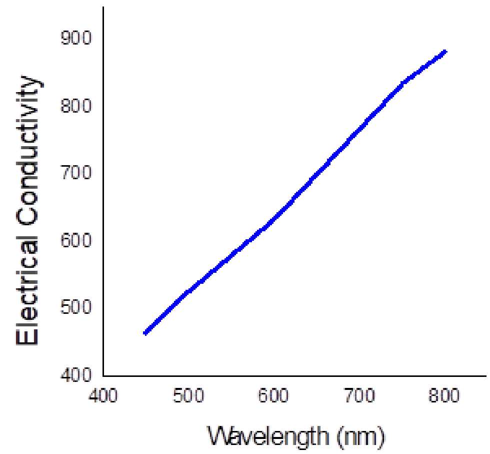

Fig.10. Wavelength versus Electrical Conductivity of Metronidazole

2.7 Electric Susceptibility

The electric susceptibility (χ_c) can be calculated from the following relation [25, 26].

$$\varepsilon_r=\varepsilon_0 + 4\pi\chi_c=\eta^2 - k^2$$

$$\chi_c = \eta^2 - k^2 - \varepsilon_0/4\pi$$

Where ε_0 is the dielectric constant in the absence of any contribution from free carriers. The complex dielectric constant is given by ε_c. The real and imaginary part of dielectric constant from extinction coefficient is given as [27, 28].

$$\varepsilon_c = \varepsilon_r + \varepsilon_i$$

$$\varepsilon_r = n^2 - k^2$$

$$\varepsilon_i = 2nk$$

Where ε_r and ε_i are real and imaginary part of the dielectric constant.

The electric susceptibility is calculated as $\chi_c = 0.4113$. The real ε_r and imaginary ε_i values of dielectric constant are 5.3001 and $7.2662*10^{-6}$.

Table.1. Optical Parameters of Metronidazole

Optical Parameters	**Metronidazole**
Cut- Off Wavelength	380 nm
Band Gap Energy	2.44 eV
Transmittance	95%
Extinction Coefficient	1.5781 X10^{-6}
Refractive Index	2.3022
Reflectance	0.1552
Optical Conductivity	1.8139
Electrical Conductivity	683.82
Electrical Susceptibility	0.4113

2.8 Photoluminescence Spectroscopy

The photoluminescence spectroscopy is a useful technique to reveal the behavior of photo induced electron hole pair and charge recombination process [29]. The emission spectrum was recorded in the wavelength range of 300 to 550 nm using the instrument Varian Cary Eclipse spectrophotometer. The intensity and spectral content of photoluminescence (PL) is a direct measure of various important material properties like band gap determination, impurity levels and defect detection. Emission spectrum gives the luminescence intensity as a function of wavelength, as the exciting radiation is kept constant. Fig 11 shows the emission spectrum of metronidazole crystal. The sample is excited at 300 nm with the excitation energy of 4.1 eV. There are four categories of luminescent peaks in the spectra. The first emission peak is observed at 360nm (3.44 eV), is due to uv radiation. The sharp peak at the wavelength of 380nm (3.26eV) is due to the emission of visible violet. The peak at 490 nm(2.53eV) shows the emission of visible blue and the sharp peak at 525 nm (2.362 eV) is due to the emission of green light. The presence of visible emission bands is because of the presence of the impurity in the crystal. Emission is associated with defects emerging during the growth of crystallites and one related to deformation of crystallinity due to dislocations and vacancies [30]. The result indicates that the grown crystal has emission in the visible region, suggests that the crystal is an excellent material for nonlinear optical applications.

The band gap energy E_g is calculated using the formula $E_g = h\gamma$ where $\gamma = c/\lambda$, λ is the wavelength, C is the velocity of light (3×10^8m/s) and h is plank's constant 6.626×10^{-34}Js.

$$\mathbf{E_g = 1240/\lambda}$$

The calculated band gap energy value for 380nm emission wavelength is observed as 3.26 eV.

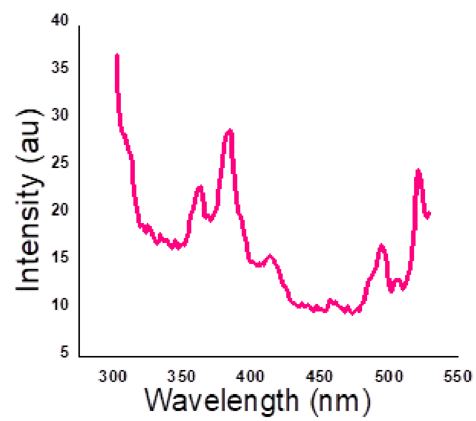

Fig.11. Photoluminescence Emission Spectrum of Metronidazole

III. Conclusion

Single pale yellow block shaped crystal of 1(2-hydroxy ethyl)- 2- methyl-5- nitro imidazole was grown by slow evaporation method. The UV-Visible spectra were recorded and from the spectrum 95% transparency was observed within the range of 425 nm to 800nm. The refractive index, extinction coefficient, reflectance, optical conductivity, electrical conductivity and susceptibility were also calculated. The grown crystal was characterized using Cary eclipse fluorescence spectrophotometer. The crystal exhibits excellent photoluminescence. The photoluminescence spectra reveal uv radiation, visible violet, visible blue and green fluorescence emission. The optical characterization studies and the results show that the drug 1-(2-hydroxyethyl) 2-methyl-5-nitroimidazole (metronidazole) is suitable for optical applications.

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