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# Growth and dielectric studies of Benzimidazole: A novel organic NLO Material

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**ABSTRACT**

*Benzimidazole single crystal was grown by slow evaporation method and confirmed by PXRD. The grown crystal was characterized by powder X-ray diffractometry (PXRD) and UV-Vis-NIR. The dielectric constant and dielectric loss of the crystal was studied as function of frequencies and the results are discussed.*

**Key words** NLO, Benzimidazole, PXRD, UV-NIR and Dielectrics.

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## INTRODUCTION

In recent years nonlinear optical materials are getting attention because of its extensive applications in the area of optical data storage, fibre optic communication and optical signal processing [1-2]. Due to its enormous applications in the above said areas, material scientists are focused their attention for the growth of variety of nonlinear optical materials. In the present study, we have grown the good quality single crystals of benzimidazole (BMZ) by slow evaporation solution growth technique at room temperature as reported by Vijayan et al [3]. The grown crystals were characterized by single crystal XRD, UV-Vis-NIR and dielectric studies.

## MATERIALS AND METHODS

The commercially available benzimidazole was further purified by repeated recrystallization process for three times, using methanol as a solvent. The recrystallized salt was the charge material for the growth of benzimidazole. Recrystallized salt of benzimidazole was dissolved in methanol at saturation temperature 35 °C. A saturated solution of 150 ml was taken and the solution was filtered using a Schleicher & Schuell filter paper (No. 595). The filtered solution was taken in a beaker, which was tightly closed with thick filter paper so that the rate of evaporation could be minimized. Good transparent single crystals were obtained after ten days. The growth procedure already reported by Vijayan et. al [3] was followed as above and good quality single crystal was harvested.

## RESULTS AND DISCUSSION

### 3.1. X-ray diffraction studies

The powder X-ray diffraction studies on the grown benzimidazole was performed using Rigaku diffractrometer (Model: Ultima III, Japan) using $CuK_{\alpha}$ (1.54 Å) radiation. It is observed that the benzimidazole single crystal belongs to orthorhombic crystal system with a space group $P_{21na}$ and unit cell dimensions a = 13.493 Å, b =6.849 Å, c = 6.896(3) Å and α=β=γ=90°: The volume of the system is V = 636.93 $Å^3$. The observed data are in very good agreement with previous determinations and thus the grown crystal is confirmed [4, 5, 6]. The XRD pattern obtained is shown in Fig.1.

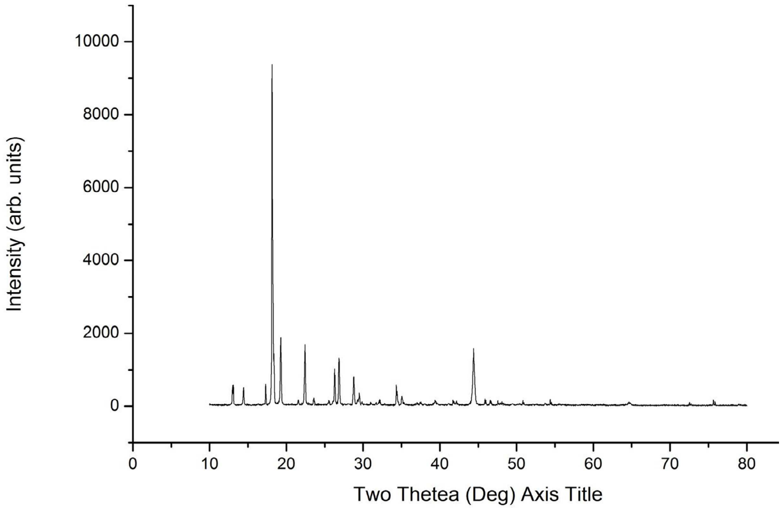


**Fig. 1. XRD Pattern of Benzimidazole**

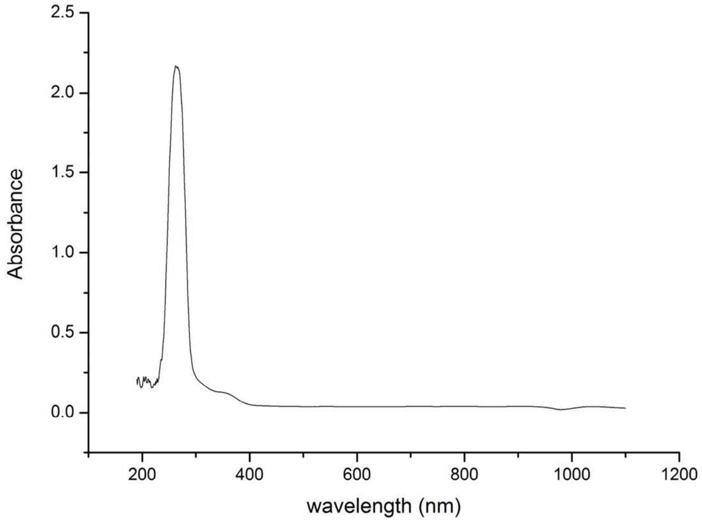


**Fig. 2. Absorbance spectrum of BMZ**

### 3.2 UV-NIR Studies

Optical absorption studies provide an easy method for the investigation of optically induced electronic transitions and furnish ideas about the band structure as well as the energy gap in crystalline and non-crystalline materials [7]. In this work, the optical transmission examined between 190 nm to 1100 nm using Perkin Elmer Make Model

Lambda 35 model UV–Vis, spectrophotometer is used to study the linear properties. The linear absorption and transmittance spectrum of benzimidazole are shown in Fig.2 and 3. It is observed that the absorption is very week in the region between 300 nm and 1100 nm is an advantage as it is the key requirement for materials having NLO properties [5].

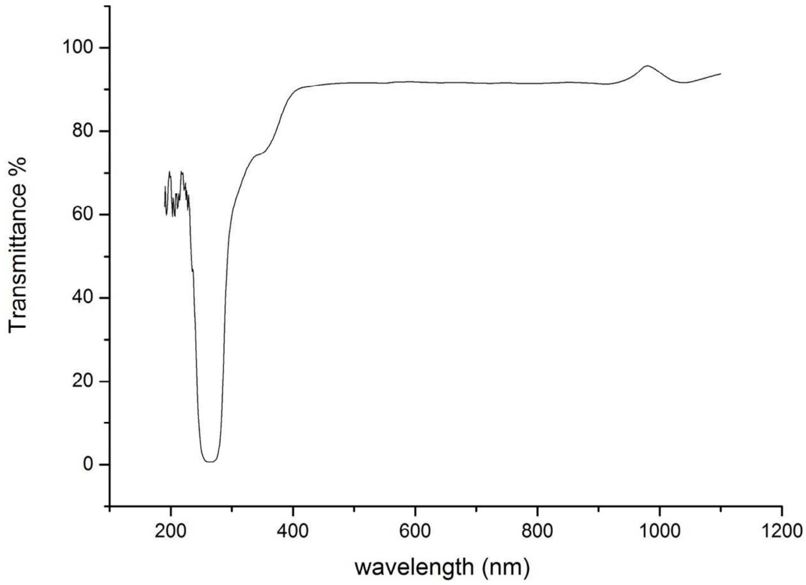


**Fig. 3. Transmittance spectrum of BMZ**

**3.3 Dielectric Studies**

Dielectric properties are correlated with electro-optic property of the crystals [8]. The dielectric constant and the dielectric loss of BMZ sample were measured using 4284A LCR METER in the frequency range of 20 Hz – 1 MHz. The sample was electroded on either side with air-dying silver paste so that it behaves like parallel plate capacitor. The studies were carried out from 318 K to 368 K for frequencies varying from 100 Hz to 1 MHz.

Figs. 4 and 5 show the variations of dielectric constant and dielectric loss with log frequency. At room temperature, both the dielectric constant and dielectric loss decrease with increasing frequency. The high value of dielectric constant is attributed to high ionic conductivity. Most of the solid electrolytes have high dielectric constant [9]. The dielectric constant of a material is composed of four contributions namely, electronic, ionic, orientational and space charge polarizations. All these may be active at low frequencies. In fact, the nature of the variation of dielectric constant with frequency indicates which type of contributions present in the sample.

In BMZ, at 100 Hz, the value of dielectric constant is found to be around 5.45 (318 K). It is also observed that as the temperature increases, the value of dielectric constant also increase to a considerable value (Fig. 6). It is observed from the plot that the dielectric constant decrease exponentially with increasing frequency and then attain almost a constant value in the high frequency region starting from 10 KHz to 1 MHz. The same trend is observed in the case of dielectric loss versus frequency also (Fig. 7). At relatively lower frequency, the higher the temperature, the larger is the dielectric constant. With increasing temperature, a high degree of dispersion in the permittivity begins to occur at lower frequency. This could be again due to the thermally generated charge carriers from the onset of space charge limited to d.c. conduction. It is in fact the space charge effect that leads the dispersion of dielectric constant at low frequencies. The very low value of dielectric constant at higher frequencies is important for extending the material applications towards photonic, electro-optic and NLO devices.

The *ac* conductivity of BMZ increases up on increase in temperature. The electrical conduction in dielectrics is mainly a defect-controlled process in the low- temperature region. It is inferred from Fig. 8 that the electrical conductivity of BMZ is low at low temperature owing to trapping of some carriers at defect sites. At any particular temperature, however, the Gibb's free energy of a crystal is minimal when a certain fraction of ions leaves the normal lattice. As the temperature increases, more and more defects are created, and as a result, the conductivity, which is predominantly due to the movement of defects produced by thermal activation, increases [10].

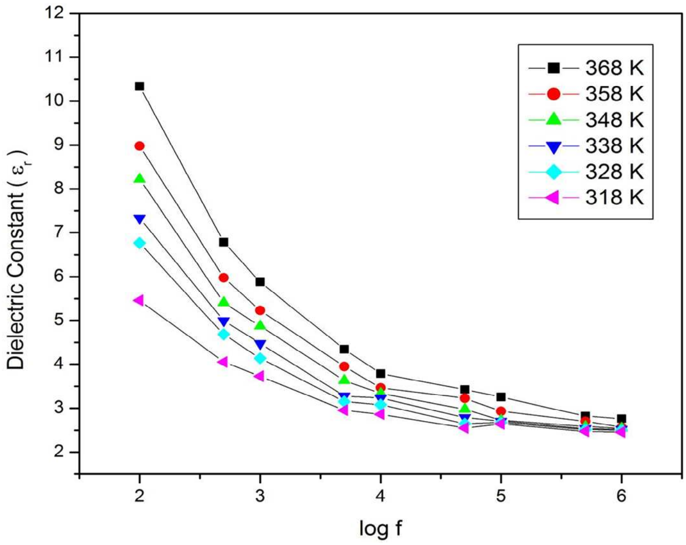


**Fig.4 Variation of dielectric constant with log frequency at different temperatures for BMZ single crystal**

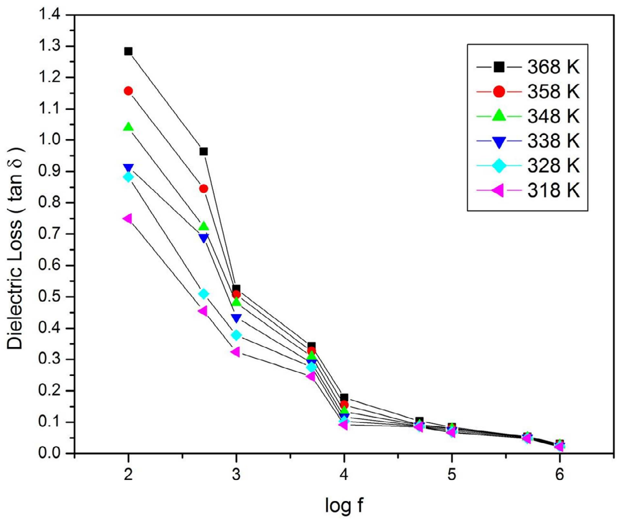


**Fig. 5. Variation of dielectric loss with log frequency at different temperatures for BMZ single crystal**

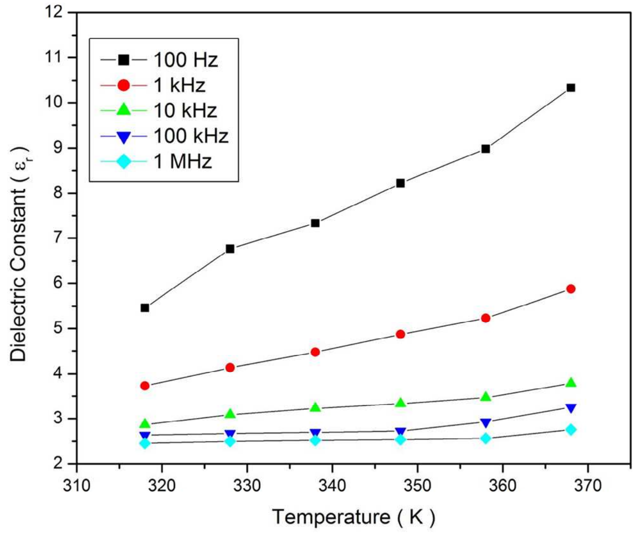


**Fig. 6. Temperature dependence of dielectric constant for BMZ single crystal**

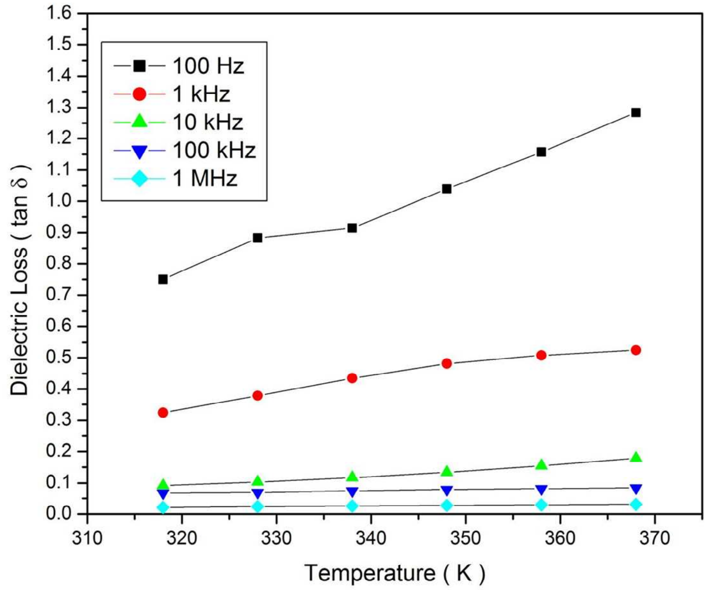


**Fig. 7. Temperature dependence of dielectric loss for BMZ single crystal**

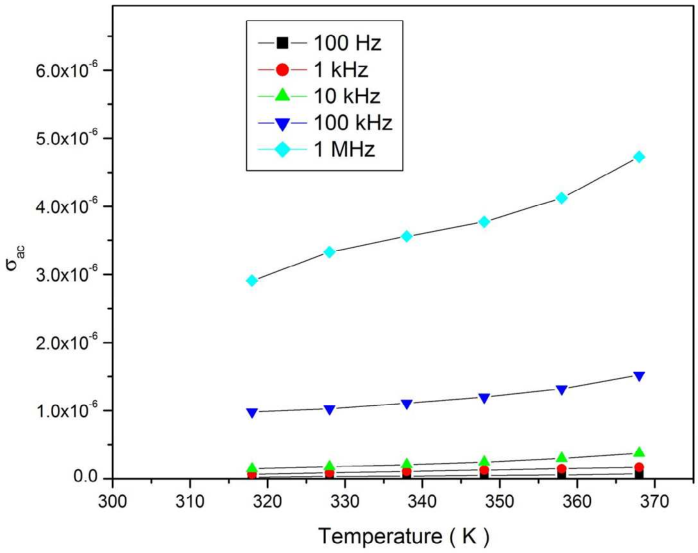


**Fig. 8. The AC electrical conductivities for BMZ crystal**

## CONCLUSION

The good quality single crystal of Benzimidazole was grown by slow evaporation solution growth technique using water as solvent and the grown crystals was confirmed by powder crystal XRD analysis. The UV-Vis-NIR spectra confirm that the crystal is transparent in the entire visible region. The frequency and temperature dependence of the dielectric constant / dielectric loss of BMZ are investigated. Based on these observations we can say that BMZ can be a promising novel NLO material, which can be possibly used for photonic application.

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