

SPECTRAL AND DIELECTRIC PROPERTIES OF TRIGLYCINE BARIUM DICHLORIDE DIHYDRATE NLO SINGLE CRYSTAL

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Abstract. Single crystals of Triglycine barium dichloride dihydrate were grown by slow evaporation technique. The unit cell dimensions and space group of the grown crystals were confirmed by single crystal X-ray diffraction. The functional groups present in the structure of the grown crystal are identified by using FTIR spectral analysis. The microhardness study shows that the Vickers hardness number of the crystal increases with the increase in applied load. Dielectric constant and dielectric loss measurements were carried out for different temperatures and frequencies.

1. Introduction

In the modern world, the development of science in many areas has been achieved through the growth of single crystals. Large sized single crystals are essential for device fabrication and efforts are taken to grow large single crystals in short duration with less cost. Over the past two decades much attention has been paid to the search of novel high quality NLO materials that can generate high second order optical nonlinearities which is important for potential applications including telecommunication, optical computing, and optical data storage and processing [1-6]. The present investigation deals with the growth of Triglycine barium dichloride dihydrate single crystal by slow solvent evaporation technique and the characterization of the grown crystal. The grown crystals were characterized by single crystal and powder X-ray analysis, FTIR and UV spectral analysis, microhardness, dielectric, and SHG measurements. The results of these studies have been discussed.

2. Experimental procedure

Triglycine barium dichloride dihydrate crystal was synthesized by dissolving glycine and barium dichloride dihydrate in the stoichiometric ratio (3:1) in double distilled water. The synthesized salt was purified by successive recrystallization process. Supersaturated solution of Triglycine barium dichloride dihydrate was prepared and filtered. The filtered solution was kept in a beaker covered with porous papers and kept in a dust-free atmosphere. After a period of 24 days, colorless and transparent crystals were obtained.

3. Characterizations

The characterization studies includes single XRD and powder XRD analysis, UV and FTIR spectral analyses, mechanical and dielectric studies of the grown crystals. The grown crystal

COO⁻ group showed the zwitter ionic nature of the glycine molecule in Triglycine barium dichloride dihydrate crystal. FTIR spectral analysis thus identifies the presence of functional group in the grown material Triglycine barium dichloride dihydrate.

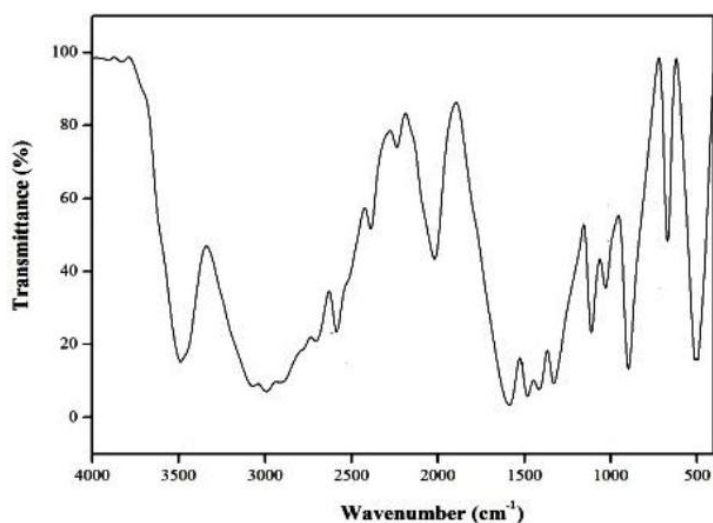


Fig. 2. FTIR spectrum of Triglycine barium dichloride dihydrate single crystal.

3.4. UV-visible spectral analysis. To determine the transmission range and hence to know the suitability of Triglycine barium dichloride dihydrate single crystals for optical applications, the UV-vis spectrum was recorded in the range of 200–1000 nm as shown in Fig. 3. The lower cut off of the Triglycine barium dichloride dihydrate crystal is at 310 nm and the range of transparency in UV and visible region makes it a very potential material for blue light emission. Hence, the material can be used for second harmonic generation (SHG) applications, using the powerful light source of wavelength below 600 nm.

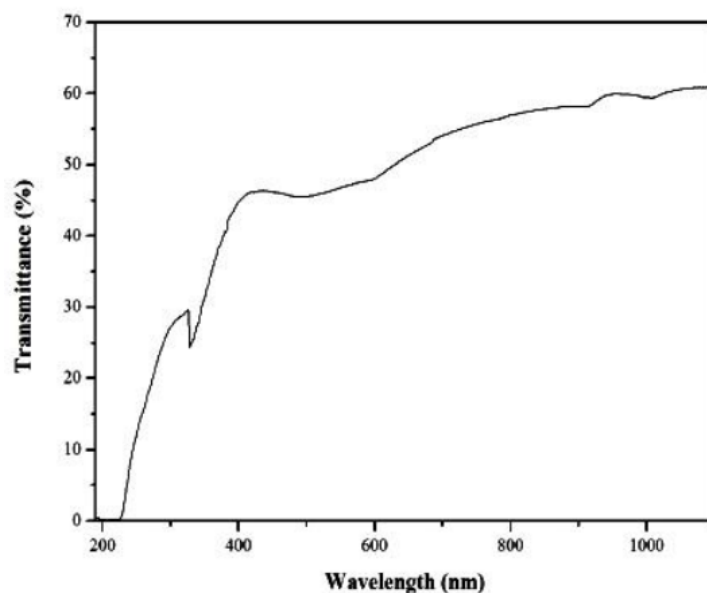


Fig. 3. UV-vis transmittance spectrum.

3.5. NLO studies. The SHG conversion efficiency of Triglycine barium dichloride dihydrate was determined by the modified version of the powder technique developed by Kurtz and Perry. The crystal was ground into powder and densely packed in a micro capillary

dielectric loss is also studied as a function of frequency at different temperatures (Fig. 7). It is observed that the dielectric constant, dielectric loss values are found to decrease with the increase in frequency at all temperatures. The high value of dielectric constant at low frequency may be due to presence of all polarizations and its low value at higher frequencies may be due to the significant loss of all polarizations gradually [8].

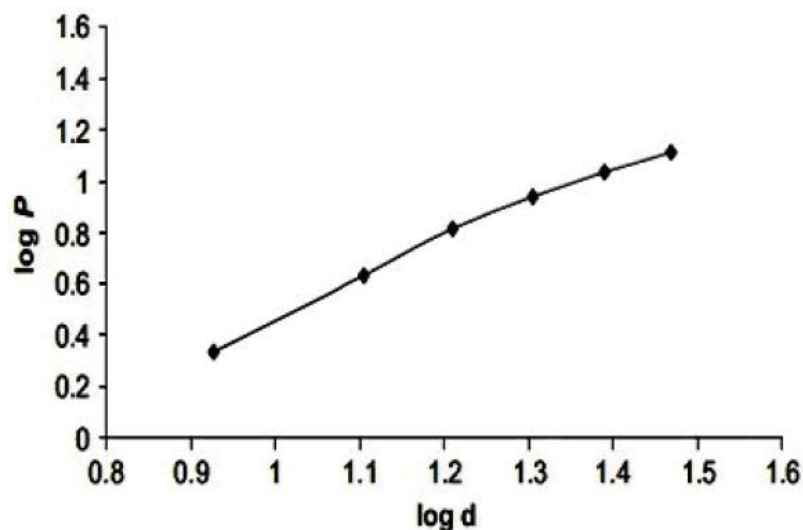


Fig. 5. Plot of log d versus log p.

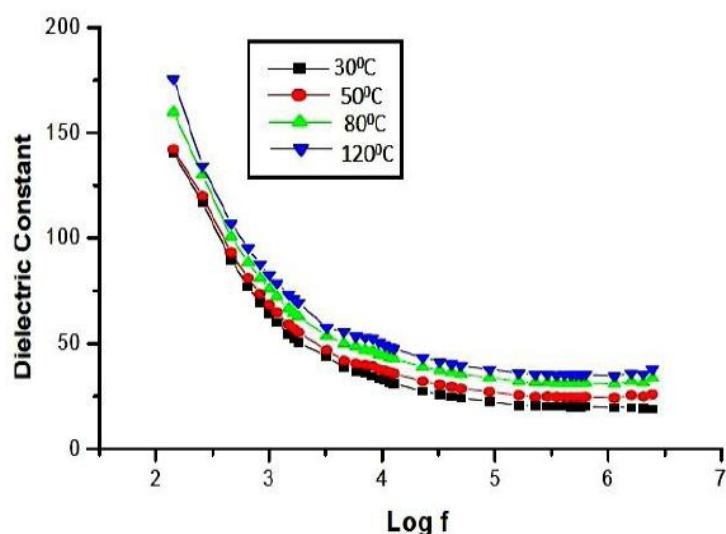


Fig. 6. Dielectric constant vs Log f.

In accordance with Miller rule, the lower value of dielectric constant is a suitable parameter for the enhancement of SHG efficiency. The variation of dielectric constant with temperature is generally attributed to the crystal expansion, the electronic and ionic polarizations and the presence of impurities and crystal defects [9]. The observed lower values of dielectric loss at higher frequencies for this sample suggest that the grown crystal contains less number of defects with high optical quality [10].

4. Conclusions

Single crystals of Triglycine barium dichloride dihydrate were grown by slow evaporation technique. The unit cell dimensions of the grown crystals were confirmed by single crystal X-ray diffraction. Functional groups present in the material have been confirmed by FTIR

analysis. UV-visible transmission spectrum shows excellent transmission in the entire visible region. NLO study reveals that the grown crystal has SHG efficiency equal to that of KDP crystal. Mechanical studies were carried out for the grown crystal. Dielectric constant and dielectric loss measurements were carried out at different temperatures and frequencies. The material exhibits NLO behaviour remarkably due to its better optical and dielectric properties.

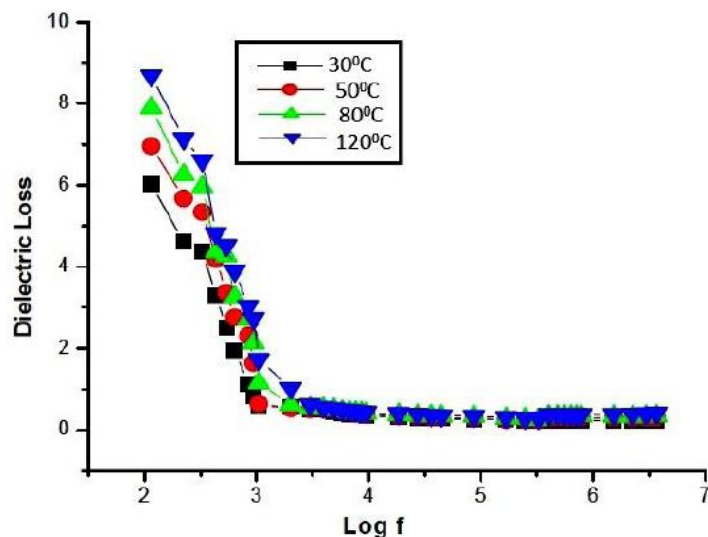


Fig. 7. Dielectric loss vs Log f.

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References

- [1] M.D. Aggarwal, J.J. Stephens // *Optoelectron. Adv. Mater.* **5** (2003) 3.
- [2] C. Razzetti, M. Ardoino, C. Paorici // *Cryst. Res. Technol.* **37** (2002) 456.
- [3] J. McArdle, J.N. Sherwood, A.C. Damask // *J. Cryst. Growth* **22** (1974) 193.
- [4] E.M. Hampton, B.S. Shah, N. Sherwood // *J. Cryst. Growth* **22** (1974) 22.
- [5] S. Dhaushkodi, K. Vasantha // *Cryst. Res. Technol.* **39** (2004) 3.
- [6] H.L. Shat // *Bull. Mater. Sci.* **17** (1994) 1233.
- [7] A. Ruby, S. Alfred Cecil Raj // *World Journal of Science and Technology* **3** (2013) 11.
- [8] C.P. Smyth, *Dielectric Behaviour and Structure* (McGraw-Hill, New York, 1965).
- [9] M. Priya, C.K. Mahadevan // *Cryst. Res. Technol.* **44** (2009) 92.
- [10] C. Balarew, R.J. Duhlew // *Solid State Chem.* **55** (1984) 1.