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Growth, Optical Studies of Meta-Nitro Aniline NLO Organic Crystal

Shobha Kulshrestha

School of studies in physics, Jiwaji University Gwalior-474011(INDIA)
E-mail: shobha011986@gmail.com

Abstract: *The single crystal of Meta nitro aniline (MNA) an organic nonlinear optical (NLO) was grown by slow solvent evaporation technique at 30-40°c temperature, acetone was used as a solvent. A good yellow –reddish colour crystal of MNA was obtained in duration of 2 weeks. The grown crystal was subjected to different characterization such as single crystal X-ray diffraction, Fourier transform infrared spectroscopy, UV-visible spectroscopy, hardness study. The grown crystal was characterized by XRD analysis, which shows that crystal was perfectly crystalline in nature and belongs to orthorhombic structure. The lattice parameters are a=6.47Å, b=19.33Å c=5.08Å. FTIR spectrum was recorded using spectrophotometer by KBr pellet technique in the region 4000-500 cm-1. This study was recorded to confirm the functional groups of respected compound. UV-visible spectrum was recorded by UV spectrophotometer in the rang 200-900 nm. UV visible transmittance studies show that the grown crystal s have wide optical transparency in the entire visible region, the cut-off wavelength is occur at 258 nm. The optical energy band gap is found to be 4.1 eV.*

Keywords: *Nonlinear optical crystal, solution growth technique, X-ray diffraction, FTIR Spectroscopy, UV Spectroscopy.*

1. INTRODUCTION

Materials with large second order optical nonlinearities find wide applications in the field of laser technology, laser communication, data storage technology and optoelectronic technology [1-3].Organic materials are emerging as an alternative to inorganic materials because of their low cost, ease to fabrication. The organic materials posses' high optical damage thresholds comparable to inorganic materials. Meta nitro aniline is favourable material for NLO application[4-7]. The molecular formula of MNA (Meta nitro aniline) has $C_6H_6N_2O_2$ and its melting point is 112°c. MNA crystals have a very large nonlinear susceptibility, which are in many cases several orders of magnitude higher than that of inorganic crystals. In present paper, we report the conditions for the growth of good quality single crystal of MNA by slow evaporation method using acetone as a solvent. The grown single crystal was subjected to characterization techniques like X-ray, FTIR Spectroscopy, and UV-Spectroscopy.

2. EXPERIMENTAL

The organic material MNA was growing by constant bath temperature method. Homogeneous solution was prepared by dissolving 10 gm of MNA in 30 gm acetone as a solvent. A saturated solution was prepared at a temperature 40°c. The solution was filtered using filter paper. The filtered solution was taken in a beaker which was sealed to avoid the evaporation of the solvent. A good yellow-reddish colour crystal of MNA was obtained in duration of time 2 weeks. As show in Fig. (1).

3. RESULTS AND DISCUSSIONS

3.1 X-ray Diffraction Analysis

The single crystal X-ray diffraction has been carried out from at RR-CAT Indore; copper K_α radiation of wavelength 1.54Å was used in all the diffraction studies. The sample was scanned over the range 0 to 60° at a scan rate of 1°/ min. The peaks were indexed by comparing the XRD data with the standard data given in the literature. It was found that crystal was perfectly crystalline in nature. It is observed that the MNA single crystals belongs to orthorhombic system with (110) orientation and unit cell dimensions were observed to be a=6.47Å, b=19.33Å, c=5.08Å [8-9]. As show in Fig. (2).

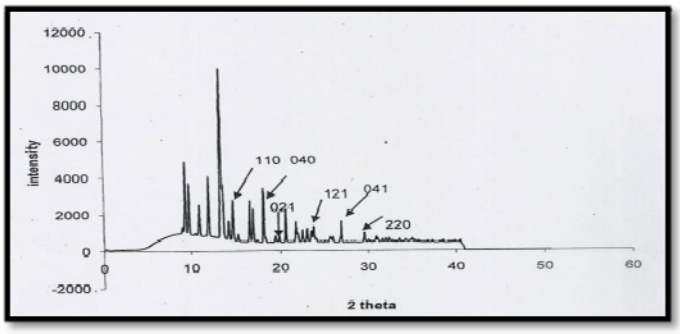

Fig. 2: XRD of MNA crystal

Table 1: Lattice Parameter of MNA Crystal

Theoretical values (Å)	a=6.48	b=19.23	c=5.06
Experimental values (Å)	a=6.45	b=19.33	c=5.08

Table 2. Wave number assignment for MNA crystal3.2 FTIR Spectroscopy

Wave number cm-1	Assignment
3211,3202	Symmetric stretching of NH2
3434,3429	Asymmetric stretching oh NH2
2297 to 2262	Sym. And asym. Stretch of C-H
1624,1622	C=O carbonyl group
1768,1740	C=N Stretching
1522,1520	NO2 Vibration
984 to 928	Presence of benzene ring in MNA

FTIR spectrum was recorded using spectrophotometer by KBr pellet technique in the region 4000-500 cm^{-1}. For the organic molecule, the FTIR region has been divided into fractional group and fingerprint region. The fingerprint region is those lying between 1340 to 900 cm^{-1}, whereas fractional group region extends from 4000 to 1300 cm^{-1}. From the spectrum shows the asymmetric and symmetric stretching modes of free NH_2 group, which are observed at 3434 & 3211 cm^{-1}. The peaks at 2297 to 2662 cm^{-1} indicates asymmetric and symmetric stretching in C-H bond, peak at 2283 cm^{-1} Indicated C=N stretching[10-11].

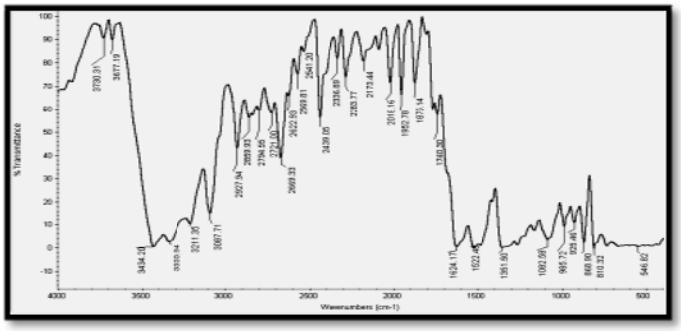

Fig. 3: FTIR spectrum of MNA crystal

The peak 1624 cm^{-1} show the C=O carbonyl groinup in the compound. The peak that appears at 1522 cm^{-1} due to vibration of NO_2 stretching modes was not much broad. The vibration at the peak 984 cm^{-1} indicated the presence of the benzene ring in the MNA molecule. The peaks 868 cm-1 show the meta position of the substituted molecules in the benzene ring of MNA.As show in Fig. (3).

3.3 UV-Spectroscopy

The UV-visible spectrum of MNA was recorded using shimadzu UV spectrophotometer in the range 200-900 nm. The crystal shows good optical transmittance up to 14% in the entire region. It shows lower cut off at 258 nm[12-13]. This reveals that in the grown crystal the absorption is almost absent in the visible region due to its high transparency. The band gap of MNA crystal is 4.1 eV. As show in Fig. s4(a,b).

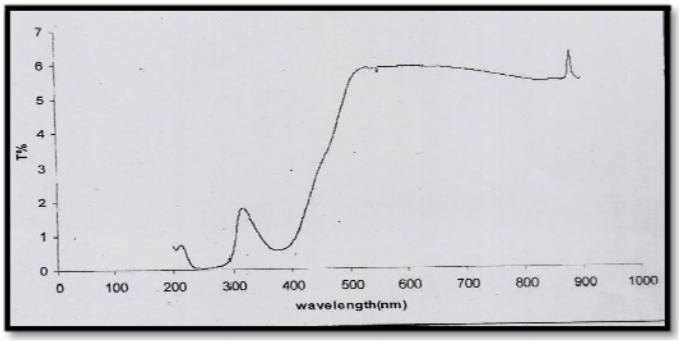

Fig. 4(a): Absorption of MNA crystal

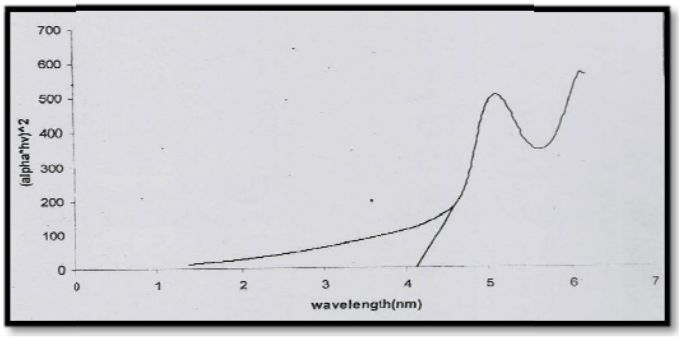

Fig. 4(b): Band gap of MNA crystal

4. MICROHARDNESS STUDIES

Hardness is one of the important mechanical properties of solid material. Microhardness analysis was carried out using Vickers Microhardness tester fitted with a diamond indenter. The selected smooth surfaces of the crystal were subjected to Vickers static indentation test at room temperature by applying loads ranging from 25-100 gm. The Vickers harness Hv was Calculated using the relation $Hv = 1.8544\ (1/d^2)\ kg/mm^2$, where P is the applied load and'd' is the diagonal length of the indentation impression. It is clear that the micro hardness number d creases with increases of load[14].

5. CONCLUSION

Single crystals of MNA, a non linear optical material has been grown in solution growth technique. It is clear that the crystals are needle like and transparent. The lattice parameters were found by single crystal X-ray diffraction technique. The FTIR spectrum reveals that the functional groups of the grown crystal. Good optical transmittance in the visible region. The band gap MNA is 4.1 of the eV. Mechanical property grown crystal has been studied by micro hardness test and noticed that there is an increase of micro hardness number.

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