



XRD, AFM, MASS SPECTRAL, CHNS, INFLUX, BEAM DISPLACEMENT OF DIETHYL 3, 3'- [(2, 4-DICHLOROPHENYL) METHYLIDENE] BIS (1H-INDOLE-2-CARBOXYLATE) CRYSTALS

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ABSTRACT

Crystalline materials have wide range of applications proportionally with isotropic materials. Here Diethyl 3,3'-[(2,4-Dichlorophenyl) Methylidene] Bis (1h-Indole-2-Carboxylate) Crystals have opto- electronic and frequency response applications and wide range of X ray analysis utility. The XRD data discloses that entitled Crystals have Chemical formula as $C_{29}H_{24}Cl_2N_2O_4$ and Crystal system is Monoclinic, Space group is $P2_1/c$ and parameters are a , b , c in (Å) as 9.778, 15.938, 17.583 and β is 101.94. The XRFL, Mass spectral data and CHNSO analysis, AFM refers the elemental analysis for the titled specimen, the influx and beam displacements are for the nature of the crystal specifications.

KEY WORDS

XRD, Mass spectral studies, CHNSO, Influx and beam displacement

1 INTRODUCTION

Crystalline materials are solid materials [1-5, 11] which have many appliances especially in industrial and medical purposes. Here, Diethyl 3,3'-[(2,4-Dichlorophenyl) Methylidene] Bis (1h-Indole-2-Carboxylate) Crystals^[11] are subjected to XRD, Mass spectral studies, CHNSO, Influx and beam displacement for filter applications....

2 SCOPE OF THE CRYSTAL

Diethyl 3,3'-[(2,4-Dichlorophenyl) Methylidene] Bis (1h-Indole-2-Carboxylate) Crystals have high NLO coefficient and high level of threshold in laser applications [12-16] and also have antibacterial activities and have cell line

representation in bio fields. So it is so chosen to grow and study the properties.

3 CHARACTERISATIONS:

The grown crystals [6-10] are subjected to XRD, XRFL, AFM, Mass spectral, CHNSO studies and influx and beam displacement (for filter applications) and they are confirmed with material grown by elemental analysis and material with crystal parameters and molecular mass and emission and angular and beam displacement by above specified methodologies.

3.1 XRD Crystal data

The XRD data [12] discloses the crystal parameters such as

Chemical formula	$C_{29}H_{24}Cl_2N_2O_4$
Crystal system, Space group	Monoclinic, $P2_1/c$
a, b, c (Å)	9.778 , 15.938, 17.583
β	101.94°
α, γ	90°

3.2 MASS SPECTRAL DATA AND CHNS DATA AND AFM

The XRFL and mass data confirms the elemental and molecular weight subjected to the diethyl 3,3'-[(2,4-dichlorophenyl)methylidene]bis(1*H*-indole-2-carboxylate) crystals and the peaks of XRFL identified the formation by elements and mass spectral data specifies the molecular weight of the titled specimen as shown in Fig.1 and found to be 534 by spectrum and 534.111 by

experimental calculations and 534.19 by CHNS analysis as shown in Table 1. The atomic force microscope (AFM) is one of the types of scanning probe microscopes used to quantify the height, friction, magnetism, with a probe. Fig.2 and Table 3 gives the porch idea of AFM of the specimen. The AFM the deviation is less and has no major flaws as well as it shows some gaps are there while nucleation in the crystals.

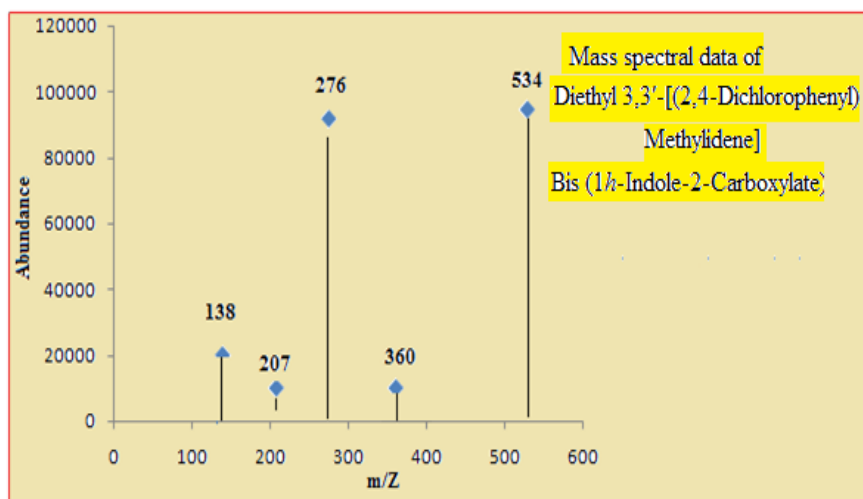


Fig.1 Mass spectra of diethyl 3,3'-[(2,4-dichlorophenyl)methylidene]bis(1*H*-indole-2-carboxylate) crystals

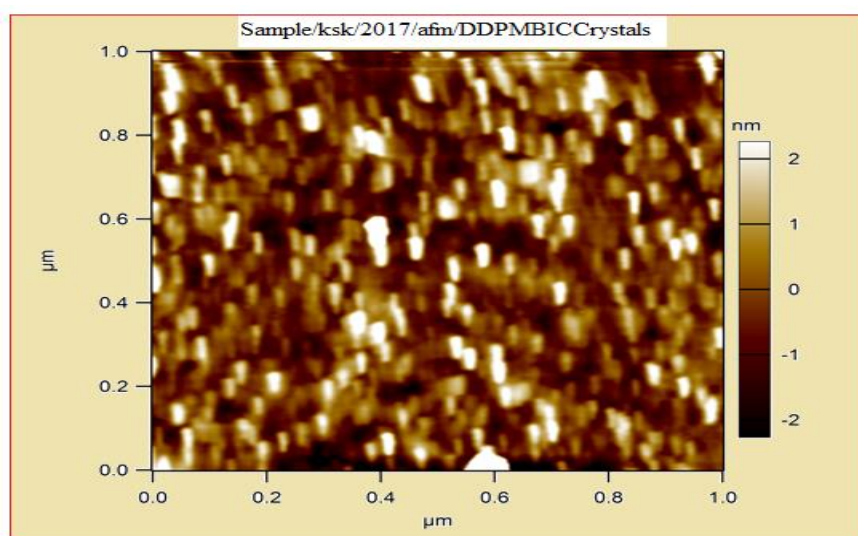


Fig.2 AFM of diethyl 3,3'-[(2,4-dichlorophenyl)methylidene]bis(1*H*-indole-2-carboxylate) crystals

3.3 BEAM DISPLACEMENT AND INFLUX MEASUREMENT

When used for filters the sample grown is with CWL of 1000nm and FWHM of 110 nm (less than 12%) and for 0 – 60° variations, with thickness of 20 mm Accuracy

within $\pm 1\text{nm}$, the following Table 2 gives the beam displacement parameters for LWP and SWP. Crystalline influx measurement specifies that 2.7668 micron for which NLO utility is predominant.

Table.1. Elemental representation of diethyl 3,3'-[(2,4-dichlorophenyl) methylidene] bis(1H-indole-2-carboxylate) crystals by theoretical calculations and by CHNSO analysis

Elements	% by calculations	% by CHNSO Analysis
C	65.08	65.01
H	4.48	4.49
N	5.23	5.25
Cl	13.25	ND
O	11.96	11.97
Total: 534.19	100.00	86.72

ND as Not Detected

Table.2. Beam displacement of diethyl 3,3'-[(2,4-dichlorophenyl) methylidene] bis(1H-indole-2-carboxylate) crystals by filter method for LWP and SWP

Pulse level / Plate level	AOI (°)	Beam displacement (mm)
LWP	426.23	1.1819
SWP	-39.05	-0.517
Compensation plate (2.0mm)	-6.02	-0.665

As the displacement is a vector, the negative sign indicates that it is in opposite direction.

Table.3 AFM of diethyl 3,3'-[(2,4-dichlorophenyl) methylidene] bis(1H-indole-2-carboxylate) crystals Roughness Data:

Sample name: ksk_1/2017	
PARAMETERS	FULL IMAGE VALUES
Number of points	65536
Standard Deviation	1.126 nm
Max	13.016 nm
Min	-3.919 nm
RMS	1.126 nm
Average deviation	791.394 pm
Skew	2.72
Kurtosis	22
Surface Area	1 sq micrometer
Area %	0.5207%

4 RESULTS AND DISCUSSIONS

The monoclinic crystals of diethyl 3,3'-[(2,4-dichlorophenyl) methylidene] bis(1H-indole-2-carboxylate) is put in ordered by slow evaporation solution growth method and Colorless crystals of the title compound by slow evaporation. In the title compound of $\text{C}_{29}\text{H}_{24}\text{Cl}_2\text{N}_2\text{O}_4$, the XRD data discloses that diethyl 3,3'-[(2,4-dichlorophenyl) methylidene] bis (1H-indole-2-

carboxylate) is $P2_1/c$ group and lattice parameters and from beam displacement as 1.1819 and -0.517 mm which is suitable for X-ray analysis were obtained in highest yield respectively, CHNSO and mass spectral data reveals the molecular weight of the enlisted material and confirmed by theoretical calculations, the influx is 2.7668 microns which is suitable for NLO

applications. AFM analysis gives the roughness and has no major flaws.

5 CONCLUSIONS

Diethyl 3,3'-[(2,4-dichlorophenyl) methylenedibis(1*H*-indole-2-carboxylate)] crystals are grown by slow evaporation method and here the grown material is subjected to XRD and Mass spectral study, CHNSO, AFM, influx and beam displacement study respectively and from this, it is well known that the entitled crystal can be used for X-ray analysis with high yield and wide range of NLO applications especially device fabrication, and in electronic filters.

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