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Archives of Applied Science Research, 2013, 5 (3):100-103
(http://scholarsresearchlibrary.com/archive.html)

ISSN 0975-508X
CODEN (USA) AASRC9

Spectroscopic (IR & Raman) studies of picolinium maleate (pm) single crystals

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ABSTRACT

Picolinium Maleate is an organic NLO material, synthesised by slow evaporation technique. The studies such as IR, Raman have been taken and analysed and reported.

Key words: PM, IR, Raman.

INTRODUCTION

In recent years organic NLO plays a vital role in Photonics, Opto - electronics, Spectroscopy....Organic materials have elevated electronic susceptibility and molecular polarizability compared with the inorganic materials [1, 2, and 3].

The reaction mechanism is as follows

$$HOOC\text{-}C\text{-}(CH)_4 - N + HOOCCHCHCOOH \longrightarrow$$

$$HOOC\text{-}C\text{-}(CH)_4 - NH^+ . HOOCCHCHCOO^-$$

The crystal diagram is shown in fig.1.

The crystallographic data and parameters ... are given in Table1.

Table1.Crystallographic data of PM single crystals

CRYSTAL DATA	
REPRESENTATION	PM
Empirical formula	$C_{10}H_9NO_6$
Molecular weight	239.18
Crystal system	Monoclinic
Space group	$P2_1/c$
Lattice parameters	a=14.649Å,b=10.3978Å,c=6.9076Å α= 90°, β=100°, γ =90°
Volume	1052.14 $Å^3$

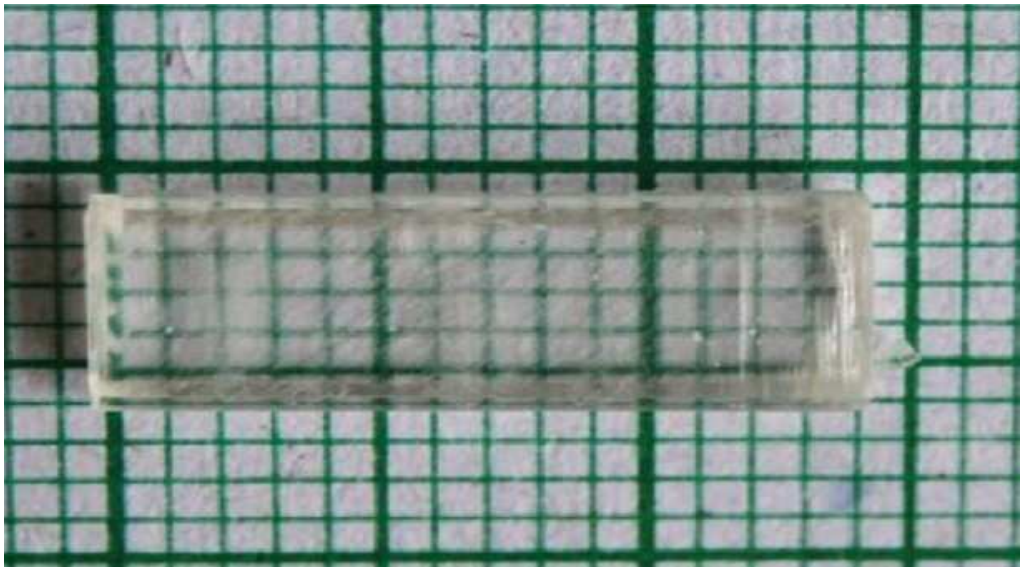

Fig.1.Crystal Diagram of PM single crystals

RAMAN SPECTRAL STUDY

Raman spectrum represents the polarizability of the molecule. Here for PM crystal the Raman wave numbers are 3102 cm^{-1},3033.24 cm^{-1}, 3066.16 cm^{-1},2816.18 cm^{-1},1668.30 cm^{-1}, 1729.01 cm^{-1},

1622.97 cm^{-1},1594.91 cm^{-1},1330.02 cm^{-1},1160 cm^{-1},860.49 cm^{-1},837.12 cm^{-1},191.50 cm^{-1} respectively.

The spectrum is given in fig.2 and the assignments, wave number interpretation are given in Table 2.

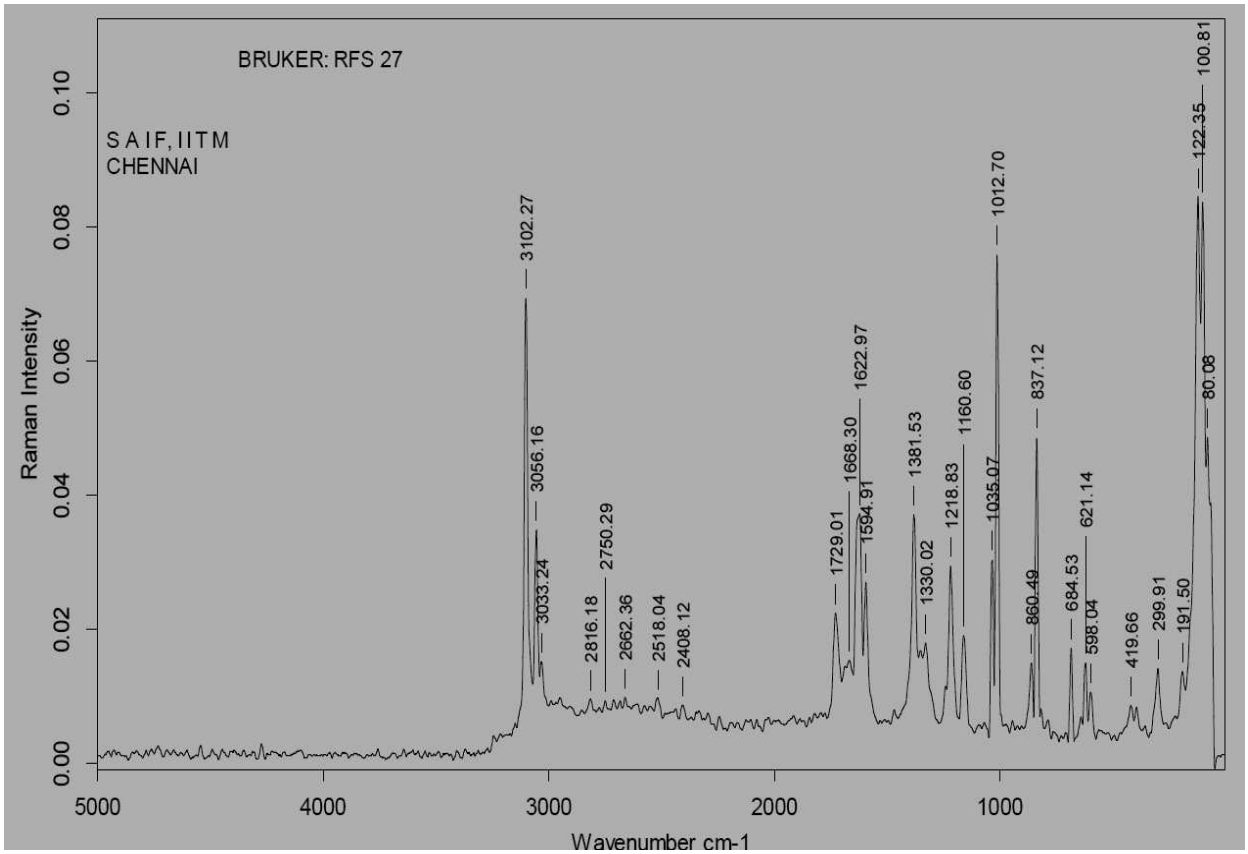

Fig.2. Raman spectrum of PM crystals

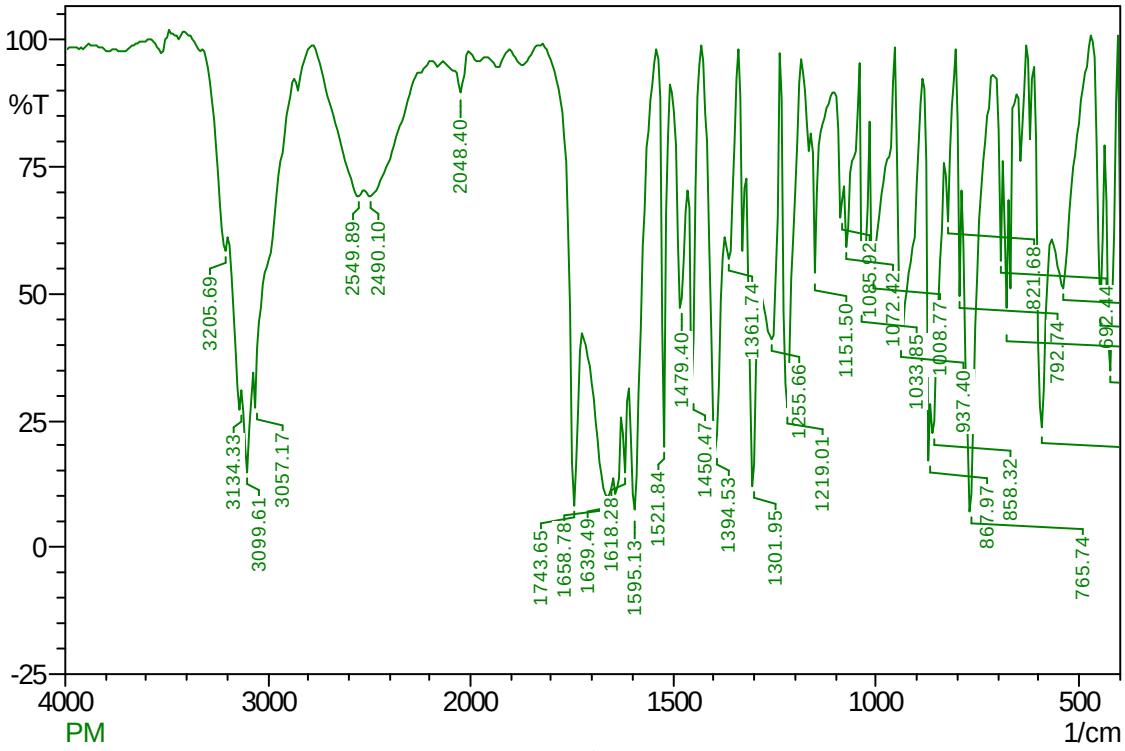

Fig 3. IR spectrum of PM crystal

Table 2. Raman spectrum data of PM crystals

WAVE NUMBER in cm^{-1}	VIBRATIONAL MODES	TYPE
3102 cm^{-1}	υ (O-H) 3100 - 3650 cm^{-1}	weak - strong
3033.24, 3066.16 cm^{-1}	υ (=(C-H)) 3000 - 3100 cm^{-1}	strong medium
2816.18 cm^{-1}	υ (C−H) 2800 - 3000 cm^{-1}	strong
1668.30, 1729.01 cm^{-1}	υ (C=O) 1680 - 1820 cm^{-1}	medium strong
1622.97cm^{-1}	υ (C=N) 1610 - 1680 cm^{-1}	strong medium
1594.91cm^{-1}	υ (C-(NO2)) asym 1530 - 1590 cm^{-1}	medium strong
1330.02cm^{-1}	υ (C-(NO2)) 1340 - 1380 cm^{-1}	strong medium
1160 cm^{-1}	υ (C-O-C) asym 1060 - 1150 cm^{-1}	weak strong
860.49 cm^{-1}	δ(C-H) 845 -900 cm^{-1}	Bending strong weak
837.12 cm^{-1}	υ (C-O-C) 800 -970 cm^{-1}	medium weak
191.50 cm^{-1}	Vibrations in crystals, LA modes 10 - 200 cm^{-1}	strong

Table 3 IR spectrum data of PM crystals

WAVE NUMBER (cm^{-1})	ASSIGNMENTS
1743.65	C = O Stretching
1639.49	C = C Stretching by Maleic acid
1595.13,1521.84,1479.40,1450.47	Pyridine ring vibrations
1219.01,1151.50,1085.92,1033.85,1008.77	COO^- Stretching
867.97,765.74	C – H Bending vibrations
2549.89,2048.40	Overtone / Combination modes of COO^- group

IR STUDY

The IR study of the PM crystal shown in fig 3 and interpretation of IR data is in Table 3. The assignments are 1743.65, 1639.49, 1595.13, 1521.84, 1479.40, 1450.47, 1219.01, 1151.50, 1085.92, 1033.85, 1008.77, 867.97, 765.74, 2549.89, 2048.40 cm^{-1} respectively [4].

CONCLUSION

Thus the Raman and IR studies of PM crystals have been studied and reported. Raman data related to polarizability where as IR gives the composition of the elements in the compound and it refers change in dipole moment.

Acknowledgement

The authors would like to thank SAIF IITM for studies / characterisation.

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