NANJIL CATHOLIC COLLEGE OF ARTS AND SCIENCE

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FOURTH NATIONAL CONFERENCE ON ADVANCED MATERIALS

(NCAM-2022)

March 26, 2022

Certificate

This is to certify that ~~Mr./Ms.~~/Dr. JEBIN R.P, ASSISTANT PROFESSOR, Muslim Arts College, Thiruvithancode. has attended the Fourth National Conference on Advanced Materials (NCAM-2022) organized by the Department of Physics, Nanjil Catholic College of Arts and Science, Kaliyakkavilai on March 26, 2022 ~~and presented a paper (Poster/Oral)~~ entitled Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde Single Crystals for NLO applications

Rev. Fr. Dr. M. Eckermens Michael
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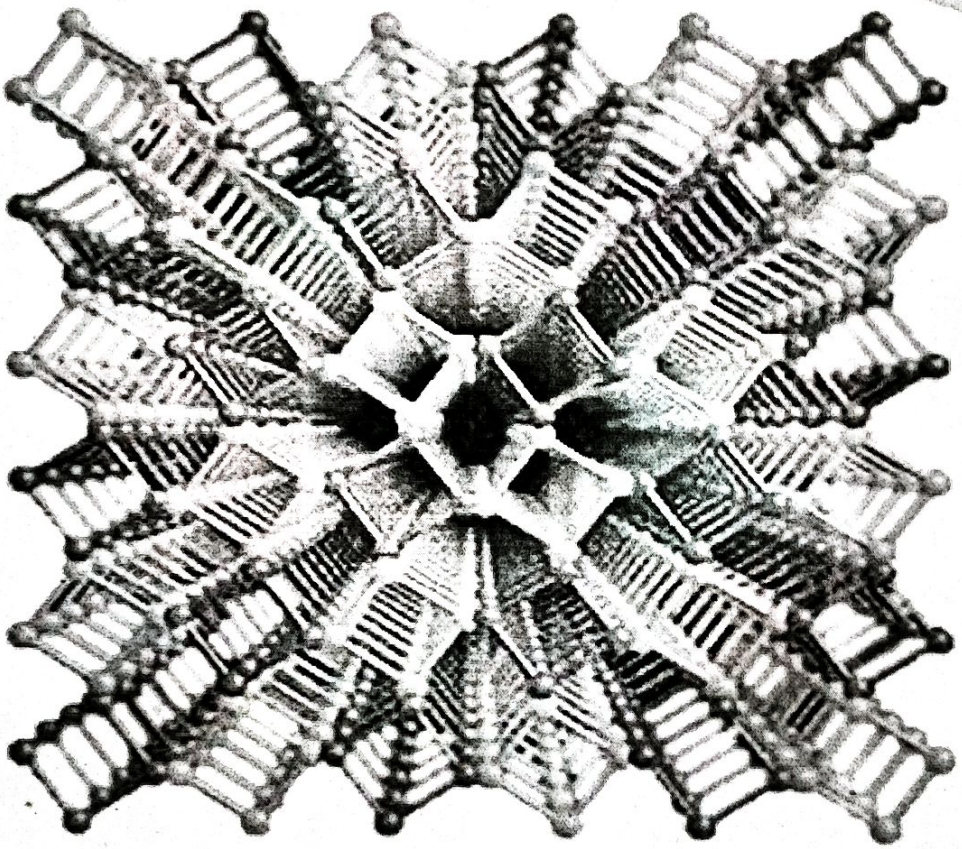
Principal

Fourth National Conference on ADVANCED MATERIALS (NCAM- 2022)



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14. Vibrational spectroscopic characterization, DFT studies and structural investigations of N-(2- Hydroxybenzylidene)-2-Iodoaniline (**D.Jayareshmi[1,*]**, D.Aruldhas[2,*])

15. Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde single crystals for NLO applications (**R.P. Jebin[a]** and T. Suthan[b])

16. Vibrational spectral investigation, DFT computational studies and charge transfer interactions analysis of l-lysine monohydrate (**T. Brintha[1]**, J. Jeni James[2], P.J. Jegan Babu[3], M. Amalanathan[4])

17. Structural, computational, C-H…O/N-H…O hydrogen bonding, homo-lumo, mesp and nbo analysis of n-2(hydroxy phenyl) acetamide (**M.Jini pramila[1]**, **D.Arul Dhas[2,*]**)

18. Single crystal growth and optical properties of glutaric acid doped potassium hydrogen phthalate single crystals (**A. Rathika[a]**, R.Ganapathi Raman[*])

19. Effect of metal doping on the properties of SnO_2 nanoparticles (**T.Regin Das[1, 2]**, M. Meena[3,*])

20. Periodic variations of sunspot activities in 24th solar maximum (**Mariya Shaniya.S[1*]**, Iren Sobia.A[2])

21. Synthesis and optical characterization of creatinium 5- sulfosalicylate (**S.S.Sherlin[a]** , C.Christal Vasanthi [b*], S.Sindhusha[b])

22. Theoretical and spectroscopic studies of orotic acid (**S.Sijana[1]**, M. Amalanathan[2])

23. Crystal growth, XRD and vibrational studies of piperazine p-nitrophenol (ppn) single crystals (**R.Suja[a]**, A.Rathika*)

24. Structural characterization of Zn and Fe doped aluminium oxide nanoparticles prepared by co-precipitation method (**R.Winston[(1)]**, T.R Jeena[(2)])

25. Synthesis and Characterization of Cu-Doped ZnSe Nanoparticles for Photocatalytic Activity (**V.Beena[1]**, S. L. Rayar[2], S.Ajitha[1])

26. Synthesis and structural characterization of zinc doped magnesium oxide (**B.C. Abhinisha [(1)]**, T.R Jeena[(2)])

27. XRD characterization of zinc oxide (ZnO) nano particles prepared by solution based method ([1]**Abhirami.U.M**; [2,*]Murugavel.S)

OP-15	Vibrational and Optical Studies of 3,4,5-trimethoxybenzaldehyde single crystals for NLO applications

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Abstract

In the recent years, studies of optical nonlinearities in materials have been become more interesting because of their useful application in integrated optics, such as optical modulation, all optical switching and optical information processing. The several NLO behaviors, such as the optical limiting is one of the most promising practical applications, as it may be protect the human eyes and the optical sensors from the damage caused by the intense optical radiations. The researchers are given the appreciable care to develop and improve the quality of the organic single crystals for the technological applications. The organic material 3,4,5-trimethoxybenzaldehyde has been grown by slow evaporation technique using methanol as solvent. The Vibration studies were recorded using FTIR and FT-Raman spectra to identify the functional groups present in the crystal. The optical property of the grown crystal was analyzed by UV-Vis-NIR measurement. The third order nonlinear optical properties of 3,4,5-trimethoxybenzaldehyde was measured by the Z-scan technique using 532 nm diode pumped continuous wave (CW) Nd:YAG laser.

Keywords: Crystal growth from Solution, FTIR, FT-Raman

Photograph of 3,4,5-TMOB Single crystals

OP-16	Vibrational spectral investigation, DFT computational studies and charge transfer interactions analysis of L-lysine monohydrate

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Abstract

In this work, using the Gaussian 09 program, the molecular structure of L-Lysine monohydrate was optimized using the DFT method with B3LYP/6-311++G(d,p) basic sets. The Mulliken atomic charge distribution, vibrational frequencies, frontier molecular orbitals and Topological analysis were calculated. The VEDA 4.0 tool was used to assign the whole theoretically estimated and experimentally observed vibrational frequencies using