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(NCAM-2023)
March 25, 2023

FIFTH NATIONAL CONFERENCE ON ADVANCED MATERIALS

Certificate

Arts College, has been through
Dr. J. Priscilla, Assistant Professor, Muslim
Chemical, Calculations and
Quantum Chemistry
Participated for Poster/Oral Presentation of the paper entitled, *Quantum Chemistry, Calculations and*
Librational Spectral Studies at the Fifth National Conference on Advanced Materials
at 2.5. at the Fifth National Conference on Advanced Materials

Science, Kallyakkavilal on March 25, 2023.

[Signature]

Rev. Fr. Dr. M. Eckermans Michael
Secretary and Correspondent

[Signature]

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Principal

Dr. M. Arulnathan

Convener

**Proceedings of Fifth National Conference on
ADVANCED MATERIALS**

(NCAM-2023)

March 25, 2023

**Organized by
DEPARTMENT OF PHYSICS**



By

Dr.M.Amalanathan M.Sc, M.Phil, Ph.D

Dr.N.Suma, M.Sc, M.Phil, Ph.D

**Nanjil Catholic College of Arts & Science,
Kaliyakkavilai – 629 153
Kanyakumari District
Tamil Nadu, India
Email: nanjil.physics@gmail.com
Tel: 04651 – 244788**

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For Copies please contact:

**Dr.M.Amalanathan,
East Kalpahaseri Vilai,
Vavarai,
S.T.Mankad Post,
Kanyakumari-629172,
Tamil Nadu,
India.**

Mobile: 9940347178**Email: ansonpublications@gmail.com, nathan.amalphysics@gmail.com**

CONTRIBUTED PAPERS - CONTENTS

1. Spectroscopic exploration, reactivity, electronic properties of different solvents, molecular docking and drug likeness of 4-Methyl-N-(4-nitrobenzylidene)-piperazin-1-amine: A theoretical approach (Bravanjalin Subi E¹, D.Aruldas²)
2. Concurrence between cosmic Ray and Solar wind during Solar cycle 23, 24 (S.Abilaa¹, S.S.Bershab², R.P.Jebin³)
3. Interplanetary coronal mass ejections at 1 AU using Multispacecraft (Abisha¹)
4. Structural, Spectroscopic on structure vibrational spectroscopic, and RDG analysis Molecular docking of biological active 4-(2, 3-Dichlorophenyl) piperazin-1-ium (W.Abisha^a, D.Aruldas^b)
5. Distribution of Linear speed and Angular width of Coronal Mass Ejections and Halo CME's Over Solar Cycle 23, 24 and 25 (Dhaiya. M.S¹, Iren Sobia. A²)
6. Soliton propagation in an alpha-helical protein system by using darbox transformation technique (R. Jeba Vijitha¹, S.Beauno²)
7. The Effect of Interaction on the Third-Order Nonlinear Optical Properties of Functionalized Reduced Graphene Oxide Nanocomposite. (Alice Noble A¹, I Hubert Joe²)
8. Non linear optical property of 2-(Methyl Amino)-1, 2-Diphenylethanone: A theoretical approach (M.Jini pramila^a, D. Aruldas^b)
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11. Structural properties and nonlinear optical absorption in Mn substituted nickel -zinc ferrites using Z scan method. (Sijo S Thomas¹, I Hubert Joe²)
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13. Spectroscopic and quantum chemical computation on molecular structure, AIM, ELF, RDG of 4-CUumene: A DFT approach, (Sukanya R¹, D. Aruldas²)
14. Synthesis and characterization of Nickel Oxide (NiO) Nanoparticles using carica papaya leaves (A. Benifa, Dr. A. Darlin Mary¹, M. Amalanathan²)

OP-09

Quantum Chemical Calculations and Vibrational Spectral Studies of 2,5-dimethoxybenzoic acid

J.Priscilla^a, D.Arul Dhas^b

^aDepartment of Physics, Physics Research Centre, Muslim Arts college, Thiruvithancode
^bDepartment of Physics, Physics Research Centre, Nesamony Memorial Christian College, Marthandam - 629 165, Kanyakumari District, Tamilnadu, India

Abstract

The molecular geometry, harmonic vibrational frequencies and bonding features of 2,5-dimethoxybenzoic acid in the ground state were calculated by using density functional theory employing B3LYP method with 6-311G(d,p) basis set. Using the same basis set NBO analysis was performed. The results show that electron density (ED) in the bonding and anti-bonding orbitals and second order delocalization energies $E^{(2)}$ confirm the occurrence of intra-molecular charge transfer (ICT) within the molecule. The fundamental vibrational transitions were explained by experimental FT-IR technique. All calculated data were compared with the experimental data of the title molecule. The calculated HOMO and LUMO energies show that charge transfer occur within the molecule.

Keywords: DFT, NBO, HOMO-LUMO

OP-10

Experimental and Theoretical Approach on NLO Studies of Benzodiazepine derivative for Optical Limiting Application

Aswathy.P¹, Hubert Joe.I¹, Narayana.B²

¹Department of Physics, University of Kerala, Kariavattom, Trivandrum -695581, Kerala,
²Department of Chemistry, Mangalore University, Mangalagangothri- 574199, India
 *hubertjoe@gmail.com

Abstract

Nonlinear optics plays a crucial role in the field of photonics and optoelectronics. One of the main challenges of researchers in photonics is to design and develop new nonlinear optical (NLO) material with high susceptibilities and hyperpolarizabilities. The NLO behaviour mainly originates from a strong donor-acceptor intermolecular interaction and delocalized π -electron system [1]. Organic materials are well known for such effects and are widely used in this area. Benzodiazepine derivatives belong to the class of organic materials having a seven membered heterocyclic ring compounds with two nitrogen atoms.

Here the present work focuses on the theoretical and experimental investigation of third-order nonlinear optical properties of benzodiazepine derivative. The optimized geometry, natural bond orbital analysis, HOMO-LUMO analysis, and theoretical hyperpolarizability values were calculated using the B3LYP/6-311 ++ G (d, p) level of theory and the structure is shown in Fig. 1. The third-order nonlinear optical properties including nonlinear absorption coefficient (β) and nonlinear refractive index (n_2) were determined using open and closed-aperture z-scan technique, respectively [2]. The third-order nonlinear optical properties, along with the optical limiting behaviour were carried out by z-scan technique using Q-switched Nd: YAG laser with 5 nanosecond pulses at 532 nm. The z-scan result confirms that the nonlinear refractive index, n_2 is positive which exhibits the self-focussing effect (Fig.2 (a)). Also, the reverse saturable absorption behaviour reveals the optical limiting property of the studied material with a positive nonlinear absorption coefficient, β (Fig.2 (b)). All the results reveal that benzodiazepine derivative is a promising candidate for photonic and optoelectronic applications.