S.NO	AUTHOR'S NAME	TITLE
1	**Dr. M. K. Murali**	Vibrational Spectra(Theoretical, Experimental) and Optimized Structure, Frontire Molecular Orbital Mulliken Atomic Charge Studies on Pentylenetetrazole(PTZ) Based on Density Functional theory.
2	**Dr. M. K. Murali**	Simulation of FT-IR and FT-Raman Spectra based on quantum Chemical Calculations, Vibrational Assisgnments, Hyperpolarizability and Homo-Lumo Analysis of 5(4 methyl phenyl)tetrazole(5MPTZ).
3	**Dr. M. K. Murali**	Biocidal property of Zinc Oxide-Titanium Dioxide-Graphene Oxide Nanocomposites via One-Pot Facile precipitation Method
4	**Dr. M. K. Murali**	Theoretical Investigations Of Molecular Structure, Vibrational Spectra And Mulliken Atomic Charge Analysis On 6-Nitrobenzimidizole, Strad Research, volume 7
5	**Dr.K. Dhanabalan**	Enhancement of Structural, Optical and Bumpy Surface Effect of Cu_2O Thin Films Through Sn Doping by Modified SILAR Technique
6	**Dr. C. Usha**	Growth and combined experimental and quantum chemical study of glycyl-L-Valine crystal. Heliyon 5 (2019) e01574.

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Vibrational Spectra(Theoretical, Experimental) and Optimized Structure, Frontire Molecular Orbital, Mulliken Atomic Charge Studies on Pentylenetetrazole (PTZ) Based on Density Functional Theory

A.Rajeswari[a], M.K. Murali[a]*A.Ramu[b]

[a] PG and Research department of physics,JJ.College of Arts & Science (Autonomous), Pudukottai-622422, Tamil Nadu, India.

[b] Department of Physics,Ganesar College of Arts and Science, Melaisivapuri-622403,Tamil Nadu, India.

***aramusir80@gmail.com**

Abstract

The vibrational spectra of Pentylenetetrazole (PTZ) have been recorded in the regions 4000−400 $cm^{-1}$for FT-IR and 3500−100 cm^{-1} for FT-Raman. The molecular structure, geometry optimization, vibrational frequencies were obtained by the density functional theory (DFT) using B3LYP method with 6-31G and 6-311+G basis sets. The complete assignments were performed on the basis of the potential energy distribution (PED) of the vibrational modes, calculated and the scaled values were compared with experimental FT-IR and FT-Raman spectra. The HOMO and LUMO energy gap reveals that the energy gap reflects the chemical activity of the molecule. The dipole moment (μ), polarizability (α), anisotropy polarizability ($\Delta\alpha$) and first hyperpolarizability (β_{tot}) of the molecule have been reported. Information about the size, shape, charge density distribution and site of chemical reactivity of the molecule has been obtained by molecular electrostatic potential (MEP).

Key words: Pentylenetetrazole,DFT, FT-IR,FT-Raman,MEP

Introduction

The biological potential molecule Pentylenetetrazole (PTZ) is a tetrazole derivative and inhibitor of the γ aminobutyric acid (GABAA) and its receptor complex[1,2]. PTZ is a convulsing agent used for inducing seizures.It can traverse the blood-brain barrier[3].As well as Pentylenetetrazole has been used to induce seizures in zebra fish larvae[4], mice[5], and male wistar rats[6]. This extensive applications of tetrazoles derivatives stimulated research in areas such as the reactivity of various tetrazolyl derivatives and the design of synthetic methodologies. In these studies, the molecular structure, vibrational spectra and HOMO-LUMO energy gap of Pentylenetetrazole (PTZ) were investigated by a concerted approach using matrix isolation

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RESEARCH ARTICLE

Simulation of FT-IR and FT-Raman Spectra Based on quantum chemical Calculations, Vibrational Assignments, Hyperpolarizability, and Homo-Lumo Analysis of 5(4 methyl phenyl)tetrazole (5MPTZ)

A.Rajeswari[1], M.K. Murali[1]* and A.Ramu[2]

[1]PG and Research Department of Physics, JJ.College of Arts & Science (Autonomous), Pudukottai - 622422, Affiliated to Bharathidasan University, Trichy, Tamil Nadu, India.

[2]Department of Physics, Ganesar College of Arts and Science, Melaisivapuri-622403, Affiliated to Bharathidasan University, Trichy, Tamil Nadu, India.

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***Address for Correspondence**
M.K. Murali
PG and Research Department of Physics,
JJ.College of Arts & Science (Autonomous),
Pudukottai - 622422,
Affiliated to Bharathidasan University,
Trichy, Tamil Nadu, India.

ABSTRACT

The spectra of 5(4 methyl phenyl)tetrazole (5MPTZ) have been recorded in the regions 4000-400 cm^{-1} for FT-IR and 3500-100 cm^{-1} for FT-Raman. The geometry optimization, vibrational frequencies were obtained by the density functional theory (DFT) using B3LYP method with 6-31G and 6-311+G basis sets. The complete assignments were performed on the basis of the potential energy distribution (PED) of the vibrational modes, calculated and the scaled values were compared with experimental FT-IR and FT-Raman spectra. The HOMO and LUMO energy gap reveals that the energy gap reflects the chemical activity of the molecule. The dipole moment (μ_0), polarizability (α), anisotropy polarizability ($\Delta\alpha$) and first hyperpolarizability (β_{tot}) of the molecule have been reported. Information about the size, shape, charge density distribution and site of chemical reactivity of the molecule has been obtained by molecular electrostatic potential (MEP).

Keywords: 5(4 methyl phenyl)tetrazole (5MPTZ) , DFT, FT-IR,FT-Raman, MEP.

INTRODUCTION

Tetrazole-related molecules have attracted considerable attention due to their biological activities. The synthesis of new members of this family of ligands is an important direction in the development of modern coordination chemistry [1,2]. Tetrazole compounds have a wide range of applications in coordination chemistry, medicinal

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Biocidal Properties of Zinc Oxide-Titanium Dioxide-Graphene Oxide Nanocomposites via One-Pot Facile Precipitation Method

V. Sri Priyanka[1] · M. K. Murali[1] · M. Abdur Rahman[1]

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Abstract

Novel multifunctional inorganic nanocomposites have enhanced the biocidal activity, towards bacterial and cancer diseases, which was useful for biomedical applications in healthcare industries. The critical parameter in preparation of multifunctional biocidal nanocomposites consists of several advantages such as low cost, smaller size, excellent yield, tunable properties, biocompatibility, multifunctionality, controllability, and reducing the toxicity levels of materials. The multifunctional biocidal zinc oxide (ZnO)-titanium dioxide (TiO_2)-graphene oxide (GO)—ZTGO—nanocomposite sample was employed via facile one-pot precipitation process. The XRD analysis revealed that ZTGO nanocomposites exhibit hexagonal structure phase formation. From the morphological analysis, the prepared ZTGO nanocomposites exhibited GO sheets were decorated with ZnO-TiO_2 nanoflakes structure with uniform distribution. EDX spectrum displays the presence of carbon (C), nitrogen (N), zinc (Zn), titanium (Ti), and oxygen (O) for ZTGO nanocomposites, respectively. The FTIR results confirmed that ZTGO samples have some oxygen-containing functional groups and defect sites, and, as a result, revealed a strong interaction between GO, TiO_2, and ZnO nanomaterials. The photoluminescence (PL) spectrum of ZTGO nanocomposites exhibited oxygen vacancies found to be 500 and 527 nm, respectively, and thus results can be responsible for the production of active radicals against the biocidal activities. The antibacterial potential of the ZTGO nanocomposites achieved against *S. aureus* and *E. coli*, results were showed that the ZTGO more antibacterial activity as compared to the standard antibiotic amoxicillin. The morphological changes of ZTGO nanocomposites treated *E. coli* bacterial cell membrane observed by SEM analysis. The anticancer activity of the ZTGO nanocomposites was studied in liver cancer cells (A549) and IC_{50} value was observed at 52.72 µg/mL. From this work, we believed that prepared ZTGO nanocomposites are a potentially important material for healthcare applications.

Keywords ZnO-TiO_2-GO nanocomposites · Biocidal activity · XRD · FESEM · PL

1 Introduction

In recent decades, the multidrug-resistant bacterial (MDR) infection has caused potentially increased noticeably over the last few years [4] and [23]. These results in increased usage of antibiotic agents in the healthcare industry. But MDR strains have developed their immunity to neutralize the biocidal action of antibiotics, and due to overcoming these problems, researchers have to develop a novel method, long-term stability, and low-cost materials treatment against MDR bacterial infections. Other important diseases worldwide cancer is unpredictable, challenging at the same time complicated issues are created by the human health system. To diagnose and treatment of cancer cells various methods such as Radiation Therapy, Surgery, and Chemotherapy [15, 17] and [18]. These methods are high risk, more side effects, and high costs. To overcome this problem, developed advanced healthcare material, it's maybe inexpensive tools, diagnosis drug are less-toxic and negligible risk factors to the normal cells. Nanoscience and nanotechnology can be developed higher prospects to cure the antibacterial and anticancer multifunctional nanomaterials for advanced clinical applications [13].

The inorganic metal oxide nanomaterials have great attention for wide applications including antibacterial, anticancer,

✉ M. K. Murali
muralimk1979@gmail.com

[1] PG and Research Department of Physics, J.J. College of Arts and Science (Autonomous), Affiliated to Bharathidasan University, Sivagnanam,Pudhukkottai-622 422., Tiruchirappalli, Tamilnadu, India

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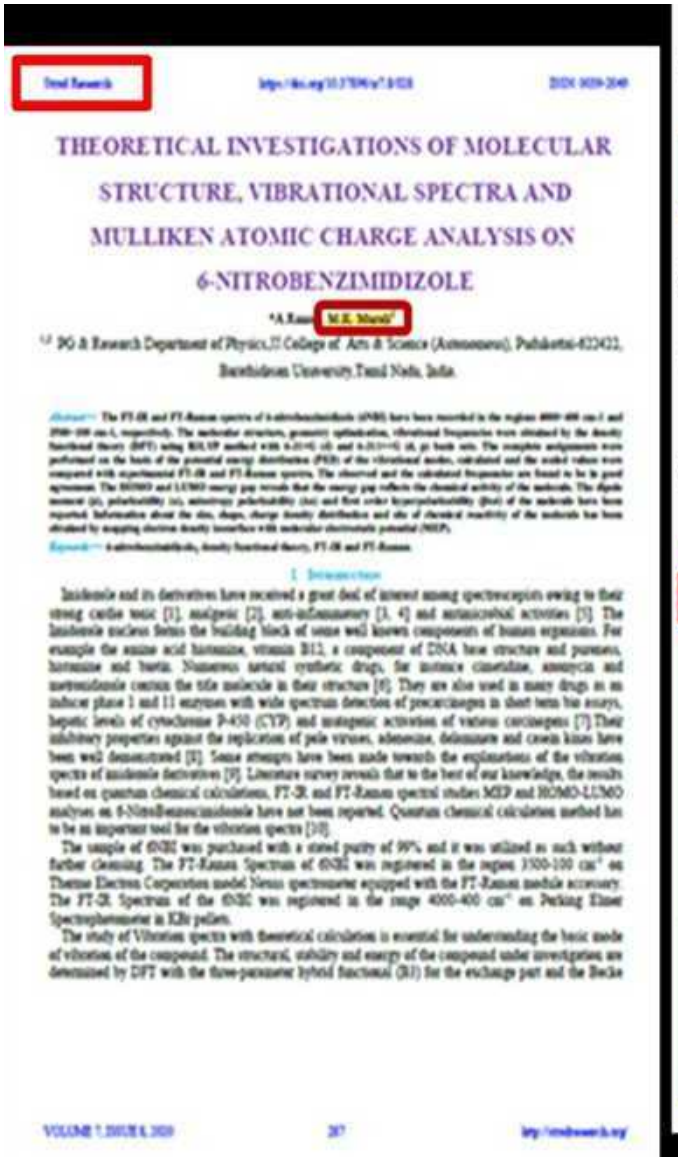

Trend Research

THEORETICAL INVESTIGATIONS OF MOLECULAR STRUCTURE, VIBRATIONAL SPECTRA AND MULLIKEN ATOMIC CHARGE ANALYSIS ON 6-NITROBENZIMIDIZOLE

A. Ramesh, M.K. Murali

PG & Research Department of Physics, JJ College of Arts & Science (Autonomous), Pudukkottai-622422, Bharathidasan University,Tamil Nadu, India.

The FT-IR and FT-Raman spectra of 6-nitrobenzimidazole (6NBI) have been recorded in the regions 4000-400 cm-1 and 3500-100 cm-1, respectively. The molecular structure, geometric optimization, vibrational frequencies were obtained by the density functional theory (DFT) using B3LYP method with 6-311G (d) and 6-311++G (d, p) basis sets. The complete assignments were performed on the basis of the potential energy distribution (PED) of the vibrational modes, calculated and the scaled values were compared with experimental FT-IR and FT-Raman spectra. The observed and the calculated frequencies are found to be in good agreement. The HOMO and LUMO energy gap reveals that the energy gap reflects the chemical activity of the molecule. The dipole moment (μ), polarizability (α), anisotropy polarizability (Δα) and first order hyperpolarizability (βtot) of the molecule have been reported. Information about the size, shape, charge density distribution and site of chemical reactivity of the molecule has been obtained by mapping electron density isosurface with molecular electrostatic potential (MEP).

Keywords: 6-nitrobenzimidazole, density functional theory, FT-IR and FT-Raman.

I. Introduction

Imidazole and its derivatives have received a great deal of interest among spectroscopists owing to their strong cardiac tonic [1], analgesic [2], anti-inflammatory [3, 4] and antimicrobial activities [5]. The Imidazole nucleus forms the building block of some well known components of human organisms. For example the amino acid histamine, vitamin B12, a component of DNA have structure and purenes, histamine and biotin. Numerous natural synthetic drugs, for instance cimetidine, azomycin and metronidazole contain the title molecule in their structure [6]. They are also used in many drugs as an inducer phase I and II enzymes with wide spectrum detection of procarcinogen in short term bio assays, hepatic levels of cytochrome P-450 (CYP) and mutagenic activation of various carcinogens [7].Their inhibitory properties against the replication of pole viruses, adenosine, deaminase and cowin kinase have been well demonstrated [8]. Some attempts have been made towards the explanations of the vibration spectra of imidazole derivatives [9]. Literature survey reveals that to the best of our knowledge, the results based on quantum chemical calculations, FT-IR and FT-Raman spectral studies MEP and HOMO-LUMO analyses on 6-Nitrobenzimidazole have not been reported. Quantum chemical calculation method has to be an important tool for the vibration spectra [10].

The sample of 6NBI was purchased with a stated purity of 99% and it was utilized as such without further cleansing. The FT-Raman Spectrum of 6NBI was registered in the region 3500-100 cm^{-1} on Thermo Electron Corporation model Nexus spectrometer equipped with the FT-Raman module accessory. The FT-IR Spectrum of the 6NBI was registered in the range 4000-400 cm^{-1} on Perking Elmer Spectrophotometer in KBr pellet.

The study of Vibration spectra with theoretical calculation is essential for understanding the basic mode of vibration of the compound. The structural, stability and energy of the compound under investigation are determined by DFT with the three-parameter hybrid functional (B3) for the exchange part and the Becke

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Enhancement of Structural, Optical and Bumpy Surface Effect of Cu_2O Thin Films Through Sn Doping by Modified SILAR Technique

A. Vanaki [1], K. Dhanabalan [2,], A. T. Ravichandran [3], R. Chandramohan [4] and Srinivas Mantha [5]*

[1]Department of Physics, H.H. The Rajah's College (Autonomous) (Affiliated to Bharathidasan University), Pudukkottai, Tamilnadu, India- 622 001
[2]Post Graduate and Research Department of Physics, J.J. College of Arts and Science (Autonomous) (Affiliated to Bharathidasan University), Pudukkottai, Tamilnadu, India -622 422
[3]Post Graduate and Research Department of Physics, National College (Autonomous) (Affiliated to Bharathidasan University), Tiruchirappalli, Tamilnadu, India- 620 001
[4]PG Department of Physical Sciences, Vidhaya Giri College of Arts and Science, Puduvayal - 630108, India
[5]Department of Electronics and Communication Engineering, SAGE University, Bhopal, 462022, India

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Abstract: Undoped and Sn doped $Cu_{2-x}Sn_xO$ (x = 0, 5.0, 10.0, 15.0 and 20.0) thin films have been deposited into glass substrates by hire a fee powerful method of M-SILAR (Modified-Successive Ionic Layer Adsorption and Reaction). The Sn doping level in the starting solution become numerous from 0 to 20.0 mol.% in steps of 5.0 mol.%. The deposited films were characterized for their structural, optical, morphological and topography properties with respective instrumentation. X-ray diffraction (XRD) evaluation found out the orientation of crystalline increase of $Cu_{2-x}Sn_xO$ films, and all the films showcase single crystalline. The preferential orientation was retained in favor of (111) plane even at the highest doping level. The presence of copper in the films turned into showed by way of energy dispersive X-ray spectrometer. Average optical transmittance (UV-vis-NIR and Photoluminescence (PL)) are varied with effect of doping concentration. The stretching vibrations of Cu-O, Sn-O and O-Cu-O have been showed by using Fourier transform infrared spectroscopy (FTIR). The morphological observe has been achieved by using a Field emission scanning electron microscopy (FE-SEM) has display as decrease the particle length with increase of doping concentration. From High resolution transition electron microscopy (HR-TEM) the crystalline growth of each line are excellent within the Sn doping of 10.0 mol.%. The atomic force microscopy method changed into employed to investigate the roughness of the films and the bumpy surface revealed at 10.0 mol.% of Sn doping level.

Keywords: Low Cost, Cu2O Thin Film, Heavily Sn-Doped, FE-SEM, HR-TEM, AFM.

1 Introduction

Metal oxide are an critical magnificence of substances from both medical and technological perspectives they gift thrilling possibilities for research. Thin films are specifically appealing as a result of their relevance in devices, and also for the ability to pursue surface-belongings family members research the usage of controlled microstructures. They are the distinguished substances gambling important function in digital device and also attractive substances for solar power conversion [1] and photo catalytic activity programs [2]. Among diverse metal oxide materials, the copper oxides are promising semiconductor substances for a extensive variety of optoelctronic devices to their semi conductivity with a band hole of ≈ 2.1 eV respectively [3]. Recently, steel oxide materials are relevant in all fields, of their pure and doping thin films. The conductivity of the Cuprous oxide (Cu_2O) film will increase, when the doping is a very vital technique to growth the conductivity of the film by increasing the variety of intermediate strength tiers created in the energy band gap location [4]. Cuprous oxide behaves because the figure compound in many p-type semiconductor for obvious undertaking oxides (TCOs) materials (TCOs : Al, Mn, Fe, Li, Ni, Ti, Zn, Co, and so on,....) [5-9]. The Sn-doped Cu_2O delafossite thin film ion be used in layer-portions and serves as the important

*Corresponding author E-mail: dhana_pgp@rediffmail.com

Heliyon

Growth and combined experimental and quantum chemical study of glycyl-L-Valine crystal

C. Usha [a], R. Santhakumari [b,*], Lynette Joseph [c], D. Sajan [c], R. Meenakshi [d], ...

[a] Department of Physics, LL. College of Arts and Science (Autonomous), Sivagiri, Pudukkottai, 622 402, Tamil Nadu, India

[b] Department of Physics, Government Arts College for Women (Autonomous), Pudukkottai, 622 001, Tamil Nadu, India

[c] Department of Physics, Bishop Moore College, Mavelikara, Kayamkulam, Kerala, 690 110, India

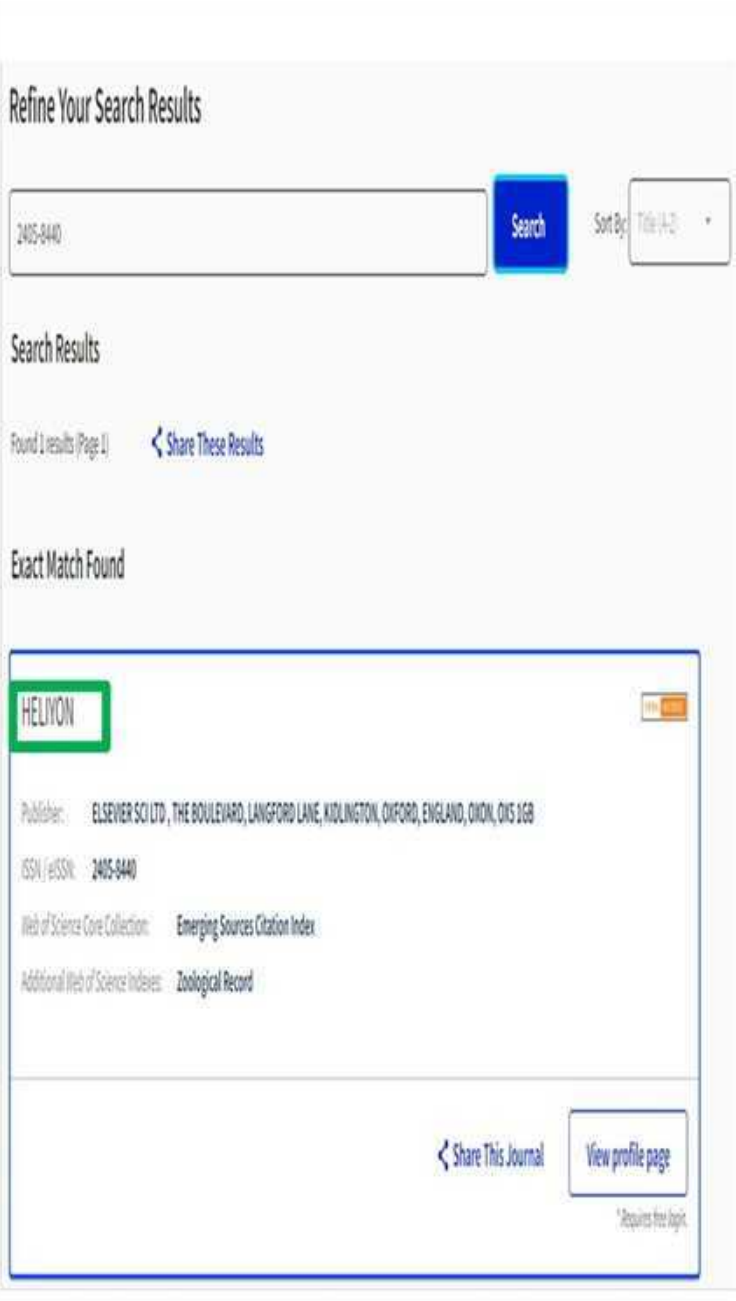
[d] Department of Physics, Cauvery College for Women (Autonomous), Tiruchirappalli, 620 018, Tamil Nadu, India

[e] Department of Physics, Srimad Andavan Arts and Science College (Autonomous), Tiruchirappalli, 620 005, Tamil Nadu, India

* Corresponding author.
E-mail address: santhakkl@yahoo.co.in (R. Santhakumari).

Abstract

Glycyl-L-Valine (GLV) crystals were grown using distilled water as the solvent at room temperature by solution growth technique. Powder X-ray diffraction confirms the crystalline quality of GLV crystal. The molecular structure of GLV crystal was identified by ^{13}C NMR spectral studies. The nonlinear optical (NLO) behavior of the crystal was found to be ~4.3 times greater than that of potassium dihydrogen orthophosphate. FT-Raman and FT-IR spectra of the GLV were recorded and complete functional group assignment of the determined vibrational bands of GLV have been reported. Density functional theoretical method (DFT) was performed using B3LYP with the 6-311++G (d, p) basis set and the results were compared with the experimental values which confirm the intermolecular interactions responsible for the enhanced NLO activity of the molecule, as evident from NBO and Hirshfeld analyses. The calculated HOMO and LUMO



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