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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

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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)

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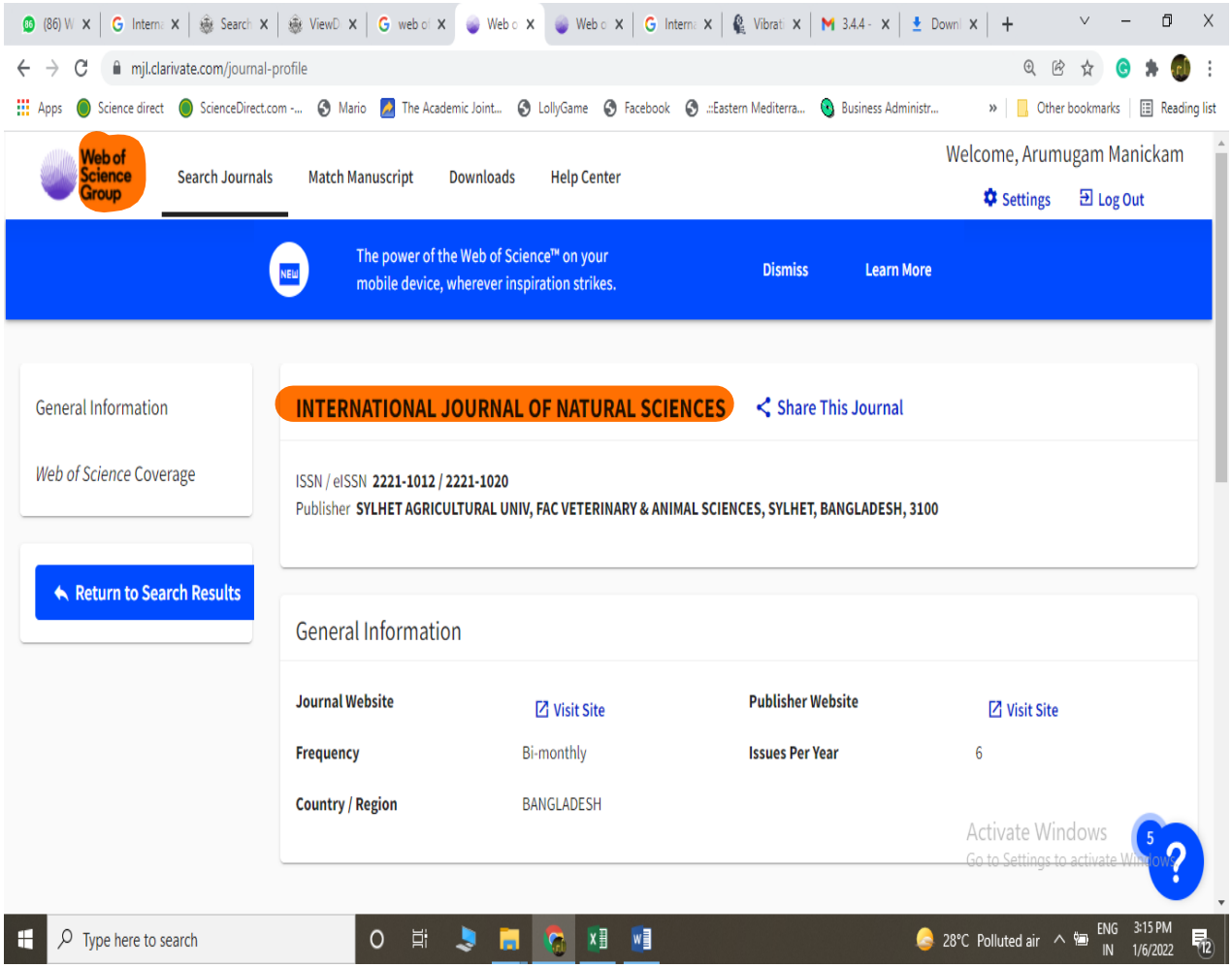
ABSTRACT

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), polarizability (α), anisotropy polarizability (Δα) 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

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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 world-wide 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 anti-cancer multifunctional nanomaterials for advanced clinical applications [13].

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

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