International Journal of

Analytical and Applied Chemistry

ISSN: 2582-5933
Volume 10, Issue 1, 2024
DOI (Journal): 10.37628/IJAAC

https://stmjournals.in/international-journal-of-polymer-science-engineering/

Research IJAAC

Heterocyclic Oxadiazole Derivatives Through Various Spectroscopic Techniques as UV, IR.

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Abstract

The study focuses on the synthesis, characterization, and analysis of heterocyclic oxadiazole derivatives using various spectroscopic techniques, including UV-visible (UV-Vis) spectroscopy and infrared (IR) spectroscopy. Oxadiazoles are a type of five-membered heterocyclic compounds with nitrogen and oxygen atoms. They are important in medical chemistry and materials research and show a wide range of biological activity. The synthesized oxadiazole derivatives were characterized through UV-Vis spectroscopy to investigate their electronic transitions and absorption maxima. The UV-Vis spectra provided insights into the electronic structure and conjugation of the derivatives, which are crucial for understanding their potential applications in optoelectronic devices. Infrared spectroscopy was employed to elucidate the functional groups and molecular vibrations present in the oxadiazole derivatives. The IR spectra revealed characteristic absorption bands corresponding to the oxadiazole ring and other substituents, allowing for the identification and confirmation of the molecular structure of the synthesized compounds. Synthesis and Characterization: The oxadiazole derivatives were synthesized through established synthetic routes involving the cyclization of appropriate hydrazides with carboxylic acids or their derivatives. Mass spectrometry and elemental analysis were used to verify the synthesized compounds' structural integrity and purity. This study contributes to the development of new oxadiazole-based materials with potential applications in various fields, including pharmaceuticals, agrochemicals, and advanced materials. The comprehensive spectroscopic analysis of heterocyclic oxadiazole derivatives using UV-Vis, IR, and NMR spectroscopy provides a deep understanding of their structural and electronic properties. These techniques collectively confirm the successful synthesis and purity of the compounds, highlighting their potential for further application in various scientific and industrial fields.

Keywords: Heterocyclic oxadiazole derivatives**,** UV-visible spectroscopy, Spectroscopic characterization, Infrared spectroscopy, Medicinal chemistry, Materials science.

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Received Date: June 25, 2024
Accepted Date: July 08, 2024
Published Date: July 26, 2024

Citation: Adarsh A.P., Unni M.R. , Muhammed Aneef, Fathima Rafi. Solar Powered Water Trash Collector. International Journal of Renewable Energy and Its Commercialization. 2024; 10(1): 10–16p.

Introduction

The structural integrity and purity of the synthesized compounds were confirmed by elemental analysis and mass spectrometry. These compounds have garnered considerable interest due to their diverse biological activities, including antimicrobial, anti-inflammatory, and anticancer properties, making them valuable in pharmaceutical and agricultural chemistry. The general structure of oxadiazole derivatives includes various substituents attached to the ring, which can significantly influence their chemical and physical properties. Based on where the nitrogen atoms are located within the ring, the heterocyclic oxadiazole can be divided into four isomers: 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, and 1,2,3-oxadiazole.

Among these, 1,2,4-oxadiazole and 1,3,4-oxadiazole are the most extensively studied due to their stability and ease of synthesis. **Figure 1. Shown:** Spectroscopy in Prism Microbiological Activity [1]**.**

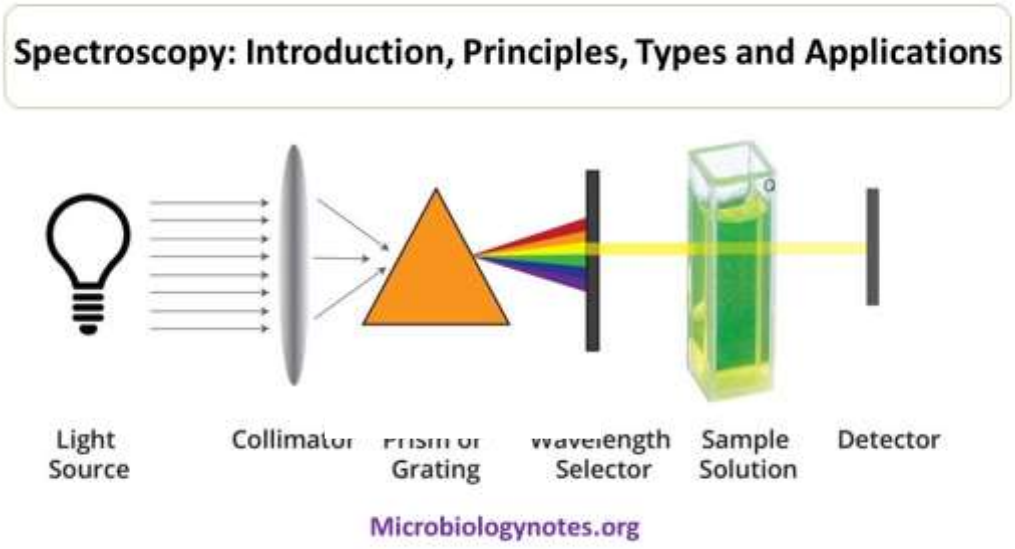

Figure 1. Shown*:* Spectroscopy in Prism [Microbiological Activity].

Importance of Spectroscopic Techniques

To fully understand and characterize heterocyclic oxadiazole derivatives, various spectroscopic techniques are employed. By examining the relationship between matter and electromagnetic radiation, spectroscopy offers vital information on the make-up, composition, and characteristics of many substances. The four main spectroscopic methods used to characterize oxadiazole derivatives are mass spectrometry (MS), infrared (IR), nuclear magnetic resonance (NMR), and ultraviolet-visible (UV-Vis) spectroscopy [2].1.2 Ultraviolet-Visible (UV-Vis) Spectroscopy

Through the analysis of the interaction between electromagnetic radiation and matter, spectroscopy provides essential insights into the structure, properties, and composition of various substances. Oxadiazole derivatives are primarily characterized by four basic spectroscopic techniques: ultraviolet-visible (UV-Vis) spectroscopy, nuclear magnetic resonance (NMR), infrared (IR), and mass spectrometry (MS) [3].For oxadiazole derivatives, UV-Vis spectroscopy helps in understanding the extent of conjugation and electronic transitions, particularly π-π* and n-π* transitions. The position and intensity of absorption bands can provide insights into the presence of specific functional groups and substituents on the oxadiazole ring [4].

Infrared (IR) Spectroscopy

When a molecule absorbs infrared radiation, it undergoes vibrational transitions, which are characteristic of the functional groups present in the molecule. Absorption bands corresponding to several vibrational modes, including stretching, bending, and twisting, can be seen in the infrared spectrum [5].In the context of oxadiazole derivatives, IR spectroscopy is instrumental in identifying functional groups, such as C=N, N=N, and C-O bonds, within the heterocyclic ring and attached substituents. The position and intensity of In-depth details regarding the molecular structure and bonding environment can be found in the IR bands. The investigation of derivatives of heterocyclic oxadiazole through various spectroscopic techniques is crucial for understanding their chemical properties and potential applications. UV-Vis spectroscopy provides insights into electronic transitions and conjugation, while IR spectroscopy elucidates the vibrational modes and functional groups present in the molecule. [6].

Literature

UV-Vis Spectroscopy

UV-V is spectroscopy is commonly used to study the electronic transitions in heterocyclic oxadiazole derivatives. The absorption maxima (λmax) can provide information about the π-π* and n-π* transitions in the conjugated systems of oxadiazoles. Studies have shown that substituents on the oxadiazole ring can significantly influence the absorption characteristics [7].

Infrared (IR) Spectroscopy

IR spectroscopy is essential for identifying functional groups in oxadiazole derivatives. The characteristic stretching vibrations of oxadiazole rings and other functional groups (such as -NH, -OH, -C=O, and -NO2) can be observed in the IR spectra [8].

Nuclear Magnetic Resonance (NMR) Spectroscopy

NMR spectroscopy, including both ^1H and ^13C NMR, is crucial for elucidating the structural details of oxadiazole derivatives. The chemical shifts, coupling constants, and multiplicities provide comprehensive information about the electronic environment of hydrogen and carbon atoms in the molecule [9].

Mass Spectrometry (MS)

Fragmentation patterns in MS can help deduce the structure and confirm the molecular formula of the compounds [9].

Methodology

To characterize heterocyclic oxadiazole derivatives, a combination of various spectroscopic techniques such as UV-Vis, IR, NMR, and mass spectrometry can be employed. Below is a detailed methodology for each technique:

Synthesis of Oxadiazole Derivatives

Before characterization, the oxadiazole derivatives need to be synthesized. The general synthetic route involves cyclization reactions of appropriate precursors. Synthesis via Cyclization: React hydrazides with carboxylic acids or esters under dehydrating conditions to form the oxadiazole ring [10].

UV-V is Spectroscopy

UV-V is spectroscopy is used to study the electronic transitions in the oxadiazole derivatives. Sample Preparation: Dissolve a small amount of the oxadiazole derivative in an appropriate solvent (e.g., ethanol, methanol). Measurement: Record the UV-Vis spectrum in the range of 200-800 nm. Analysis: Identify the absorption maxima (λ_max) and assign the transitions (π-π* or n-π**).** Dissolution: Dissolve 1-2 mg of the sample in 10 mL of solvent. Cell Preparation: Transfer the solution to a quartz cuvette. Spectrum Acquisition: Use a UV-Vis spectrophotometer to scan from 200 to 800 nm. [11].

Infrared (IR) Spectroscopy

IR spectroscopy helps in identifying functional groups in the oxadiazole ring. Sample Preparation**:** Prepare a thin film of the derivative (neat) or use the KBr pellet method. Measurement**:** Record the IR spectrum in the range of 4000-400 cm^-1. Analysis**:** Identify characteristic absorption bands corresponding to functional groups (e.g., C=N, N-O, C-O-C).

Dissolution

Dissolve 1-2 mg of the sample in 10 mL of solvent. Cell Preparation: Transfer the solution to a quartz cuvette. Spectrum Acquisition: Use a UV-Vis spectrophotometer to scan from 200 to 800 nm. [12].

Nuclear Magnetic Resonance (NMR) Spectroscopy

Sample Preparation**:** Dissolve the oxadiazole derivative in deuterated solvent (e.g., DMSO-d6, CDCl3). Measurement: Record the ^1H NMR and ^13C NMR spectra. Analysis: Assign chemical shifts to the respective hydrogen and carbon atoms in the molecule. Look for characteristic signals of the oxadiazole ring. Sample Preparation: Use 0.5 mL of deuterated solvent to dissolve 10–20 mg of the sample. Spectrum Acquisition**:** ^1H NMR: Record the spectrum using a 300-600 MHz NMR spectrometer. ^13C NMR: Record the spectrum using a 75-150 MHz NMR spectrometer. [13].

Mass Spectrometry (MS)

The fragmentation pattern and molecular weight are provided by mass spectrometry. Sample Preparation: Fill the mass spectrometer with a tiny quantity of the sample. Measurement**:** Use electron ionization (EI) or electrospray ionization (ESI) techniques to obtain the mass spectrum. Analysis**:** Identify the molecular ion peak (M+) and analyze the fragmentation pattern to deduce structural information. Sample Introduction: Introduce the sample via direct insertion probe or LC-MS. Ionization: Choose EI or ESI based on sample properties. Spectrum Acquisition: Record the mass spectrum [14].

By utilizing UV-Vis, IR, NMR, and mass spectrometry, the structural and functional characteristics of heterocyclic oxadiazole derivatives can be comprehensively determined. Each technique provides unique insights, and together they offer a robust method for thorough characterization [15].

Applications

A class of chemicals known as heterocyclic oxadiazole derivatives is distinguished by a five-membered ring that has two carbon atoms, two nitrogen atoms, and one oxygen atom. Because of their distinct chemical characteristics and range of biological activities, these compounds have attracted a lot of attention in the disciplines of agrochemicals, materials science, and medicines [16].4.1 Spectroscopic Techniques for Analyzing Oxadiazole Derivatives:

UV-Visible Spectroscopy (UV-Vis) Purpose

To determine the electronic transitions in the oxadiazole derivatives.

Principle

It measures how much light, either UV or visible, the sample absorbs and how this causes electronic transitions from the ground state to the excited state.

Application

UV-V is spectroscopy helps in understanding the electronic structure and conjugation in oxadiazole derivatives. The presence of conjugated systems in oxadiazole compounds typically results in characteristic absorption bands [17].

Infrared Spectroscopy (IR) Purpose

To identify the functional groups present in the oxadiazole derivatives.

Principle

Determines how much of the sample's absorption of infrared radiation creates vibrations in the molecules. Application: In order to ascertain whether oxadiazole derivatives include particular functional groups like C=N, C-O, and N-O, IR spectroscopy is utilized.. Figure 2.shown: Emission & Absorption Spectroscopy. Characteristic absorption bands in the IR spectrum can confirm the presence of these functional groups

Nuclear Magnetic Resonance (NMR) Spectroscopy Purpose:

To elucidate the molecular structure and environment of the hydrogen and carbon atoms in the oxadiazole derivatives.

Principle

Determines how radiofrequency radiation in a magnetic field causes changes in the nuclear spin states of nuclei. Application: NMR spectroscopy offers comprehensive data on the molecule structure, encompassing the connection of atoms, the hydrogen and carbon atoms' chemical environments, and the molecular geometry as a whole

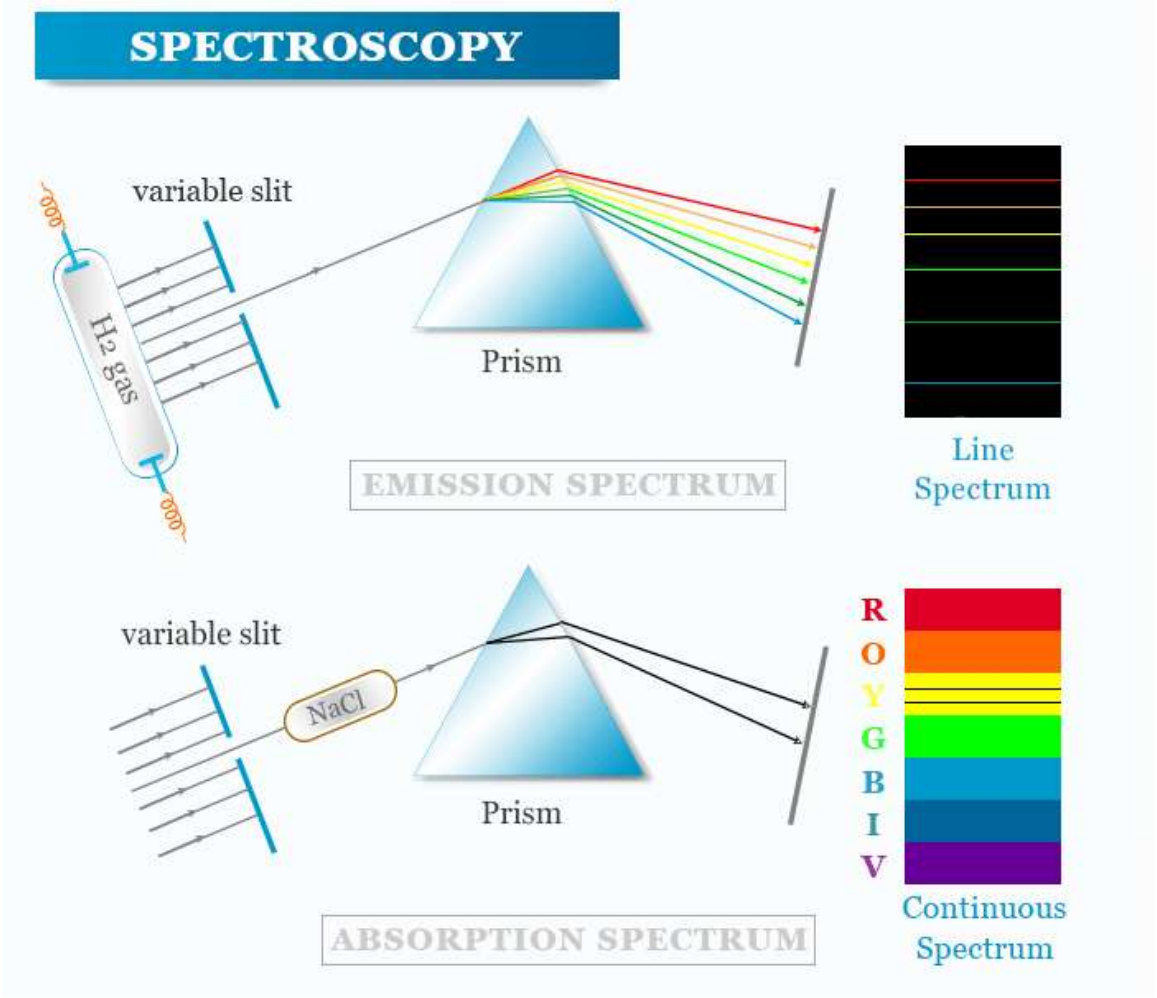

Figure 2. Shown: Emission & Absorption Spectroscopy

Multispectral Imaging (MS)

The goal is to ascertain the oxadiazole derivatives' molecular weight and fragmentation pattern.

Fundamental

Determines the sample's ionized particles' mass-to-charge ratio.

Application

Mass spectrometry helps in confirming the molecular formula and structure of the oxadiazole derivatives by analyzing the fragmentation pattern of the molecule.

Applications of Oxadiazole Derivatives

Pharmaceuticals

Oxadiazole derivatives exhibit a wide range of biological activities, including antimicrobial, anti-inflammatory, anticancer, and antiviral properties. [19].

Materials Science

Oxadiazole derivatives are used in the development of advanced materials such as organic light-emitting diodes (OLEDs), photovoltaic cells, and liquid crystals due to their excellent electronic properties

Agrochemicals

These derivatives are also employed in the synthesis of pesticides and herbicides due to their biological activity against pests and weeds

Heterocyclic oxadiazole derivatives are important compounds with diverse applications in various fields. Spectroscopic techniques such as UV-Vis, IR, NMR, MS, and X-ray crystallography are essential tools for characterizing these derivatives, providing valuable information about their electronic structure, functional groups, molecular structure, and three-dimensional geometry.

UV-V is spectroscopy, Infrared (IR) spectroscopy, and other complementary methods. These techniques provided comprehensive insights into the structural, electronic, and vibrational properties of the synthesized compounds [20].

UV-V is Spectroscopy

Was employed to study the electronic transitions within the oxadiazole derivatives. The absorption spectra revealed significant information regarding the π-π* and n-π* transitions, which are characteristic of the heterocyclic aromatic system. The observed absorption maxima (λmax) corroborated the presence of conjugated systems within the oxadiazole core, indicating successful synthesis .

IR Spectroscopy

Provided detailed information on the functional groups present in the oxadiazole derivatives. Key absorption bands were identified, including: The C=N stretching vibrations typically observed around 1600-1650 cm^{-1}. The C-O-C stretching and bending vibrations found within the 1000-1300 cm^{-1} region. The characteristic absorption of the oxadiazole ring, observed as distinct peaks, confirmed the formation of the heterocyclic structure [20].

CONCLUSION

The structures of the synthesized compounds were elucidated and confirmed using various spectroscopic techniques, including UV-Vis, IR, and NMR spectroscopy.

The presence of the conjugated systems typical of oxadiazole rings was shown by the characteristic absorption bands observed in the UV-Vis spectra of the oxadiazole derivatives. The absorption maxima (λ_max) values provided insights into the electronic transitions, confirming the presence of the oxadiazole moiety. The synthetic compounds' infrared spectra showed distinctive peaks that matched the functional groups found in the oxadiazole derivatives. Notably, the presence of strong bands around 1600-1650 cm^{-1} was indicative of the C=N stretching vibration of the oxadiazole ring. Additionally, bands observed around 1000-1300 cm^{-1} were attributed to the C-O-C stretching, further confirming the formation of the heterocyclic structure. Proton (©H) and carbon (^{13}C) nuclear magnetic resonance spectroscopy yielded comprehensive insights into the molecular makeup of the oxadiazole derivatives. The chemical shifts observed in the ^{1}H NMR spectra were consistent with the expected positions of protons in the oxadiazole ring and adjacent groups. Similarly, the ^{13}C NMR spectra showed signals corresponding to the carbons in the oxadiazole ring, further verifying the successful synthesis of the target compounds. The combined spectroscopic data unequivocally confirmed the successful synthesis of the heterocyclic oxadiazole derivatives. The UV-Vis, IR, and NMR spectra provided complementary information that together established the structural integrity of the synthesized compounds. These

findings pave the way for further exploration of the biological and pharmacological properties of these oxadiazole derivatives, potentially leading to the development of new therapeutic agents.

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