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Indian Journal of Natural Sciences
Vol.12 / Issue 66 / June / 2021

International Bimonthly
www.insroindia.org.in ©IJONS
ISSN: 0976 - 0997

RESEARCH ARTICLE

Imidazole and Ag⁺ Nano Material as Corrosion Inhibitor for Mild Steel in Hydrochloric acid Solutions

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Received: 03 Apr 2021 Revised: 19 Apr 2021 Accepted: 13 May 2021

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ABSTRACT
The corrosion inhibition efficiency of Imidazole in controlling the corrosion of mild steel immersed in 0.1N HCl for 60 min in the presence and absence of Ag⁺ has been studied by weight loss method. The formulation consisting of 240 ppm of Imidazole and 60 ppm Ag⁺ offers 95% inhibition efficiency. The synergistic effect exists between Imidazole and Ag⁺ system. Polarization study shows that the formulation system controls anodic reaction predominantly. The FTIR spectra study reveals that protective film consists of Fe²⁺ - C=O group and N-H stretch on metal surface. The mechanism of corrosion inhibition is proposed based on the results obtained from weight loss study and polarization study. Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) were used to investigate the nature of protective film formed on the mild steel surface.

Keywords: Imidazole, corrosion inhibition, mild steel, FT-IR and SEM.

INTRODUCTION
The study of corrosion of steel and Iron in acid media remains a global scientific problem which affects all kinds of Industries. The economic cost of corrosion is enormous and has been estimated to be in the range of 2-4% of an industrialized country's gross national product. In the field of combating corrosion, both economic and scientific

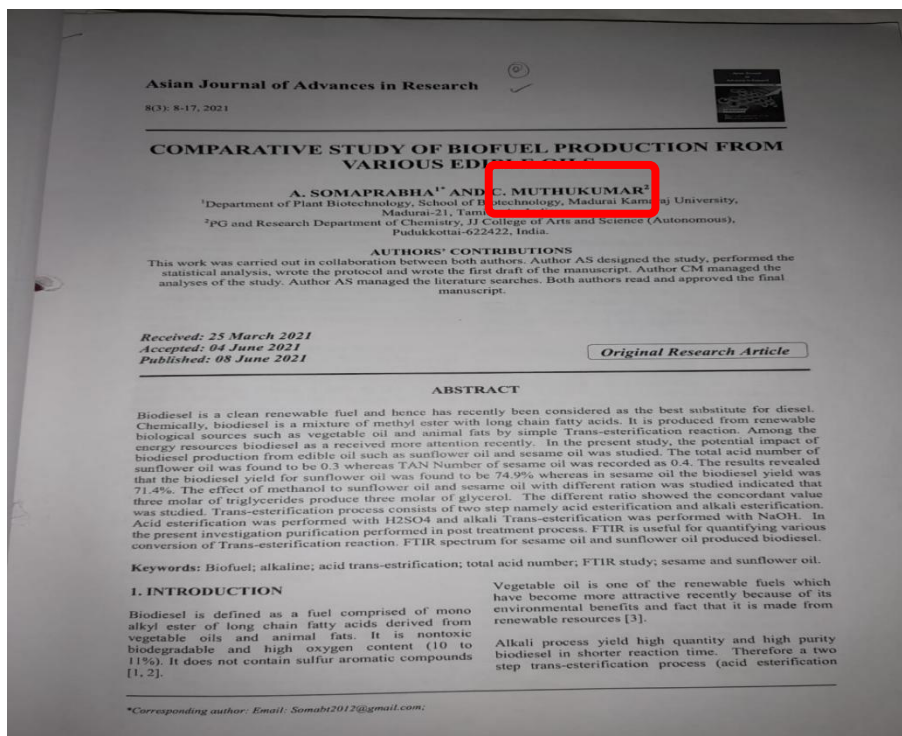
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Volume 38, Issue 01, 2018



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42(15), 1-11, 2021
ISSN: 0256-971X (P)

EVALUATION OF PYRAZOLE AND ITS BIOLOGICAL APPLICATIONS

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AUTHORS' CONTRIBUTIONS

This work was carried out in collaboration among both authors. Both authors read and approved the final manuscript.

Article Information

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Revisions:
(1) Adnan Ahmed Farah Niaz, University of Kordofan, Sudan.
(2) K. Ajay Kumar, University of Mysore, India.

Received: 05 May 2021

Accepted: 10 July 2021

Published: 16 July 2021

Original Research Article

ABSTRACT

Heterocyclic bearing nitrogen constitutes the core structure of number of pharmacological and biologically active interesting compounds. Heterocyclic compounds show vital role in the field of pharmaceuticals. In the present investigation treatment of diseases possess challenging problems due to emerging infectious disease and also due to increased multi drug resistance pathogens in spite of commercially available antibiotics and drugs search for novel compound with theoretical values are mandatory. Pyrazole was screened for anti-bacterial activity against *shigella flexneri*, *E. coli*, *Pseudomonas aeruginosa*, *Pseudomonas fluorescence* respectively. The anti-fungal activity of three fungal namely as *Aspergillus niger*, *Aspergillus flavus* and *Odium coriace* were evaluated and it was found to be pyrazole was found to be effectively. The anti-inflammatory performance of pyrazole compound was tested with formalin induced paw edema test activity by oral administration at a dose level of 100mg/kg compared to reference drug paracetamol. The potential analgesic activity of pyrazole using animal model was carried out with oral administration of pyrazole 100mg/kg of body weight. The anti-pyretic activity of pyrazole was determined on yeast induced pyrexia in albino mice. FTIR is an important tool analyzed to analysis functional group modification of pyrazole and its derivatives. In my research findings, strongly recommended for pyrazole as best drug to the enzyme and greater the number of sites occupied, the more effective the drug is likely to be in inhibiting the action of the enzymes.

Keywords: Pyrazole; anti-microbial; anti-fungal; anti-inflammatory; anti-pyretic and FTIR studies.

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Krishnaveni S., J. Adv. Sci. Res., 2020, 11 (3) Suppl 7: 287-293 287

Journal of Advanced Scientific Research
Available online through <http://www.scienceage.info>

ISSN
0976-9595
Research Article

A STUDY ON BIOSORPTIVE REMOVAL OF HEAVY METAL CHROMIUM FROM AQUEOUS CHROMIUM SOLUTION USING APONOGETON NATANS ROOT POWDER

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ABSTRACT
Pollution is the main problem due to heavy metal discharges from industries. In this study *Aponogeton natans* roots powder (Family: Aponogetonaceae), a biosorbent was selected to remove the heavy metal chromium ion from aqueous chromium solution. Various parameters like pH, biosorbent dose, equilibrium time and metal ion concentration were investigated using batch studies for optimization. A kinetic model study and isotherm model fitting study were studied using Langmuir and Freundlich isotherms. The results revealed that it follows pseudo first order kinetic model and also fit in the Langmuir and Freundlich isotherms. The thermodynamic parameters ΔG , ΔH and ΔS are investigated and reported. The results are very much encouraging. So, it can be used as low cost biosorbent in controlling the pollution.

Keywords: Biosorbent, *Aponogeton natans*, Chromium, Kinetics, Thermodynamic study.

1. INTRODUCTION
The discharge of heavy metals into drain water through industrial actions has become a big issue for humans and aquatic lives. The most familiar toxic pollutants are chromium, lead, cadmium, copper, and mercury. Chromium as a heavy metal is one of the top 16 toxic metals that have destructive effects on human health [1]. Cr(VI) is a strong oxidizing agent and is extremely toxic than Cr(III) [2]. It defectively influences the human being by oxidizing the building block of DNA and some protein molecules. The toxicity of Cr(VI) has negative effects such as skin irritation, asthma, ulceration, and severe diarrhoea. It harms the kidney, circulatory tissues, liver, and nerve tissues. Disclosure to high chromium quantity causes cancer in the digestive tract and lungs [3-5]. Therefore, extensive discharge of Cr(VI) roughly into aquatic sources of potable water has to be regulated through the enactment of legal standards and strict environmental control mechanism [6]. The maximum permitted concentration limit for Cr(VI) for drinking waters that is recommended by the Environmental Protection Agency (EPA) is 0.05 mg/L. Several techniques, such as membrane process, electrochemical precipitation, electrodialysis, ultrafiltration, reverse osmosis, and ion exchange, are possible to remove harmful metals from the aquatic medium [7, 8]. But, these methods are inadequate or costly when Cr(VI) is present in the wastewater at a low concentration. The adsorption technique stays the most preferred procedure because of its efficiency, non-hazardous technique, and low-priced method [9]. The recent adsorbents supply an attractive material, especially if the adsorbent is cheap and ready for use. As a result, we should pay close consideration to the use of natural biomass feasible in large quantities. In recent times, many researchers have achieved the sufficient elimination of Cr(VI) from wastewater, applying natural biomasses such as rice straw [10], *Sterculia guttata* shell [11], fish scales and egg shells [12], activated carbon derived from *Leucaena leucocephala* [13], mangrove leaf powder [14], garlic stem and horse chestnut shell [15], *Juniperus procera* sawdust, avocado kernel seeds and papaya peels [16], *Cornus mas* kernel shell, *Rosa canina* seed shell and *Musa cavendishii* peel [17]. The economic price of these adsorbents is insignificantly correlated to the price of ion-exchange resins or activated carbon. Most of these biomaterials consist of functional groups combined with polysaccharides, proteins, lignin, cellulose, and hemicellulose as major components. Cr(VI) uptake process is united with these functional groups [18]. The search for substituted advanced, cheap,


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

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DFT and Vibrational Studies on 2-(Hydroxymethyl)-3,5-dimethyl-6-(1-aziridinyl)-1H-indole-4,7-dione

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Abstract

In this work vibrations Spectral examination of 2-(hydroxymethyl)- 3,5-dimethyl-6-(1-aziridinyl)- 1H-indole-4,7-dione (2HD6AID) have been explored by theoretical vibration information showed the presence of variable useful gatherings with the all out of atom vibration recurrence. FT-IR and FT-Raman have been determined with the assistance of theoretical and hypothesis techniques. The tasks of vibration spectra have been completed the ordinary co-ordinates examination following the scaled quantum mechanical power field counts. The First hyperpolarizability (β_{ind}) of the novel atoms framework and related properties (μ , α and $\Delta\alpha$) are determined utilizing B3LYP/631G+ (d) and B3LYP/631G++ (d, p) strategy on the limited field approach. The determined HOMO and LOMO energies show that charger move happens inside the particle. Data about the size shape, charge thickness dispersion and site of compound reactivity of the particles has been acquired by planning races thickness is surface with sub-atomic electrostatics potential.

Keywords: DFT Study, Indole, Vibrational Analysis, HOMO-LUMO

1.INTRODUCTION

Bicyclic and heterocyclic structures are widely prevalent in many biologically active molecules [1]. Among various bicyclic and heterocyclic structures represents one of the most significant structures in designing novel drugs. The nitrogen atom present in aromatic heterocycles can interact with the other molecular targets through hydrogen bond [2]. Indole is an N-heterocyclic organic chemical compound, containing benzene ring, fused with the nitrogen-containing pyrrole ring, which is an important building block in pharmaceutical industry [3]. Many bioactive indole compounds have got importance because of their pharmacological and therapeutic activities, such as anticancer, antiviral, anti-inflammatory, anti-hyperglycemic [4]. Indole derivatives have distinct property of representing the structure of peptides and binding reversibly to enzymes [5].

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DFT and Spectral Analysis of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

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ABSTRACT
 In this work vibrational Spectral analysis of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione (SHHMID) have been investigated by theoretical vibration data indicated the presence of variable functional groups with the total of molecule the equilibrium geometry, bonding features, harmonic vibration frequency, FT-IR and Raman intensities have been calculated with the help of density functional theory methods. The assignments of vibration spectra have been carried out the normal co-ordinate's analysis following the scaled quantum mechanical force field calculations. The First hyperpolarizability (β_{xxx}) of the novel molecules system and related properties (μ, α and β_{xxx}) are calculated using B3LYP/6-31+G (d) and B3LYP/6-311++G(d, p) method on the finite-field approach. The calculated HOMO and LUMO energies show that charge transfer occurs within the molecule. Information about the size, shape, charge density distribution and site of chemical reactivity of the molecules has been obtained by mapping electrons density surface with molecular electrostatics potential.

Keywords: Vibrational Spectra, DFT Calculations, HOMO-LUMO, MEP Surface.

INTRODUCTION

Indole is a fragrant heterocyclic compound comprising of intertwined benzene and pyrrole rings through the 2-and 3-places of the pyrrole part. Since its first combination in 1866, indole was found in numerous characteristic items like parasitic metabolites and marine normal items in different bioactive agrochemicals and drugs [1]. The nitrogen particle present in fragrant heterocycles can communicate with the other sub-atomic focuses through hydrogen security [2]. Indole subsidiaries have unmistakable property of addressing the construction of peptides and restricting reversibly to catalyst [3]. Because of this property, indole subordinates clear an astounding method to find novel medications on natural focuses with an alternate method of activity. Indole containing compounds are notable to show an assortment of pharmacological exercises, for example, mitigating [4], cancer prevention agent [5] antidiabetic [6], antiviral [7], antifungal [8], antibacterial [9], and anticancer [10]. Indole may be utilized as a promising platform in the advancement of novel nicotinic opponents [11]. Characteristic cell reinforcements can dodge or if nothing else fundamentally diminish the peroxidation of lipids by free extremists, which are identified with an assortment of issues and infections [12]. Indole is a chromophore of the amino corrosive tryptophan that has acquired obvious premium of numerous scientists to research the instruments of the different photophysical responses going on inside tryptophan particle in different conditions. Because of these properties bright emanation range and fluorescence lifetime to its nearby environmental factors, makes it a fundamental boundary in understanding protein usefulness just as dissolvable availability [13]. In the new time, endeavours have been fixated on the fluorescent conduct of indole compounds in non-fluid conditions. It has been discovered that expansion of modest quantity of alcohols to a non-polar

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DFT Analysis of 1,2 dimethyl -3-(hydroxymethyl)-5-(2-hydroxy ethyl amino)-1H-indole-4,7-dione

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Abstract: In this work vibrations Spectral examination of 1,2 dimethyl -3-(hydroxymethyl)-5-(2-hydroxy ethyl amino)-1H-indole-4,7-dione (D3HSHAD) have been explored by theoretical vibration information showed the presence of variable useful gatherings with the all out of atom vibration recurrence. IR and Raman have been determined with the assistance of theoretical and hypothesis techniques. The tasks of vibration spectra have been completed the ordinary co-ordinates examination following the scaled quantum mechanical power field counts. The First hyperpolarizability (β_{ω}) of the novel atoms framework and related properties (μ , α and $\Delta\alpha$) are determined utilizing R3LYP/631G+ (d) and R3LYP/6311G++ (d, p) strategy on the limited field approach. Data about the size shape, charge thickness dispersion and site of compound reactivity of the particles has been acquired by planning races thickness is surface with sub-atomic electrostatics potential.

Keywords: DFT Study, Vibrational Analysis, Molecular Electrostatics Potential, Indole.

INTRODUCTION

The indole alkaloids and their manufactured analogs have shown critical anticancer [1], cell reinforcement [2], antiviral [3], antimicrobial [4], hostile to material exercises [5]. These characteristic and engineered analogs of indoles additionally show some agrarian as plant development controllers, fungicidal, insecticidal, herbicidal [6-9] and mechanical applications like colors/shades, food supplements, fundamental oils [10-12]. Keeping in see all former meaning of indole moiety and having computational just as manufactured examination foundation [13-14]. Bicyclic and heterocyclic constructions are broadly pervasive in numerous organically dynamic atoms. [15] Among different bicyclic structures, N-heterocyclic construction addresses quite possibly the main designs in planning novel medications. The nitrogen particle present in sweet-smelling heterocycles can collaborate with the other atomic focuses through hydrogen security [16].

The present study is used to predict the optimized molecular structure and vibrational studies of the 1,2 dimethyl -3-(hydroxymethyl)-5-(2-hydroxy ethyl amino)-1H-indole-4,7-dione (D3HSHAD) molecule with the aid of quantum chemical calculations. The vibrational investigations were carried out based on the potential energy distribution (PED) calculation were performed. The present research work predominantly focused on 1,2 dimethyl -3-(hydroxymethyl)-5-(2-hydroxy ethyl amino)-1H-indole-4,7-dione (D3HSHAD) the and its FT-IR, FT-Raman vibrational spectral characterizations.

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DFT and FT-IR, FT-Raman Studies on 1,2-dimethyl-3-(hydroxymethyl)-5-[(2-methoxyethyl)amino]-1H-indole-4,7-dione

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Identification of phytochemical compounds are present in the *senna auriculata* flower with using of FTIR, UV and GC-MS analysis

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ABSTRACT: *Senna auriculata* unremarkably called "tanner's cassia", is wide employed in the Indian System of medicines. The aim of this education was to conclude the view on phytochemical investigation. *Senna auriculata* Flowers are collected in between January and march from hot regions of Pudukkottai in Tamil Nadu, India. To evaluate the phytochemical investigation on ethanolic and aqueous extract of dried powder of *senna auriculata* Flowers. The phytochemical studies carried out by a standard procedure and support of FTIR, UV-Visible and GC-MS analysis. Overall, the studies of Ethanolic and Aqueous extract of *Senna auriculata* flowers shows various phytochemicals which may be used for several diseases as an herbal drug.

KEYWORDS: *senna auriculata*, FTIR, UV-Visible and GC-MS analysis.

INTRODUCTION:

Medicinal plants play a vital role in primary health care for overall population in world. The plants are vital sources for development of potent antimicrobial drugs, they are continued to play a dominant role in maintenance of human health since ancient days [1]. E. O. Fasombi, (2003). The World Health Organization has estimated that 80% of people in Asia and Africa rely on herbal medicines and 25 to 50 % of pharmaceuticals bestowed around the world are of plant origin and few among them have been used as antimicrobials [2]. P. Bharathi et al., (2011). India, the botanical garden of the world is rich in biodiversity and most plants were recognized for their remedial purposes. Herbal technology is India's one of the biggest revenue sources [3]. A. Sharma et al., (2008). The potential of plants as a source of drugs is mostly unexplored. The medicinal properties of the plants are mainly due to the antioxidant, antimicrobial and antipyretic effect of the phytochemicals present in them [4]. A. A. Adesokan et al., (2008). The medicinal properties of a plant are mainly due to the presence of phytochemicals like alkaloids, glycosides, volatile oils, tannins, saponins, etc [5]. Satheesh Kumar Bhandary et al., (2012). The main benefits of using plant-derived medicines are that they are comparatively safer than synthetic alternatives, offering deep therapeutic benefits and more inexpensive treatment [6]. Iwu et al., 1999.

Senna auriculata are evergreen shrub that grows in many parts of India and in other parts of Asia. It is also known as *senna auriculata*. The flower, leave, stems are used especially in ayurvedic medicine. The State flower of Telangana is *senna auriculata*. The dry regions of India and Sri Lanka are the yielders of *senna auriculata*. It is common along the sea coastline and the dehydrated zone in Sri Lanka.

The plant has been reported to treat hyperglycaemia and associated hyperlipidemia [7]. Jayaraj et al., 2011]. This plant is said to contain a cardiac glycoside (oumaphacin) and sap, leaves and bark yield anthraquinones, while the latter contains tannin [8]. JAYAWEEERA, D.M.A., 1981]. The roots of avaram is employed in decoctions against fevers, diabetes, diseases of urogenital system and constipation. The leaves have purgative properties. The dried flowers and flower sprouts are used as a substitute for tea in occasion of diabetes patients. It also improves the complexion. In case of chronic purulent conjunctivitis, the powdered seed is applied to the eye. In Africa the bark and seeds are said to give relief in rheumatism, eye diseases, gonorrhoea, diabetes and gout [9]. JAYAWEEERA, D.M.A. 1981]. The plant has been shown to have antibacterial activity in the laboratory [10]. Manosegulari, S. and T. Navern, 2010]. The powdered dried flower bud is used as a substitute for tea in the case of diabetic patients and it is also fictional to improve the complexion in women and also considered to be one of the important dyes yielding plants in India [11]. Vandana Meena et al., 2019]. Leaves and fruits are used as an anthelmintic and diuretic. Sometimes *Senna auriculata* is cultivated as a decorative. A most interested use of *Senna auriculata* is stated from India. It is believed that branches were formerly used in the fabrication of sweet Damascus steel [12]. Dr. Vustlanuri Padmavathi., 2018].

