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ABSTRACT BOOK

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Table of Contents

BIBLIOMETRIC ANALYSIS IN SCIENTIFIC ARTICLES ON NITROGEN FIXATION IN LEGUMES

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Legumes has a great important in sustainable agriculture because roots are aerate and improve the physical, chemical and biological properties of soil. Legumes also enrich soil for nitrogen throughout simbiyotic nitrogen fixation by rhizobia bacteria in nodules on roots and they provide products with low input. There are many studies about nitrogen fixation in legumes. However, indicating status and trends of researches are great important by bibliometric analysis. Bibliometric analysis is a useful method in literature review that reveals where research is done on a topic, models and mapping of research fields. In this study, 356 publications on nitrogen fixation of legumes between 1980-2022 were investigated using Web of Science (WoS) data and VOS viewer programme by bibliometric analysis methods. The highest number of publication on nitrogen fixation of legumes was produced in 1987, while the lowest one was in 1989. Peoples, M. had number of highest documents and citations followed by Sprent, J. The most citation was achieved from year of 2021 with 1038 while the lowest was in 1980. Journal Plant and Soil has the most record count of publications. The organization with most publications was CSIRO. Swedish University Agricultural Sciences and CSIRO had the number of highest citations. USA and Australia had the largest numbers of publications. As a results, the aim of the study revealed fields of research, identify the main journal, authors, countries, research trends on nitrogen fixation of legumes by bibliometric analysis methods.

Keywords: bibliometric analysis, legumes, nitrogen fixation, web of science

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IN SILICO IDENTIFICATION OF NATURAL COMPOUNDS AS PESTICIDES AGAINST PLUTELLA XYLOSTELLA

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Plutella xylostella (diamondback moth), a major invasive pest of Brassica crops, feeds on cruciferous plants and causes serious economic loss. The moth has spread worldwide owing to its short life cycle, high fecundity, and capability to migrate long distances. Chlorantraniliprole is a human-made insecticide widely used to control P. xylostella. On the other hand, resistance to chlorantraniliprole was reported in the literature. The use of natural compounds as pesticides can eliminate resistance and reduce potential harm to humans. In the present study, natural compounds were identified as potential pesticide candidates in silico. To achieve this goal, the binding potentials of over 3000 natural compounds found in the MPD3 database to the diamondback moth ryanodine receptor N-terminal domain (PDB:5y9v) were scanned using AutoDock Vina. The active sites of the target proteins were identified using PyMOL software. The first filtration was applied according to the binding energies, with a threshold of -6,0 kcal/mol. Second, the binding affinities to the N-terminal region of the human ryanodine receptor 2 (PDB:4jkq) of the candidates were checked. Candidates were then filtered according to the ADME properties based on Lipinski's rule of five using DruLiTo software. Finally, toxicity (oral toxicity, hepatotoxicity, carcinogenicity, immunotoxicity, mutagenicity, and cytotoxicity) was evaluated using ProTox II online server. In addition, the binding energy and toxicity of chlorantraniliprole were compared. Chlorantraniliprole binds to 5y9v with a binding energy of -3,5 kcal/mol while binds to 4jkq with higher affinity (-6,8 kcal/mol). Moreover, it may cause hepatotoxicity. Dorsmanin B, chartaceone B, and 7-O-galloyltricetifavan bind to 5y9v with a binding energy of -6,1 kcal/mol, -6,0 kcal,/mol, -6,1 kcal/mol, respectively while binding to 4jkq with lower affinity (0,1 kcal/mol, -2,4kcal,/mol, -2,9 kcal/mol, respectively). In addition, these candidates did not show any toxicity. These natural compounds can be used instead of chlorantraniliprole to control Plutella xylostella.

Keywords: plutella xylostella, natural compounds, pesticide

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INVESTIGATION OF TOTAL PHENOLIC, TOTAL FLAVONOID CONTENT AND ANTIOXIDANT ACTIVITY OF ONOBRYCHIS MEGATAPHROS LEAF EXTRACT

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This study aims to determine the total phenolic, flavanoid and antioxidant activity levels of Onobrychis megataphros plant leaves. Therefore, firstly, O.megataphros (Sainfoin) bicry samples were collected, laid on blotting papers in shady places away from sunlight and dried. The completely dried plant samples were pulverized. The powdered bicry samples were extracted with methanol using Soxhlet device. The methanol was removed by evaporation in a rotary evaporator and stored at +4ºC until the experiment starts. Phenolic and flavanoid content and antioxidant activity properties of O.megataphros plant leaf extracts were investigated. To determine total phenolic content, sample solution (0.25 mL) was mixed with diluted Folin-Ciocalteu reagent (1 mL, 1:9) and shaken vigorously. After 3 min, Na_2CO_3 solution (0.75 mL, 1%) was added and the sample absorbance was read at 760 nm after 2 h incubation at room temperature. For total flavonoid content, sample solution (1mL) was mixed with the same volume of aluminum trichloride (2%) in methanol. Similarly, a blank was prepared by adding sample solution (1mL) to methanol (1mL) without $AlCl_3$. The sample and blank absorbance were read at 415 nm after 10 min incubation at room temperature. Absorbance of the blank was subtracted from that of the sample. Total antioxidant activity of the samples was evaluated by phosphomolybdenum method. Sample solution (0.2mL) was combined with 2mL of reagent solution (0.6M sulfuric acid, 28mM sodium phosphate and 4mM ammonium molybdate). The sample absorbance was read at 695nm after 90 min incubation at 95°C. As a result, it was determined that the total phenolic content in O.megataphros plant leaf extracts was 20.62±0.15 mg GAE/g extract and total flavonoid content was 24.55±0.22 mg QE/g extract. As a result of our study, it was determined that TAS and TOS levels increased with the increase in concentration.

Keywords: onobrychis megataphros, total phenolic content, total flavonoid content, antioxidant activity

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DETERMINATION OF THE COEFFICIENT OF THERMAL EXPANSION IN A NON-LINEAR ELASTIC ROD OF TWO CONCENTRIC LAYERS

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Layered material systems find wide application in different sectors of modern technics (components of load-carrying structures, electronics, optical devices, sport facilities, engineering infrastructure, aeronautics, aerospace, etc.). In many applications, layered components are subjected to temperature change during their life-time. Besides, some layered material systems have non-linear elastic mechanical behaviour, i.e. their stress-strain constitutive law is non-linear. In such cases the Hook's law is not applicable. Also, the coefficients of thermal expansion of the layers are different. The present theoretical paper treats the problem of determination of the coefficient of thermal expansion of a rod with two concentric longitudinal layers. The layers exhibit non-linear elastic behaviour. Besides, the layers have different thickness. The rod is exposed to temperature change. The coefficient of thermal expansion of the rod is derived by analysing the thermal strains in the two layers. Since the layers are soundly connected, the strains in the layers are equal (this fact is used to work out an equation for determining the coefficient of thermal expansion of the rod). The case when the two layers of the rod are continuously inhomogeneous along the rod length is also considered. In this case the material properties of the layers vary continuously along the rod length. Here again the layers have non-linear elastic mechanical behaviour. Analysis of the distribution of strains along the length of the rod is carried-out when deriving the coefficient of thermal expansion of the rod. A comparison with the coefficient of thermal expansion of a rod having linear-elastic mechanical behaviour is performed for check-up of the solutions obtained in the present paper.

Keywords: concentric layers, rod, circular section, coefficient of thermal expansion, temperature

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CURVATURE ANALYSIS IN A BI-LAYERED NON-LINEAR ELASTIC BAR UNDER UNIFORM HEATING

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Bi-layered materials are frequently applied in various areas of up-to-date engineering. They are used for manufacturing of components of different structures, facilities and devices in car industry, aeronautics, civil engineering, power plants, optics and electronics. These materials are preferred to traditional homogeneous engineering materials because of their superior properties especially in applications in extreme conditions (high temperature, humidity, etc.). However, the layers of a bi-layered material system have different coefficients of thermal expansion. This fact indicates the importance of studying various aspects of the behaviour of structural components made of bi-layered materials subjected to hitting. Also, in some cases the mechanical behaviour of bi-layered material systems is non-linear elastic (this necessities application of non-linear stress-strain relationships since the Hook's law does not hold). Very often the bi-layered structural components have rectangular section. Therefore, the present theoretical paper is concerned with analysis of the curvature in a bi-layered bar of rectangular cross-section. The bar is subjected to uniform heating. The two layers of the bar have different thickness and material properties. Besides, the layers exhibit non-linear elastic mechanical behaviour that is treated by applying a power-law stress-strain constitutive relationship. The bi-layered bar curvature is derived analytically. For this purpose, the mechanical response of the bar to uniform heating is investigated. The strains in the two layers due to heating are analyzed. An equation is compiled by using the fact that the prolongations of the bar layers are equal. Two equations are work out by considering the equilibrium of the layers. The solution of the curvature derived is checked-up by comparing with a known solution for the curvature in a bi-layered linear-elastic bar under uniform hitting. The temperature induced curvature of a bar whose two layers are continuously inhomogeneous in longitudinal direction is also derived.

Keywords: curvature, bi-layered bar, uniform heating, non-linear elastic behaviour, continuously inhomogeneity

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ORGANIC CHEMICAL SYNTHESIS OF NAPHTHALENE DERIVATIVE CARBAZOLE MONOMER AND DETERMINATION OF ITS HOMO-LUMO ENERGY LEVELS

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The use of renewable energy sources, which is becoming increasingly widespread in the world, is increasing. Among these energy sources, solar energy has an important place. Photovoltaic devices are systems that can directly convert solar energy into electrical energy. Electron donor carbazole is widely used in solar cells due to its wide band gap, optical and photoconductive properties. In this study, naphthalene derivative carbazole was synthesized as a monomer to be used in solar cell design. This monomer contains n-octylcarbazole as electron donor and naphthalene as π-spacer group. Naphthalene with high π bond conjugation emits strong fluorescence in the range of 200-400 nm. The synthesized new carbozol-derived monomer structure was analyzed by FT-IR, ^{1}H-NMR, ^{13}C-NMR, CHN methods. To investigate the electrochemical performance of the monomer, the oxidation of the monomer was examined on three different electrode (Au, Pt, Gc). surface in dichloromethane solution containing tetrabutylammonium hexafluoraphosphate using the cyclic voltammetry method. The optimum oxidation performance of the monomer was obtained from voltammograms taken between -0.2 and 1.6 V on the glassy carbon (Gc) electrode surface. The HOMO-LUMO energy levels and UV absorption of the synthesized compound were determined. $Eg_{(el)}$ and $Eg_{(opt)}$ values obtained from CV and UV graph and band gaps were compared.

Keywords: solar cells, carbazole, elektrochemistry

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ELECTROCHEMICAL POLYMERIZATION OF A NOVEL THIOPHENE-DERIVED MONOMER AND ITS USE AS SUPPORT MATERIAL FOR METHANOL OXIDATION

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This research, conductive polymer supported modified electrode system which was prepared for usage in direct methanol fuel cells. To test the behavior of these electrode system for methanol oxidation, cyclic voltammetry (CV), chronoamperometry (CHR) and electrochemical impedance spectroscopy (EIS) methods were used as electrochemical methods. As the working electrode, pencil graphite electrode (PGE) was preferred because of its porous structure, good ion conductivity, practicality in application and ease of preparation and obtaining. Thiophene derivative 4,4')-2,2'-(diazen-1,2 diylbis(4,1 phenylene))bis(4 (thiophene-2-ylmethylene) oxazol-5(4H)-one), (DiAzBiPhBiTyOx) monomer was prepared and electrochemically polymerized by CV method in 0.01M TBAP and 0.05 $HClO_4$ containing ACN solution on the surfaces of PGE. The spectroscopic characterization of the synthesized monomer was performed by NMR spectroscopy. Optimum polymerization conditions of monomer was determined according to scanning rate, potential range and acid density. The obtained modified electrode system (PGE/PDiAzBiPhBiTyOx) was doped with chloroplatinic acid hexahydrat-Pt2Cl6.6H2O (Pt) at different densities and the optimum catalyst density was determined as 3.25mM (PGE/3.25mMPt@PDiAzBiPhBiTyOx). The methanol oxidation performances of conductive polymer film, platinum and conductive polymer supported platinum catalyst systems were investigated separately. While the methanol oxidation responses of the conductive polymer film and platinum are almost similar, the methanol oxidation response of the platinum doped conductive polymer film catalyst system is higher. The modified electrode characterization was performed by CV, CHR and EIS methods. Furtheremore obtained modified electrode systems were characterized by FESEM/EDS, XRD to confirm the structures and morphologies. Also, the theoretical values such as electrochemical surface area (ECSA) and specific capacitance (Cs) were calculated in aqueous acidic solution with and without methanol. Cs values of the PGE/3.25mMPt@PDiAzBiPhBiTyOx electrode in aqueous acidic solution with and without methanol were 3.861 and 3x10-4Fg^{-1} respectively. Also, the electrochemical surface area values of the same electrode in aqueous acidic solution with and without methanol were 196.437 and 21.150m2g^{-1} respectively.

Keywords: methanol oxidation, platinum, conductive polymer

SYNTHESIS AND CHARACTERIZATION OF 3,6-DISUBSTITUTED CARBAZOLE CONTAINING FLUORENE AND DSSC APPLICATIONS

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Heterocyclic compounds containing nitrogen are regarded as essential structural motifs present in numerous natural products and organic materials. Within this group, carbazoles are important hetero-aromatic molecules which play a significant role in the development of materials with various functionalities. Carbazole derivatives play a crucial role in various organic electronic devices such as organic transistors (OTFTs), organic light-emitting diodes (OLEDs), and organic solar cells. In this study, the solubility of the carbazole nucleus, which initially had limited solubility in organic solvents, was increased by adding an octyl group. Next, a carbazole-based compound 3,6-di(fluorene-9)-9-octyl-9H-carbazole (IV) was synthesized via the Suzuki-Miyaura cross-coupling reaction (Scheme 1). The photophysical and thermal properties of this compound were determined by UV-Vis, thermogravimetric analysis (TGA) and differential thermal analysis (DTA). the HOMO and LUMO energy levels and the optical band gap (Eg,opt) were obtained by cyclic voltammetry (CV) and absorption bands. TiO_2-based dye-sensitized solar cells (DSSCs) were fabricated using compound IV. The photoelectrochemical properties of the resulting TiO_2-DSSCs were measured.

Keywords: carbazole, suzuki-miyaura cross coupling, cyclic voltammetry, dssc.

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SYNTHESIS OF SOME CARBAZOLE-DERIVED MOLECULES AND INVESTIGATION OF THEIR ELECTROCHEMICAL AND PHOTOPHYSICAL PROPERTIES

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Carbazole is an aromatic compound due to its conjugated double bond system. Aromatic stability is achieved through the delocalization of π-electrons across the two benzene rings and the nitrogen atom. It is noteworthy that electron-withdrawing groups such as -F, -CN, -CF_3 are commonly used to adjust the electronic properties of carbazole derivatives. The fluorine atom, possessing high electronegativity and a small atomic radius, has the capacity to modulate molecular energy levels and enhance electron mobility when attached as a substituent to the molecule. Structures containing C-F bonds are extensively employed in biomedical active systems and electronic material design (such as OLEDs, DSSCs). Organic compounds containing fluorine atoms gain high stability against oxidation due to their lower HOMO/LUMO energy levels. Additionally, these compounds exhibit increased reduction potentials, facilitating the electrochemical decomposition of fluorine compounds. In this study, two carbazole-based compounds 3,6-bis(4-(trifluoromethyl)phenyl)-9-octyl-9H-carbazole (IVa) and 3,6-bis(3,4,5-trifluorophenyl)-9-octyl-9H-carbazole (IVb) was synthesized via the Suzuki-Miyaura cross-coupling reaction (Scheme 1). The photophysical and thermal properties of this compound were determined by UV-Vis, thermogravimetric analysis (TGA) and differential thermal analysis (DTA). The oxidation potentials of the molecules were determined on the gold electrode surface in dichloromethane solution containing tetrabutylammonium hexafluorophosphate using the cyclic voltammetry method. The HOMO and band gap (Eg,opt) energies were calculated from oxidation potential and absorption bands. Similarities in the electronic structures of compounds with similar structures containing CF_3 and F were identified using the obtained data.

Keywords: suzuki-miyaura cross coupling, cyclic voltammetry, homo/lumo

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SYNTHESIS AND SOME ELECTROCHEMICAL PROPERTIES OF CARBAZOLE DERIVATIVE MONOMERS FOR OPTOELECTRONIC DEVICE DESIGN

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Low-cost instruments are used to achieve high sensitivity, accuracy and precision with electrochemical techniques, making them the most suitable analytical methods used to investigate the electrochemical properties of a new molecule. Among these techniques, cyclic voltammetry, which is widely employed, allows for the determination of electronic characteristics such as molecular energy levels and orbital structure, redox properties, sensor capabilities, surface activity, and more. The carbazole molecule can undergo derivatization from various positions, allowing for alterations in its electrical and optical properties. These compounds serve as heterocyclic building blocks that can be utilized as materials for organic sensitizers and semiconductors in optoelectronic devices. Due to the presence of a hydrogen atom in the nitrogen-hydrogen (N-H) bond within the carbazole structure, which can be replaced with different functional groups, carbazole is highly suitable for nitrogen-based derivatization studies. In this study, two different carbazole monomers (IIa and IIIa), which could be potential optoelectronic, were synthesized using the Ullman and Suzuki-Miyaura reaction and characterized using ^{1}H NMR, ^{13}C NMR, UV-Vis, and Flouresence spectroscopy techniques. The cyclic voltammetry experiments were performed using three different working electrodes (Au, Gc, Pt disk electrodes) for each compound. Since the optimum oxidation of the compounds was obtained from the voltammograms on the gold disk electrode, this electrode was used in the calculation of energy levels. HOMO and Eg values of the compounds were deduced from cyclic voltammetry experiments and the optical absorption bands, respectively.

Keywords: organic optoelectronics, suzuki-miyaura reaction, cyclic voltammetry, band gap energy levels.

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SOME FIXED POINT RESULTS OF (α, β, ϕ, δ)-CONTRACTIONS IN EXTENDED B-CONE METRIC SPACE

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The study of fixed points of various functions in generalized metric spaces is an important issue of Fixed Point Theory. Recently the generalization of metric space plays a crucial role in this theory such as extended metric space. The extended metric space was defined for the first time in 2017, by Kamran et al. They replaced the constant in the triangle inequality of the metric by a two variable function and studied some fixed point theorems in it. In 2022, Das and Bag introduced extended cone metric spaces by using a three variable map in third condition of cone metric. Later, Selko and Sila gave the notion of extended quasi cone b-metric space and proved Banach contraction in it. Alqahtani et al., in 2018 proved some fixed point results for a couple of orbital cyclic functions in extended metric space. In this paper, we prove some fixed point theorems for (α, β)-orbital cyclic functions in extended quasi cone metric spaces by using the continuous maps ϕ and a nonnegative constant δ.

Keywords: (α β)-orbital cyclic functions, fixed point, extended quasi cone metric space, cone metric space

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ON FIXED POINT RESULTS FOR NONLINEAR CONTRACTIONS IN FUZZY CONE METRIC SPACE

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Fixed Point Theory has been the object of study for many authors during the years, especially for its applications in a wide range of metric spaces such as cone metric spaces. fuzzy metric spaces, fuzzy cone metric spaces, etc. The Fuzzy metric space concept was introduced by Kramosil and Michalek as an approach of probabilistic space in Fuzzy sets Theory which was studied for the first time by Zadeh. Many researches have studied the topologies of these spaces and proved fixed point theorems on them. The mathematicians Huang and Zhang defined the cone metric spaces by generalizing the metric using a subset of a real Banach space. Initiating by above, Oner et al. gave the definition of fuzzy cone metric space by operating with a cone. The concept of nonlinear contraction was given by Boyd and Wong. Dutta and Choudhury generalized this contraction by using two auxiliary functions. In this paper we prove some theorems which guaranties the existence and the uniqueness of a fixed point for a generalized nonlinear contraction.

Keywords: fixed point, fuzzy cone metric space, generalized nonlinear contraction, auxiliary function

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SYNTHESIS, MOLECULAR STRUCTURE, SPECTRAL ANALYSIS, HOMO-LUMO AND MOLECULAR DOCKING STUDY ON A THIAZOLIDIN-4-ONE DERIVATIVE

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Thiazolidinone compounds have garnered significant attention in recent decades due to their crucial role in the realm of organic chemistry. Their importance stems from their proven utility in the material sciences as well as their theoretical significance. This work focuses on the synthesis, characterization, and structural study of the thiazolidinone derivative compound of chemical formula $C_{26}H_{21}N_3O_5S$. The synthesized compound was characterized with spectroscopic analysis (FTIR-IR, UV-visible, (^{1}H, ^{13}C) NMR) and single crystal X-ray diffraction. To interpret the intramolecular charge transfer (ICT), natural bond orbital (NBO) analysis is performed. HOMO-LUMO orbitals and global reactivity descriptors are determined, considering the charge transfer within the molecule. Reactivity and stability are assessed using global chemical parameters obtained from HOMO-LUMO analysis. Furthermore, the electrophilicity index is calculated based on electronic chemical potential and chemical hardness. A lower chemical potential and electrophilicity index indicate a more reactive nucleophile, while a higher value suggests a good electrophile. UV-Visible spectroscopic studies and calculated band-gap energy help to interpret charge transfer within the molecule. Additionally, Mulliken population analysis, molecular electrostatic potential (MEP), and thermodynamic parameters are investigated. All calculations were performed using the DFT/B3LYP method in the gas phase. Furthermore, molecular docking was performed in order to develop the biological application of the synthesized derivative.

Keywords: thiazolidinones, molecular structure, dft, homo-lumo, molecular docking.

STUDY OF THE INHIBITORY EFFECT OF THIAZOLE DERIVATIVES AGAINST TUMOR NECROSIS FACTOR (TNF-α) BY MOLECULAR DOCKING

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Tumor necrosis factor alpha (TNFα) is a pleiotropic cytokine that facilitates immune evasion, survival, and resistance to the treatment of malignant cells by generating a favorable environment for them [1]. Several attempts have been made to develop potential inhibitors against TNFα, and protein-based drugs have been approved by the FDA [2], however, these inhibitors have several adverse effects [3]. Therefore, the development of small molecules against this receptor is ideal for long-term use [4]. Thiazole derivatives are actually a considerable group of heterocyclic compounds that have therapeutic effects against several diseases [5]. In this study, we carried out the molecular docking of new hemi-synthesized thiazole derivatives, with TNFα whose three-dimensional structure was extracted from the RCSB protein database, and the structures of the thiazole derivatives were drawn and converted into files. pdb using ChemDraw 16.0 and ChemDraw3D 16.0 successively, and geometry optimization was performed with Gaussian 03 software and Gauss-View program using DFT (B3YLP) with basis set 6-31G(d, p). Molecular docking was performed by Autodock 4.2 using the Lamarkian genetic algorithm method. Molecular docking results revealed that all complexes formed between the newly synthesized ligands and TNFα exhibited well-established hydrogen and Van Der Waals bonds between the ligand and several amino acids in the active pocket of the receptor. The binding energies of the complexes formed vary between -8.25 and -7.71 kcal/mol, and the inhibition constants are between 0.901 and 2.240 μM. Compared to the drug Methotrexate and Molecule 307, synthesized heterocyclic compounds may be good candidates for inhibiting TNFα.

Keywords: molecular docking, tnfα, thiazole derivatives, hemi-synthesis

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SYNTHESIS, MOLECULAR STRUCTURE, DFT ANALYSIS AND MOLECULAR DOCKING OF THE THIAZOLOBENZIMIDAZOLE DERIVATIVE

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Heterocyclic compounds occupy an important place in chemistry and the medicinal field; they constitute the basis of many natural, semi-synthetic, or totally synthetic drugs. Due to their biological activities, thiazolobenzimidazole derivatives have been evaluated for their antibacterial, anti-inflammatory, antidiabetic, anticonvulsant, and antidepressant agents. In this work, the organic compound 5-(furan-2-ylmethylidene) thiazolo[3,4-a] benzimidazole-2-thione with the chemical formula $C_{14}H_8N_2OS_2$ was synthesized and characterized by FTIR, UV-Vis, NMR, and single crystal X-ray diffraction. By molecular modeling and using the GAUSSIAN program, we performed theoretical calculations by the DFT method using the 6-311G (d, p) basis set. The calculation carried out makes it possible to obtain the IR and UV-visible spectrum, molecular electrostatic potential, gap energy, and other properties of the studied compound. The structural parameters obtained by theoretical calculations are compared with those obtained by XRD. DFT analysis indicates a good agreement between the experimentally determined and the theoretically calculated molecular structures. By molecular docking, the title molecule was tested as an inhibitor for the C-Met protein (PDB ID: 5EOB), Alzheimer's protein (PDB ID: 6LVM), and COVID-19 (PDB ID: 6LU7) as targets. The AutoDock vina program was chosen for the molecular docking and the results were visualized using the BIOVIA Discovery Studio Visualizer software. The calculation shows different types of interactions between the ligand and receptors. According to the results obtained, the organic molecule studied could be a good inhibitor for all proteins.

Keywords: synthesis, dft, thiazolobenzimidazole, docking, covid-19

RECOVERY OF AGRICULTURAL WASTE FOR WATER TREATMENT

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This work consists of studying the biosorption of Congo red on the peel of cactus and forest leaves in continuous mode (fixed bed column) by developing the performance of this sorption column. Supports prepared from cactus peel and forest leaves were characterized by SEM/EDS, IRTF, and iodine numbers. The characterization of the biomaterials used indicated the presence of several functional groups, heterogeneous air, and significant values of the iodine value of the adsorbent surfaces of PC and FF. The study showed that increasing the initial concentration accelerates the breakthrough due to the high availability of RC substances at bed surface sorption sites. The strong flows make the breakthrough curve faster and quickly reach saturation. The adsorption kinetics were analyzed using the kinetic models of Thomas and Yoon-Nelson. Kinetic data were well described by both models. The maximum sorption capacity calculated from the Thomas model generally increases with increasing flow rate and initial RC concentration. For Yoon and Nelson's model, the time required for 50% breakthrough decreases with increasing flow rate and initial dye concentration. The kinetic data are well correlated with the two models. Comparison of the experimental breakthrough curve to the breakthrough profile obtained from the method of Thomas and Yoon-Nelson showed a satisfactory fit for Congo red sorption on peels of cactus and forest leaves continuously.

Keywords: congo red, cactus peel, forest leaves, sorption, column.

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NANO πG*S-SEPARATION AXIOMS IN NANO TOPOLOGICAL SPACES

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Lellis Thivagar introduced the notion of Nano topology by using theory approximations and boundary region of a subset of a universe in terms of an equivalence relation on it and also defined Nano closed sets, Nano-interior and Nano-closure in a Nano topological spaces. In 2018, P. Satish Mohan, V. Rajendran and P. Jeevitha introduced a new class of sets called Nano π generalized star semi-closed (πg*s-closed) sets and Nano πg*s-open sets and studied their basic properties in Nano topological spaces. They showed that a new class of sets lies between the class of Nano πg-closed sets and the class of Nano πgs-closed sets. Further the notion of Nano πg ∗s-open sets, Nano πg ∗s-neighbourhoods, Nano πg∗s-interior and Nano πg ∗s-closure were discussed. Several examples were also provided to illustrate the behaviour of new sets and functions. The class of sets namely πg*s-open sets are playing more important role in topological spaces, because of their applications in various fields of Mathematics and other real fields This paper is devoted to the introduction of Nano πg*s-Separation Axioms namely Nano πg*s-T0 space, Nano πg*s-T1 space, Nano πg*s-T2 space, Nano πg*s-Regular space, Nano πg*s-Normal space, almost Nano πg*s-Normal space, mildly Nano πg*s-Normal space, Nano πg*s-Compact space and Nano πg*s-Connected space in Nano topological spaces. We investigate the fundamental properties and characterizations of these spaces in Nano topological spaces.

Keywords: nano πg*s-ti-space, nano πg*s-regular, nano πg*s-normal, nano πg*s-compact space, nano πg*s-connected space

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SOFT G*β-SEPARATION AXIOMS IN SOFT TOPOLOGICAL SPACES

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During recent years, soft theory emerged as a best mathematical tool to deal with uncertainties, imprecision and vagueness. Many engineering, medical science, economics, environment problems have various uncertainties, and the soft set theory came up with the reasonable solutions to these problems. Some researchers have provided some applications of soft set theory in software engineering, innovation, medical diagnosis, data analysis, decision making etc. Recently several researchers introduced the notion of soft topology and established that every soft topology induces a collection of topologies called the parametrized family of topologies induced by the soft topology. They discussed soft set-theoretical operations and gave an application of soft set theory to a decision-making problem. Several mathematicians published papers on applications of soft sets and soft topology. Soft sets and soft topology have applications in data mining, image processing, decision-making problems, spatial modeling, and neural patterns. Research works on soft set theory and its applications in various fields are progressing rapidly. Decision-making and topology have a long joint tradition since the modern statement of the classical Weierstrass extreme value theorem. In 2020 Punitha Tharani and H. Sujitha introduced a new class of soft generalized star β-closed (soft g*β-closed) sets and soft g*β-open sets in soft topological spaces. They investigated some basic properties of soft g*β-closed sets and soft g*β-open sets. They also studied the relationship between this type of closed sets and other existing closed sets in soft topological spaces. The aim of this paper is to introduce some soft separation axioms called soft g*β-R0 space, soft g*β-R1 space, soft g*β-T0 space, soft g*β-T1 space, soft g*β-T2 space, soft g*β-regular space and soft g*β-normal space in soft topological spaces. We investigate several properties and characterizations in soft topological spaces.

Keywords: soft g*β-open set, soft g*β-ri space, soft g*β-ti space, soft g*β-regular space, soft g*β-normal space

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G**β-CONTINUOUS AND G**β-IRRESOLUTE MAPPINGS IN TOPOLOGICAL SPACES

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Topology being somehow very recent in nature but has got tremendous applications over almost all other fields. Theoretical or fundamental topology is a bit dry but the application part is what drives crazy once we get used. Topology has applications in various fields of Science and Technology, like applications to Biology, Robotics, GIS, Engineering, Computer Sciences. Topology though being a part of mathematics but it has influenced the whole world with so strong effects and incredible applications. The concept of continuity is fundamental in large parts of contemporary mathematics. In the nineteenth century, precise definitions of continuity were formulated for functions of a real or complex variable, enabling mathematicians to produce rigorous proofs of fundamental theorems of real and complex analysis, such as the Intermediate Value Theorem, Taylor's Theorem, the Fundamental Theorem of Calculus, and Cauchy's Theorem. In the early years of the Twentieth Century, the concept of continuity was generalized so as to be applicable to functions between metric spaces, and subsequently to functions between topological spaces. Topology is an area of mathematics concerned with the properties of space that are preserved under continuous deformations including stretching and bending but not tearing. In 2023, Dr. T. Delcia and M. S, Thillai introduced a new type of closed sets called g**β-closed sets and investigated their basic properties including their relationship with already existing concepts in Topological Spaces. In this paper, we introduce g**β-continuous function, g**β-irresolute function, g**β-open function, g**β-closed function, pre-g**β-open function, and pre-g**β-closed function, and investigate properties and characterizations of these new types of mappings in topological spaces.

Keywords: topological space, g**β-closed set, g**β-continuous function, g**β-irresolute function, g**β-open function

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LARGE PARTICLES ZNO POWDERS FOR PHOTOCATALYTIC REMOVAL OF PARAQUAT DICLORIDE

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ZnO photocatalysts was applied in the photocatalytic removal of paraquat dichloride. The synthesized ZnO was characterized via XRD, FESEM-EDX, FTIR, and XPS. Findings indicated that ZnO allowed degradation of paraquat dichloride under UV irradiation by the rate of ~42%. XRD pattern indicated the presence of ZnO (zincite) crystalline. FESEM results revealed that the observed shape of ZnO is nanorods indicating large particle sizes. FTIR analysis clearly demonstrated the spectra of ZnO powder catalyst. Kinetic study of the degradation process was performed and the influence of ZnO dosage and initial paraquat concentration were investigated on the treatment performance for the reaction. Under the optimized condition (pH = 7, PQ =15 mg/L and catalyst loading =0.8mg/L), the stability and reusability of the powder catalyst was also evaluated over five sequential treatment runs, and the catalyst maintain some reactivity. Recyclability of the ZnO as catalyst in photodegradation processes are also reported in this study.

Keywords: keywords: zinc oxides, photocatalyst, removal, paraquat dichloride, characterization, zinc oxides

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NUMERICAL COMPUTATION OF NMR MAGNETIZATION FOR VARIOUS TISSUES IN THE HUMAN BODY USING ORINGINPRO

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Nuc1ear magnetic resonance (NMR) spectroscopy and imaging arexarguab1y the most versati1e techniques use in biomedica1 research today. NMR spectroscopy is a powerfu1 and theoretica1 ana1ytica1 too1s. Since the deve1opment of NMR spectroscopy it is has become a very important too1s in the fie1d of medicine because of it being safer than the X-ray crysta11ography which has radiation effects on the human body. The most attractive features of NMR techniques are the wide range of bio1ogica1 processes that can be investigated using these methods and the variety and versati1ity of the specific MR techniques that can be app1ied. diagnosis of diseases. With the advent of computer programme, different computer programme has a1so being deve1oped for NMR spectroscopy for performing different ana1ysis on how e1ectromagnetic radiation interact with various form of matter. This research perform NMR ana1ysis of different tissue in the human body using Originpro. The research investigates various tissues of the human body, with the aid of Bloch flow equation the research obtained the transverse magnetization equation that was used for the tranverse magnetization map for the different tissues. Three different relaxation times consider for the different biological tissues are 0.5 T, 1.0 T and 1.5 T. The transverse magnetization for the various tissues are ca1cu1ated at different magnetic f1ux density, at range of 0-0.02 seconds and a length for the tissues were in the range of $4.5x10^{-12\ to}$ $4.5x10^{-}$m. The result shows that transverse magnetization was greater at 0.5 T for the tissues considered at the range of $4.5x10^{-12}$ to $4.5x10^{-5}$ m.

Keywords: bloch equation, nmr, relaxation time, tissues, originpro

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APPROXIMATE ANALYTIC SOLUTION FOR FRACTIONAL DIFFERENTIAL EQUATIONS WITH A GENERALIZED FRACTIONAL DERIVATIVE OF CAPUTO-TYPE

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This paper introduces the analytic series solution of the differential equation with fractional Caputo-type derivative including two parameters using the homotopy analysis method (HAM). The main properties of the fractional derivative with two parameters are illustrated. The standard HAM converges for a short domain, so we modify the method to overcome this issue by dividing the domain into finite subintervals and applying the method to each one. The initial conditions in each subinterval can be obtained from the previous one In this way, a continuous piecewise function that converges to the exact solution can be constructed. The effect of each fractional parameter on the solution behaviors is presented in figures and tables. Several examples are presented to verify the validity of the algorithm. A comparison with the exact solution in the case of integer derivative and with the Adaptive predictor corrected algorithm in the case of fractional one demonstrates the efficiency of the method.

Keywords: homotopy analysis method, fractional calculus, numerical methods

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SYNTHESIS, BIOLOGICAL EVALUATION AND THEORETICAL STUDIES OF HYDRAZONE DERIVATIVES

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The Hydrazones possesses some particular properties which make them a potential candidate for designing new moieties. They contain a C=N bond in conjugated form with a functional nitrogen electron pair. They are distinguished from other members of this class (imines, oximes) by the presence of two interlinked nitrogen atoms . These nitrogen atoms are nucleophilic, while the carbon has both an electrophilic and nucleophilic nature and further combining hydrazones with numerous functional groups leads to the formation of products with unique biological properties. The aim of this work is to synthesize, characterize and evaluate the biological activity of a series of hydrazone derivatives. These new compounds were characterized by elemental analysis, IR spectroscopy, mass spectrometry, UV-Vis Spectroscopy, Scanning Electron Microscopy (SEM) and ^{1}HNMR spectra and thermogravimetric analysis (TGA). In vitro, Their antibacterial and antifungal activities were screened against bacterial species (Staphylococcus aureus, Bacillus subtilis and Escherichia coli) and fungi (Candida albicans). In silico, The Toxicity were studied by ADMET simulations. A structural, energetic and electronic theoretical study was carried out using the DFT method, with the functional B3LYP and the gaussian program 09. A complete optimization of geometries was made, followed by a calculation of the frequencies of the normal modes of vibration. The UV spectrum was also interpreted. The theoretical results were compared with the experimental data.

Keywords: hydrazone derivative , synthesis , theoretical study, antibacterial activity

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DFT STUDY OF A SERIES OF NICOTINIC ACID BENZYLIDENEHYDRAZIDE DERIVATIVES: STRUCTURE, STABILITY AND REACTIVITY

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Hydrazones constitute an important class of compounds that has received much interest in recent years, due to their diverse biological characteristics, such as antimicrobial, anticonvulsant, analgesic, anti-inflammatory, antiplatelet, antituberculous and antitumor activities. These compounds have donor sites such as N and O which have non-bonding doublets which allow them to coordinate with metal ions. For this purpose, six hydrazine structures were optimized in the DFT method, using the B3LYP functional, with the basis 6-31G** for all atoms, in the gas phase using the Gaussian 09 program. the structural, energetic (energies, EHOMO-LUMO gaps), electronic (dipolar moments, atomic charges) parameters were determined. A study of the stability of the ligands was carried out based on the relative energies To study the chemical reactivity of the optimized structures, we calculated the global reactivity parameters (ionization potential, electronic affinity, electronic chemical potential, absolute hardness, overall softness and overall electrophilicity) the results obtained show that All the systems considered are stabilized by two types of electronic effect. Either; an inductive attractor effect, with a coexistence of mesomeric effects Analysis of chemical hardness values indicates that the most stable isomers found are the hardest, with larger HOMO/LUMO gaps, and therefore less reactive. As a result, charge transfer will be predominant. The most nucleophilic systems are also determined based on the calculation of the eletrophicity and nucleophilicity indices. The theoretical results obtained are compared to the available experimental ones.

Keywords: hydrazones, dft, reactivity, stability

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COMPUTATIONAL EVALUATION ON MOLECULAR STABILITY AND REACTIVITY OF SOME DIMETHYLGLYOXIMATO-NICKEL COMPLEXES FROM DFT

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Complexes Nickel constitute a very widespread axis in coordination chemistry and in medicine, because of their application as well as their activity. The Ni(III) species which aroused the interest of many biochemists, the three last decades, was identified to be the active entity of many enzymes, in particular, in hydrogenases. It is also mentioned for its powerful catalytic properties in biological and chemical processes. The Ni(IV) species, for its part, is known for its marked oxidizing capacities. In this work, we were interested in the theoretical study of Two complexes of dimethylglyoximato-nickel , using the DFT method, with the functional B3LYP function and LANL2DZ basis set in the gaseous phase, using Gaussian 03 program package. No symmetry constraints were imposed. We used the GaussView software to draw the optimized geometries and visualize the vibrational modes. For this purpose, a complete geometry optimization was performed for each compound followed by a frequency calculation of the normal modes of vibration to confirm the stability. Thus, the structural parameters and electronic parameters, the energies, the HOMO/LUMO gaps, and the NBO atomic charges were evaluated of the ligand and complexes obtained.To compare the stability of the two studied complexes, we computed the bending energies. The population analysis was carried out using the natural orbital bond program (NBO) implemented in the Gaussian program 03. in order to reproduce the experimental electronic spectra. The experimental results, IR, ^{1}H NMR, ^{13}C NMR and electronic spectra (UV) were compared to those obtained theoretically.

Keywords: nickel, dimethylglyoxime, dft, reactivity

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CHEMICAL COMPOSITION AND BIOLOGICAL POTENTIAL OF DIFFERENT EXTRACTS OF TWO MEDICINAL PLANTS FROM NORTHERN ALGERIA

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This work aime to study the chemical composition and the main biological properties contained in the extracts of Lavandula stoechas and Pistacia lentiscus collected in northern Algeria.Lavandula stoechas and Pistacia lentiscus are two medicinal plants belonging to the botanical family Labiatae and Anacardeacea respectively. They are grow wild in the northen Algeria and widely used in traditional Algerian medicine. The GC/MS analysis of the essential oils of Lavandula stoechas extracted by hydrodistillation showed that the latter are of fenchone chemotype whatever the period and the site of harvest. LC/MS analysis of tannin powders extracted by maceration of the leaves in a hydroalcoholic solvent reveals that they mainly contain rosmarinic acid. Essential oils extracted from the leaves of Pistacia lentiscus showed a large variability in terpenoid. The antioxidant activity of the different essential oils varied according to the harvesting period and the altitude. The highest antiradical effects were observed with the FRAP test. An another side the Pistacia lentiscus extracts showed to have an α-glucosidase inhibition effect that was more or less impactful according to the plant's living environment (mountain or littoral) and the considered organ (leaves, stem barks or fruits).

Keywords: lavandula stoechas, pistacia lentiscus, essential oils, antioxidant activity, α-glucosidase inhibition

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A NUMERICAL STUDY OF THE EFFICIENCY OF THE SONO-GALVANO-FENTON PROCESS AS A TERTIARY TREATMENT TECHNIQUE FOR THE WASTEWATER REUSE IN AGRICULTURE

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In the present study, the Sono-Galvano-Fenton process is studied numerically as a tertiary treatment process for treated wastewater reuse in irrigation, with in situ generation of the Fenton's reagent and catalyst, i.e., $H_2O_2$and Fe^{2+}. The sonochemical pathway is examined as a source of hydrogen peroxide under the pre-optimized condition of acoustic frequency, 300 kHz. The macroscopic model accounting for the performance of the single acoustic cavitation bubble and the bubble population density is combined with the Fe/Cu galvanic cell operating in acidic conditions (pH 3), following a cumulative and instantaneous production approach in terms of Fenton's reagent. The combination is optimized based on the rate of hydroxyl radicals generated by the Galvano-Fenton process, as a non-selective powerful oxidant against recalcitrant pollutants, then considering the synergetic effect of the hybrid process in terms of $HO^{\bullet}$pumped sonochemically and via the Fenton based pathway, treated using simulations of the isolated processes then their combined configuration following both aforementioned approaches.

Keywords: numerical model, synergy, hydroxyl radical, ultrasounds, galvano fenton, simulation

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PV SUPPLIED ELECTROCHEMICAL PRODUCTION OF HYDROGEN PEROXIDE: A GREEN PATHWAY FOR FENTON BASED ADVANCED OXIDATION PROCESSES

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Hydrogen peroxide is the common reagent of the Fenton Based advanced oxidation processes, it is generally added in stochiometric yields to the Fenton catalyst (Ferrous or ferric ions) to produce hydroxyl radicals. In the present study, a green technique for the in-situ production of hydrogen peroxide is examined numerically, using modelling and simulation, based on PV supplied electrochemical process and carbon-based electrodes. The PV supply model is based on Maximum Power Point Tracking using ET-Solar M53640 panel, while the modelling of the performance of the electrochemical cell is based on an electrical equivalent schema of activation, ohmic, and concentration resistances. Two production pathways of hydrogen peroxide under acidic conditions are considered, namely the reduction of $O_2$and the oxidation of H_2O. The performed simulations under 3 scenarios of solar radiation (low, middle and high) demonstrated that 300 W/$m^2$of incident global radiation results in 0.35 A of feeding current, against 0.88 A under 600 W/$m^2$and 1.41 A under 900 W/m^2. Both pathways for hydrogen peroxide production under the three scenarios have been compared, and the reduction of $O_2$is proved to be more performant, especially with the lower H_2O_2cathodic decomposition.

Keywords: simulation, pv supply, fenton, hydrogen peroxide, model, production

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SBA-15 – ZN – FE COMPOSITE MATERIAL: SYNTHESIS, CHARACTERIZATION, AND APPLICATION IN HIGH-EFFICIENT ADSORPTION OF P-NITROPHENOL

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In this study, SBA-15 – Zn – Fe composite was synthesized, characterized, and used as an adsorbent for the efficient removal of p-nitrophenol (p-NP). Firstly, SBA-15 was synthesized using the triblock copolymer P123 (PEO20PPO70PEO20). The characterization studies of SBA-15 were performed with FT-IR, XRD, SEM, and BET analysis methods. Then, SBA-15 – Zn – Fe composite was prepared. The characterization studies of SBA-15 – Zn – Fe are carried out using FT-IR, XRD, and SEM analysis. According to FT-IR spectrum of SBA-15, the obtained peaks and vibrations were determined to belong to functional groups specific to SBA-15. The peaks at 1070. 92 cm-1and 802.78 cm-1are due to Si-O-Si asymmetric and symmetric stretching vibration of SiO2. The weak band obtained at 973 cm-1belongs to the Si-OH stretching vibration. According to the XRD analysis, a characteristic broad peak of amorphous SBA-15 was obtained in the range of 2-theta =23°- 27°. SEM images of the synthesized SBA-15 at different magnifications showed that the material exhibited spherical morphology in average particle sizes ranging from 3 to 16 µm. The specific BET surface area of the SBA-15 was determined as 662.19 m2/g and the pore diameter of 43.61 Å. The batch adsorption experiments were carried out to investigate the adsorption performance of SBA-15 – Zn – Fe composite in the efficient removal of p-NP. When the experimental conditions for treating p-NP were initial pH of 3.0, an adsorbent concentration of 1.0 g/L, and a temperature of 25°C, 84.16% adsorption yield was obtained at the end of 1 h contact time at the initial p-NP concentration of 25 mg/L. Equilibrium, kinetic, and mass transfer modeling for p-NP adsorption were elucidated. Consequently, the synthesized SBA-15 – Zn – Fe composite material showed good adsorbent properties in the elimination of p-Nitrophenol.

Keywords: adsorption, sba-15, composite material, p-nitrophenol

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THERMAL OXIDATION KINETICS OF NICKEL AND DILUTE (NI- AL) ALLOYS

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Oxidation of high purity nickel and of a dilute Ni-Al (0.11 wt%) polycrystalline alloy were performed in the temperature range 700°- 1200°C, under P_{O2}=1 atm. At T<1100°C, Al leads to a reduction of the oxidation kinetic, while at higher temperatures its beneficial effect disappears. The results were analysed from a formal treatment, taking into account the thermodynamic and transport properties of undoped and Al-doped $Ni_{1-x}O$ single crystals. At temperatures below 1000°C, it was found that the results are in agreement with the thermal oxidationof undoped and doped $Ni_{1-x}O$ samples. They are due to the kinetic demixing of cations in the alloy layer growth, leading to both, a lower concentration of aluminium and a decrease of D_{Ni}in the outer oxidation scale. At higher temperatures, the Ni-Al alloy oxidises faster than Ni. This increase was explained by an inward oxygen gas transport within the layer through fissures, whose formation was attributed to compressive stresses due to the growth of nickel oxide units in grain boundaries. The mechanism whereby nickel oxide units form is explained.

Keywords: oxidation rate, kinetic demixing, thermodynamic, diffusion, point defects.

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