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தோன்றின் புகழோடு தோன்றுக அஃதிலார்
தோன்றலின் தோன்றாமை நன்று

ABSTRACT PROCEEDINGS

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APPLICATION ORIENTED MATERIALS IN SCIENCE AND TECHNOLGY

ICAOMSAT-2018

Abstract Proceedings-Volume 8| Issue 3| 2018

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Abstract-1

Synthesis of Silver doped Zinc Oxide Nanorods and its Structural and Biological Studies

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Abstract

ZnO and Ag doped ZnO ($Ag_xZn_{1-x}O$ were synthesized by using soft chemical route. The synthesized materials were characterized by using XRD, HRSEM, EDS and HRTEM. The powder XRD pattern indicates that the ZnO and $Ag_xZn_{1-x}O$ samples exhibits hexagonal wurtzite structure and also the Ag doping decreases the grain size of ZnO nano particles. The micro structural characterizations (HRSEM and HRTEM) reveal the incorporation of Ag into the ZnO lattice and also the formation of nano rods. At the length, the antimicrobial response was also brought against human pathogenic Gram +ve (S. Aureus), Gram –ve (E. Coli) bacteria and Fungi (C.Albicans). Thus, the above work brings out the presence of antimicrobial response against the microbes from these nano composites.

Keywords:

ZnO, Ag doped ZnO, nanorods, antimicrobial, XRD.

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Abstract-2

Green synthesis and characterization of zinc oxide nanoparticles using cuminum cyminum seeds

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[d]Department of Physics, Thirumalai Engineering College, Kilambi, Kancheepuram, 631 551, India.

Abstract

ZnO NPs is synthesized via eco-friendly synthesis using cuminum cyminum (cumin) seed extract with simple solvothermal method using a domestic microwave oven. Lattice parameters are determined by carrying out X-ray powder diffraction measurements. Scanning electron microscopy (SEM) shows the morphology. Dielectric studies are carried out on palletised samples at various temperatures 308 K - 368 K. The electrical parameters increase with the increase in temperature. Results of the present study reveal that the space charge contribution plays a significant role in the charge transport process and polarizability in the nano particles studied. Electrical properties of green synthesized ZnO may be used in nano and electronic devices.

Key words:

Zinc oxide nanoparticles, cuminum +cyminum seeds, solvothermal method.

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Abstract-3

Emerging trends in Nanotechnology Future for All

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Abstract:

Nanotechnology has been considered as an interdisciplinary field of advanced research on different types of nano materials and nano devices and their applications in various fields of scientific advancements. New nano products and nano technology could be applied in almost all fields of human activity. Potential applications of nano materials are not limited to medicine, drug delivery, electronics, data storage, construction, space materials, etc. It offers advances in industry, engineering, information and communication technology, electronics, environmental science and energy savings, economics etc. Nanotechnology, which is a cross-border technology transforming the world's economy, plays a crucial role in recent science and technology developments.

Key words:

Nanotechnology, Cross-border technology.

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Abstract-4

Studies on some amino acids substituted Hydroxyapatite

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Abstract

Calcium phosphate, otherwise, Hydroxyapatite (HA; $Ca_{10}(PO_4)_6(OH)_2$) is a major component of bones and teeth. A deeper understanding of the role of amino acids doped in hydroxyapatite will not only help to increase our fundamental knowledge related to bone formation. But it could also lead to new methods for calcium mineralization and its related disorders. The substitution of amino acid modifies the structural properties. Glycine, proline and alanine are essential and non-polar amino acids present in the collagen protein and 10% of these amino acids are substituted in HA by sol-gel method. The effect of substituting the arginine polar amino acid in HA was also studied. Sol-gel method is preferred well over the other methods for its homogeneity and molecular level of mixing. The present studies concentrate in substitution of amino acids in hydroxyapatite and the study of their physicochemical properties. Pure HA and amino acids substituted HA powders are characterized by powder X-ray diffraction patterns, Fourier transform infrared spectrum, Laser Raman spectrum and Scanning electron microscopy. The crystallite size, crystallinity and the lattice parameter values were found using powder X-ray diffraction method. The SEM micrographs showed agglomerated spherical particles.

Key words:

Nanotechnology, Cross-border technology.

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Abstract-5

Failure Investigation on Two Numbers of Tubes at the Old High-Pressure Feed Water Heater

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Abstract

The fracture of old high-pressure feed water heater SA688 TP304 Welded Austenitic Stainless Steel was the results of Stress Corrosion Cracking (SCC) and the corrosion fatigue under repeated impact type load exerted by the sudden discharge of exhaust steam at high temperature and pressure in the environment of corrosion. The depleted matrix was selectively attacked halide ions causing extensive pitting. These pits under the influence of crack propagated under the influence of high internal stresses and may the chloride ion attacks be fracturing the stainless-steel tube transgranularly and intergranularly.

Key Words:

SA688 TP 304, SS304 Tube Failure, HP FWH Tube, Creep Rapture.

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Abstract-6

Comparative analysis on nonlinear optical property of 2-amino 5-chloropyridine derivative crystals

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Abstract:

The 2- amino 5- chloropyridine derivative crystals are grown by solution growth method. One of them is SHG and other is THG. NLO property is the predominant in case of materials especially crystals for which the frequency parameters are properly analyzed and Second harmonic efficiency of powdered 2A5CPLTA is determined by Kurtz and Perry method and it is 1.2 times that of KDP. The third harmonic efficiency of powdered 2A5CPC is determined by Z - scan technique and the nonlinear parameters are calculated.

Keywords:

Single crystal X-ray diffraction; Recrystallization process; Nonlinear optical properties; Z- scan technique.

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Abstract-7

Computational measurement of parameters of PM crystals (B3LYP and HF methods) A Comparative analyzation by theoretical way using Software

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Abstract

Organic crystals have high NLO coefficients especially Picolinium Maleate (PM) crystals have wide range of NLO applications and the theoretical calculations reveal that the crystal has Homo and Lumo values of -8.9697 and -1.5477 eV and the optimized structure parameters of PM by ab initio HF and DFT (B3LYP) levels with the 6-311G basis set in accordance with the atom numbering.

The molecules possessing C1 point group symmetry with 72 fundamental modes of vibrations and are active in IR region.

Keywords:

PM crystals, Homo, Lumo, B3LYP, DFT, HF.

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Abstract-8

Antimicrobial Properties of Nano materials

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Abstract

Nano materials of nanotechnology have emerged as source for antimicrobial therapy. With the invention of copper, silver and magnesium nano particles having antimicrobial properties its application is widened in biomedical and pharmaceutical sciences (Shirin Mahmoodi_*et al.*, 2018). With the developments in nanotechnology new and effective antimicrobial nano particles are designed which are more affective in killing bacteria targeting at various sites of bacterial cell. The bacterial cell death can be noticed very clearly identifying the target site by using transmission electron microscope (Tiwari DK 2008). Metallic nano particles are designed with extremely high surface area and numerous reactive sites (Stoimenov PK *et al.*, 2002).

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Abstract-9

Gaussian computational characterization and spectroscopic (NMR and Mass) investigation on 3,6-Dimethylphenanthrene

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Abstract

In this attempt, in order to the physical and chemical properties, a thorough investigation has been made by recording Mass and ^{13}C and ^{1}H NMR spectra of pharmaceutically important compound; 3,6-Dimethylphenanthrene. The keen observation is made over the excitations between the electronic energy levels of the molecule which lead to the study of electronic properties. The variation of thermodynamic properties; heat capacity, entropy, and enthalpy of the present compound at different temperatures are calculated using NIST thermodynamical function program and interpreted. The low energy electronic excited states of the molecule are calculated at the B3LYP/6-311++G(d,p) level using the TD-DFT approach on the previously optimized ground-state geometry of the molecule. The calculations are performed in gas phase and with the solvent of DMSO and CCl_4.

Key words:

3,6-Dimethylphenanthrene; ^{13}C and ^{1}H NMR electronic properties; NIST.

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Abstract-10

Growth, Structural, Optical, Mechanical and Electrical Properties of Amino Acid Single Crystal Of γ-Glycine

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Abstract

An organic nonlinear optical single crystal of gamma glycine (GGLY) has been grown by slow evaporation of the saturated solution at room temperature. Single crystal of gamma glycine (GGLY), an organic nonlinear optical (NLO) material, has been grown by slow solvent evaporation technique. Good optical quality single crystals with dimension up to 31 × 30 × 6 mm^3 are obtained. The crystals are characterized by optical absorption spectrum, FTIR and X-ray diffraction studies. The dielectric response of the sample is studied as a function of frequency and temperature. The mechanical, photoconductivity and ac/dc behavior of the grown crystals are also investigated.

Key words:

NLO materials; Crystal growth; Dielectric measurement; Conductivity; Mechanical properties.

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Abstract-11

Spectroscopic, thermal and dielectric characterization of Tutton salt crystals

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Abstract

A good quality single crystal of Tutton salt with dimensions 6 x 7 x 3 mm^3 was successfully grown by the slow evaporation growth technique at ambient temperature. The grown crystal was subjected to single crystal X-ray diffraction study which confirms that the grown crystal is monoclinic in nature with the space group $P2_1/c$. Spectroscopic studies reveals that the grown crystal has good optical transparency in the entire visible region and its energy band gap was determined. The thermal behavior of the grown crystal was investigated by thermogravimetric and differential thermal analysis. The dielectric measurements were carried out to determine the dielectric behavior of the crystal.

Keywords:

Crystal growth; Tutton salts; XRD; UV-Visible-NIR; Thermal stability; Dielectric characteristics.

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Abstract-12

Synthesis, crystal growth spectral characterization and optical studies of 1,4 Dihydropyridine (1,4-DHP)derivative single crystal

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Abstract

1,4 Dihydropyridine derivative (1,4 DHP) organic crystal has been synthesized by employing slow evaporation method. The grown crystals were characterized by single crystal XRD, FT-IR and UV-Visible studies. Single crystal X-ray diffraction reveals that the crystal belongs to monoclinic crystal system with centrosymmetric space group. The presences of functional groups were confirmed by FT-IR analysis. The UV-Vis absorption spectrum has been recorded and the cut off wavelength is exhibit in 398 nm. The energy band gap was found to be 2.92 eV.

Keywords:

Single crystal XRD, FTIR, UV-Visible.

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Abstract-13

Influence of Sno_2 Nano Particles on the Structural and Optical Behaviour Of PVA Film

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Abstract

Addition of inorganic nanoparticles to polymers allows the modification of physical properties of polymers as well as the implementation of new features in polymer matrix. In this present work, we have made an attempt to disperse SnO_2 nanoparticle in the polyvinyl alcohol (PVA) and to understand the change in structural and optical properties of the polymer film. The proposed films were characterized by XRD and optical measurements. The results are reported herein.

Keywords:

Inorganic nanoparticles, Polyvinyl alcohol

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Abstract-14

Cost Effective Synthesis of Magnesium Ferrite Nano particles for its Structural and Magnetic Behaviour Analysis

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Abstract:

Magnesium ferrite ($MgFe_2O_4$) nanoparticles were synthesized by a Cost technique of self-combustion, where egg white (albumen) plays the role of fuel in the combustion process. The powder X - ray diffraction (PXRD) and Fourier Transform Infrared Spectroscopy (FTIR) results indicated that the synthesized nanoparticles are of single phase and show evidence of spinel structure. Also, the functional groups present in the synthesized nanoparticles were identifiedfrom FTIR spectra. Magnetic moment and retentivity of the as synthesized Magnesium ferrite ($MgFe_2O_4$) nanoparticles were obtained using Vibrating Sample Magnetometer (VSM) analysis.

Keywords:

ferrite; egg white; PXRD; FTIR; VSM.

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Abstract-15

Studies on Photocatalytic activity of $CuS_xO_{(1-x)}$ Nanocomposites

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Abstract

A facile microwave assisted solvothermal method was adopted for the synthesis of $CuS_xO_{(1-x)}$ nanocomposites (with x values 0.0, 0.5, 1.0). The as-prepared samples were annealed at 200 °C to improve ordering. Relevant properties of annealed samples were characterized by powder X – ray diffraction (PXRD) analysis and photocatalytic activity. The broadening peak in the PXRD pattern indicates the nano crytalline nature of the samples and the particle size was calculated from Debye Scherrer equation. Photocatalytic activity of $CuS_xO_{(1-x)}$ nano composites was carried out by using methylene blue (MB) dye. The degradation efficiency with respect to irradiation time was calculated for the prepared nanocomposites. The result showed that $CuS_xO_{(1-x)}$ nanocomposites have suitable photocatalytic activity in degradation of MB dye. The result obtained were discussed and reported.

Key words:

Catalyst, methylene blue, photo catalytic degradation, UV irradiation.

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Abstract-16

A study on the influence of hydrogen bonding interaction between organic and inorganic moiety over the third order nonlinear optical properties of semi organic crystal: Diammonium Fumarate

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Abstract

Nonlinear optics owes to many applications towards the development of many disciplines of research and in industries. Variety of nonlinear optical materials can serve as radiation detectors, solid state lasers, harmonic generators, transducers and crystalline thin films for microelectronics and computer industries. Organic materials are prominent owing to its good nonlinear optical response, but they suffer from low mechanical and thermal stability. The inorganic materials exhibit good mechanical, thermal and deep UV transmission properties, but have low nonlinear efficiency. The combination of organic and inorganic materials with large nonlinear optical characteristics, leads to the investigation of semi organic materials. The semi-organic single crystals of diammonium fumarate were grown from aqueous solution by slow evaporation method. The lattice parameters and the crystal system are estimated from single crystal X-ray diffraction studies. The transmission range of the crystal was revealed from UV-Vis-NIR analysis and the lower cutoff wavelength is found at 300 nm. The vibrational modes of different molecular groups present in the crystal were identified from IR and Raman analyses. The NMR analysis confirms the molecular structure of the grown crystal. The thermal studies were analysed from TG/DTA experiment. The nonlinear refractive index and susceptibility was determined from z-scan technique.The third order susceptibility value of the grown crystal is found to be 9.33 x 10^{-6}esu and this value is greater when compared with some semiorganic crystals. This greater value is due to the hydrogen bonding interaction between cations and anions in organic and inorganic moiety.

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Abstract-17

Synthesis, structural, spectral, thermal and third order nonlinear optical studies of L-threoninium p-toluenesulfonate monohydrate crystal

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[1]Department of Physics, Government Arts College (Autonomous), Kumbakonam 612001, Tamilnadu, India.

Abstract

L-threoninium, p-toluenesulfonate monohydrate single crystal is a new organic nonlinear optical (NLO) material grown by solution growth solvent evaporation method. Single crystal X-ray diffraction studies reveal that the crystal belongs to monoclinic crystal system with non centro symmetric space group $P2_1$. The FT-Raman spectral studies reveal the presence of various functional groups and also the formation new compound is confirmed through NH_3^+ and SO_3^- moieties peaks. Thermal stability and the various decomposition stages of grown crystals were analysed through the thermo gravimetric (TG) and differential thermal analysis (DTA). The lower cutoff wavelength was found at 235 nm and the wide transparency window was observed using ultraviolet-visible-near infrared (UV–vis–NIR) spectral analysis. The third-order nonlinear optical parameters of the grown crystal were calculated by Z-scan technique and the third order nonlinear susceptibility values were found to be $\chi^{(3)} = 1.3035\times10^{-7}$ esu and this is greater than the values of some reportedcrystals.

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Abstract-18

Construction of Bioreactor for The Effective Degradation of Acid Blue-25 In Textile Effluents Using Bacterial Consortium A Pilot Study

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Abstract

Discharging of industrial effluents into natural water resources without any treatment causes a serious problem and leads to the ecological imbalance in nature. In India alone, the dyestuff industry produces around 60,000 metric tons of dyes, which is approximately 6.6% of total colorants used worldwide. During dying processes in the textile industries produce large volumes of effluents, often rich in color, containing dye residues and chemicals which requires proper treatment before being discharged into the environment. Unfortunately, most of these dyes escape conventional effluent treatment processes and persist in the environment as a result of their high stability to light, temperature, detergents, chemicals, soap and other parameters such as bleach and perspiration. The technologies for dye removal have been divided into three principal categories: physical, chemical and biological methods. Among these biological methods offers a cheaper and environmentally friendly alternative for the textile effluent treatment. The utilization of microbial consortia offers considerable advantages over the use of pure cultures in the degradation of synthetic dyes. Hence, we constructed a bioreactor with 5 lit capacity with locally available materials and studied the dye degradation of Acid blue-25 at 100ppm concentration and achieved a significant degradation (85%) within 48 hours of HRT.

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Abstract-19

Vibrational (FT-IR, FT-Raman), UV–Visible, NMR spectroscopic studies, HOMO–LUMO, NBO, MEP, TG-TDA of 3-Chloro-6-fluorobenzo [b]thiophene-2-carbonyl chloride

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Abstract

This paper is a report on the molecular structures and vibrational spectral analysis of 3-Chloro-6-fluorobenzo[b]thiophene-2-carbonyl chloride have been reported by using DFT calculations at B3LYP/6-311G(d,p) level of theory. The molecular electrostatic potential MEP showed the electrophilic and nucleophilic region of the molecule. NBO analysis is carried out to show the charge transfer between the localized bonds and lone pairs. HOMO-LUMO energies which confirm the occurring of charge transformation within the molecule.TG-DTA is to obtain its thermal stability.^{1}H and ^{13}C NMR were investigated to understand the shielding and deshielding nature. Non-covalent interactions were also analyzed using RDG analysis and color filled electron density diagram.

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Abstract-20

Molecular spectroscopy investigation on Pharmacodynamic activity and biological property analysis on anti-bacterial drug; Chloramphenicol using computational tools

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Abstract

The Detailed physical, chemical, thermal and circular vibrational investigations have been made on FT-IR, FT-Raman, NMR and UV-Visible spectra of Chloramphenicol. The modification of the basic property (deficit hyperactivity disorder) of the base compound (Amphetamine) is favored by the insertion of two methoxy and ethyl-methyl groups have been discussed in detail. The transitional pattern among NBO emphasized the inducement of the psychedelic activity in the compound. The strong interpretation made on the physical and chemical properties by intense observation using excitations between the electronic energy levels within the molecule have been carried out. The arrangement of the dipole moment of the bonds and the change of resultant magnetic moment were observed from the average Polarizability first order diagonal hyperpolarizability. The receptor and inhibition property of the molecule were interpreted by the identification of reactive sites from molecular electrostatic potential contour map. The chemical reaction continuity is keenly observed from thermodynamical analysis.

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Abstract-21

Studies on some amino acids substituted Hydroxyapatite

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Abstract

Calcium phosphate, otherwise, Hydroxyapatite (HA; $Ca_{10}(PO_4)_6(OH)_2$) is a major component of bones and teeth. A deeper understanding of the role of amino acids doped in hydroxyapatite will not only help to increase our fundamental knowledge related to bone formation. But it could also lead to new methods for calcium mineralization and its related disorders. The substitution of amino acid modifies the structural properties. Glycine, proline and alanine are essential and non-polar amino acids present in the collagen protein and 10% of these amino acids are substituted in HA by sol-gel method.

Key Words:

Hydroxyapatite, amino acids, powder X-ray diffraction, FTIR and Laser Raman spectroscopy.

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Abstract-22

A novel synthesis of nano Palladium using 1-carboxy ethyl-3-methyl imidazolium bromide

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Abstract

Palladium nanoparticles (Pd NPs) have been successfully synthesized in imidazolium based ionic liquid (IL)under mild conditions. In this self-ordered medium, particles with narrow size distribution can be formed. No ligand is required to stabilize the suspension, which can be directly used to coat technological substrates. Several parameters are examined: the nature of IL, stirring, dihydrogen pressure and temperature. Under optimal conditions, well dispersed, zero-valent Pd NPs of 97 nm with narrow size distribution are obtained. These stable suspension of Pd (0) NPs is a promising starting material to form conformal palladium seed layers in high aspect ratio interconnect structures.

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Abstract-23

Effect of 60 MeV Si^{5+} Swift Heavy Ion Irradiation on the surface modification of Hydroxyapatite and Polystyrene composite

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Abstract

The extensive use of biomaterials for biomedical implantation depends on its bioactivity and biocompatibility. Hydroxyapatite (HAP) has been used clinically as substitute for autografts in filling bone defects. Unlike, other implant materials, HAP is biocompatible, nontoxic, possesses excellent osteo conductive ability and has the structure similar to bone mineral and forms direct bond with bone. Despite these advantages it has poor mechanical strength that limits its application in the load bearing applications. In order to improve the strength of HAP, polymers were used. In the present work, HAP and polystyrene (PS) composite was prepared and to improve its bioactivity and biocompatibility, the surface of the sample was modified by swift heavy ion irradiation using Si^{5+} ion beam.

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Abstract-24

Synthesis, characterization and antimicrobial investigation of silver doped ZnO nanoparticles

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Abstract

Pure and different concentration of *Ag (1, 3 and 5 at. %)* doped ZnO nanoparticles were synthesized by Sol-Gel technique. The products were characterized by UV-Vis absorption, X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), FT-Raman and *antibacterial activity were studied.* UV–visible spectrometry study revealed surface plasmon resonance at 403, 409, 412 and 423 nm undoped ZnO, and Ag *doped* ZnO nanoparticles respectively, the optical band gap of the nanoparticles was tuned from 3.08 to 2.93 eV. The X-ray diffractometer were characterized Crystal structure and the average crystallite size varied from 17 to 11 nm, Scanning Electron Microscopy (SEM), Energy dispersive analysis of X-rays spectroscopy (EDAX) spectrum indicates that the successful dopants of Ag peaks in the ZnO lattice and which indicates the purity of the sample. The structural bond vibrations of pure and Ag doped ZnO nanoparticles were analyzed by FTIR spectroscopy, From the Raman spectrum all the peaks observed in samples matched with the Raman active modes of ZnO wurtzite structure. The antibacterial studies performed against a set of bacterial strains showed that Gram positive (G+) bacteria were relatively more susceptible to the NPs than Gram negative (G–) bacteria.

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Abstract-25

FluoreneMolecule for nano devices using condensed matter applications

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Abstract

Fluorene based single molecule nano devices are constructed with different electrodes in order to study the effect of electrodes on the electronic transport properties of Fluorenenano devices using non-equilibrium Green's function method. The electrodes are constructed along the (111) plane and they are connected with the Fluorene molecule through a linker atom. This is confirmed by the corresponding V-I spectra obtained for these devices.

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Abstract-26

CuS molecule for nano devices using condensed matter applications

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Abstract

Covellitec opper sulphide (CuS) is a p-type transition metal chalcogenide material with a wide band gap. In the form nano structures, CuS has a wide range of applications such as solar cells, gas sensors, hydrogen storage devices, battery electrodes and as catalyst. They have been prepared experimentally by various methods such as soft chemical method, wet method, sonochemical, electrodeposition method, microchemical methods etc. Nanostructures of CuS are prepared in various forms like nano tubes, nano ribbons, flakes, nano wires etc.

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Abstract-27

Synthesis and spectral characterization of Zn (II), and Fe (III) complexes derived from thiourea Schiff base ligand and pyridine

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Abstract

Chemistry of Schiff base metal complexes have been studied extensively because of their attractive chemical and physical properties and their wide range of application in numerous scientific areas. Metal ions play a vital role in a vast number of widely differing biological processes. Research work was directed towards the synthesis and Characterization of mixed ligand Schiff base complexes of Zn (II), Fe (II) and Ni (II) with high thermal stability, adequate solubility and low toxicity. To synthesis and characterization of a series of N-functionalized Schiff base complexes by reflux method of corresponding metal salts like Cu (II), Mn (II), Zn (II) and Fe (III) with pyridine. The structure of the complexes was established and analyzed by IR, UV and CV spectral studies.

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Abstract-28

Mixed ligand copper (II) ferrous (II) and zinc (II) complexes derived from 2,2' bipyridine and acetyl acetone ligands: Antimicrobial and Antibacterial studies

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Abstract

Nitrogen and oxygen coordinated ligands are common in coordination chemistry. The imine nitrogen is basic and exhibits good pi-acceptor properties. Furthermore, pyridyl substituted metal complexes have pivotal role in biological field. Current Research work was focused on the synthesis and Characterization of mixed ligand complexes of Zn (II), Fe (II) and Cu (II) with high thermal stability, adequate solubility and low toxicity. A series of N-functionalized and O-functionalized complexes were obtained by reflux method of corresponding metal salts like Cu (II), Zn (II) and Fe (III) with bipyridine and di oxalate ion. The structure of the complexes was established and analysed by IR, UV and CV spectral studies and biological studies has been recorded.

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Abstract-29

Refractive influx of 4-Benzeneazoaniline with Taxol

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Abstract

A new organic nonlinear optical material Single crystal of 4-Benzeneazoaniline with Taxol was grown by slow evaporation with methanol solution at room temperature.

Transparent crystals with size up to 13x5x6 mm^3 were obtained. Single crystal X-ray diffractometer was utilized to measure the unit cell parameters and to confirm the crystal structure.

The structure of compound was further confirmed by FTIR, NMR and mass spectral analyses, CHNS and theoretical calculations.

The refractive influx is calculated and is found in the order of microns and is necessary predominant property for NLO crystals.

Keywords:

4-Benzeneazoaniline, Taxol, crystal, influx.

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Abstract-30

Effect of cerium on meta Nitroaniline single crystal

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Abstract

A nonlinear optical material of meta-Nitroaniline cerium (mNACe) was grown by slow evaporation solution growth technique. The presence of cerium in mNACe crystal was tested by energy dispersive X-ray diffraction (EDAX) analysis. The structure of the grown crystal was confirmed by single crystal X-ray diffraction (SXRD). The Fourier transform infrared (FT-IR) study was used to reveal the functional groups present in the grown crystal. The optical properties of the grown crystal have been studied by means of transmission measurements in the wavelength region between 200 and 1100 nm. The optical constants such as refractive index (n) and extinction coefficient (k) have been determined from the transmittance data. The optical band gap (Eg) also calculated. Second harmonic generation (SHG) efficiency of the grown crystal has been studied using Nd:YAG laser and was measured as 1.05 times that of standard potassium di hydrogen phosphate (KDP) crystal. The nonlinear optical (NLO) property of the crystal was tested by pulsed Nd: YAG laser as a source. The closed aperture Z-scan studies reveal the negative nonlinearity in the crystals and open aperture Z-scan reveals the saturation absorption. Also, various parameters such as nonlinear refractive index, absorption coefficient, and nonlinear susceptibility were calculated for the grown crystal.

Key words:

Solution growth technique; Etching studies; X-ray diffraction; Nonlinear optical material; Z-scan technique.

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Abstract-31

Catalytic Performance of Mn (II), Co (II) and Sm (II) salen complexes immobilized mesoporous SBA-15: Selective epoxidation of Alkene

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Abstract

Mn (II), Co (II) and Sm(II)–schiff base complexes were immobilized over mesoporous SBA-15 through the reaction of mesoporous SBA-15 functionalized 3-aminopropyltrimethoxy silane (3-APTES) and salicylic aldehyde via schiff base condensation. The surface properties of the functionalized catalysts were analyzed by a series of characterization techniques like elemental analysis, XRD, SEM, AFM, FTIR, TGA, DRS UV–Vis, etc. The catalytic activity of the functionalized metal-salen complexes examined in the liquid phase oxidation of styrene and cyclohexene shows that the functionalized salen complexes are more active and selective than the corresponding neat metal complexes.

Keywords:

SBA-15, Mn (II), Co (II) and Sm(II) salen complex Oxidation reaction

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Abstract-32

Synthesis, characterization and photocatalytic performance of Sn_6SiO_8 nanoparticles

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Abstract

Sn_6SiO_8 nanoparticle was synthesized by a hydrothermal method. This material was characterized by XRD, Raman, DRS-UV, FT-IR and Field emission Scanning electron microscopy studies. The Sn_6SiO_8 nanoparticles hexagonal phase was confirmed by XRD and functional groups were monitored by FT-IR spectroscopy. The obtained band gap energy at 2.5 eV, the flakes like morphology was carried out by FE-SEM. This nanomaterial was testing for photocatalytic dye degradation of Methylene blue under visible light illumination.

Keywords:

Sn_6SiO_8 nanoparticle, hydrothermal method and photocatalytic dye degradation.

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Abstract-33

Development of Silicon Quantum Dots for the Selective Detection of Organic Pollutants

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Abstract

Synthesis of Silicon Quantum Dots (SiQDs) has recently more attentions due to their inertness, abundant, biocompatible and nontoxicity. Besides, SiQDs exhibits size and shape dependent optical properties, which includes tunable emission, photo stability, and brightness. In this work, we report the surface modified highly stable aqueous suspensions of SiQDs using for the detection of organic pollutants. The functionalization of surface in the SiQDs was confirmed by FT-IR and NMR spectroscopy. The adsorption and photoluminescence (PL) spectra of the SiQDs dispersion were measured by UV-visible and fluorescence spectrometer. The size and shape of the QDs was measured by transmission electron microscopy (TEM) and dynamic light scattering techniques (DLS). The synthesized SiQDs can be used as probe for detection of organic pollutants such as Aldrin, dieldrin and hexachlorobenzine.

Keywords:

Silicon quantum dots; Detection; Optical properties; Organic Pollutants:

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Abstract-34

Synthesis, Characterization and electromagnetic interference shielding effectiveness of tetrapod lead sulphide blended few layered graphene nanosheets filled semi flexible conjugated microporous polymer composites

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Abstract

In this paper, few layered Graphene nanosheets prepared *via* modified Ullmann reaction. Semi-flexible conjugated microporous polymer was synthesized by modified Chichibabin reaction. Although conventional EM wave Shielding materials are blended with few layered Graphene nanosheets, such blended shielding materials have many limitations in their electrical and mechanical performance. A thin and lightweight Tetrapod lead sulfide blended few layered Graphene nanosheets structure (with a thickness of 1.80, 1.82 and 1.90 mm, respectively) having good EM wave shielding in the X-band (8.2-12.4 GHz) was designed with dispersing tetrapod lead sulfide blended few layered graphene nanosheets in the Semi-flexible conjugated microporous polymer matrix. The functional group, morphology, element composition, phase identification, Porosity and polymer nanocomposites stability were examined by FTIR, SEM, EDS, XRD, BET, TGA and DSC. Consequently, considering the EM wave Shielding performance, Semi-flexible conjugated microporous polymer/ Pbs blended Graphene nanosheets synthesized nanocomposites to in this work can be evaluate the Dielectric and electromagnetic interference (EMI) shielding effectiveness (SE).

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Abstract-35

Synthesis, characterization of carbon dots (CDs) from sucrose(disaccharides) application as an efficient potentiometric sensor for Cu^{2+}metal ions

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Abstract

In this study was, synthesis of highly fluresent carbon dots (CDs) is one of the hot research areas in the present-day context C-dots synthesis from sucrose (disaccharides) is a carbohydrate material. The C-dots synthesis using hydrothermal method using 180°C for 24 hrs reaction. We have synthesized highly fluresent CDs in a can be adopted for large-scale production of fluresent CDs. In the newly synthesized C-dots characterizations including UV-Vis using electronic transition state, FT-IR, Raman using the functional groups conformation, PL, XRD, DLS is using particle size of CDs materials, and FE-SEM using surface morphology study's etc. The newly prepared CCPE was using C-dots and potentiometric heavy toxic metal ions sensing. We have demonstrated the CDs as a sensitive and selective potentiometric sensor for the determination of Cu^{2+}ions.

Key words:

Carbon Dots (CDs), Composite carbon paste electrode (CCPE), Potentiometer, Cu^{2+}metal ions.

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Abstract-36

Spectrophotometric Determination of Atorvastatin Calcium Using Sulphonphthalein Dyes

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Abstract

The proposed methods are simple, rapid, cost effective and successive spectrophotometric determination of atorvastatin calcium in pure and pharmaceutical formulations using sulphonphthalein dyes like bromothymol blue (BTB), bromocresol purple (BCP) and bromocresol green (BCG). The developed methods are based on the formation of ion-pair complexes between drug and acid dyes. The formed ion-pair complexes show maximum absorbance which is measured at 637nm for BTB, 606 nm for BCP and 631 nm for BCG. The optimization conditions such as effect of solvents nature, effect of reagent concentration, effect of time and stability profile of the formed ion –pair complexes are studied. Under the optimized conditions, the calibration curve shows the excellent linearity which is experimentally proved by high values of correlation coefficient and again conforms by Beers laws. The methods are validated according to ICH guidelines by doing accuracy, precision, limit of detection, limit of quantification, robustness, ruggedness and selectivity. The recovery studies show the good results because co-formulated substances don't interfere in the analysis of the developed methods. The developed methods are applicable in routine quality control for the determination of atorvastatin calcium in pure and pharmaceutical dosage forms.

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Abstract-37

Synthesis and photocatalytic activity of Cd doped ZnS nanoparticles

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Abstract

Pure and Cd-doped ZnS nanoparticles were synthesized by an inexpensive solid-state reaction method at different percentage (0.5, 1.0, 1.5 and 2.0 wt. %). The structural, functional, optical, morphological and photocatlytic properties were characterized by using X-ray diffraction analysis, Fourier transform of infrared (FTIR) spectroscopy, UV-Vis spectroscopy, photoluminescence (PL) spectroscopy and scanning electron microscopy (SEM) with energy dispersive X-ray analysis. XRD pattern confirms the crystalline nature with cubic structure of the prepared products. Crystallite size, microstrain, dislocation density, stacking fault were also evaluated from XRD data. A blue shift absorption edges were noticed in the UV and visible emissions. SEM and TEM revealed the abundance of spherical shaped particles and the elements ZnS and Cd alone identified from EDS. The photo-degradation rate was strongly influenced by activation of ZnS photocatalyst with photon and production of hydroxyl radicals, hence suggested Cd doping enhanced catalytic activity in the ZnS lattice.

Keywords:

ZnS, Cd doped ZnS, Methyl Orange dye: Photo catalytic.

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Abstract-38

Synthesis, characterization and antibacterial activity of cerium oxide (CeO_2-NPs) nanoparticles by using Sol-Gel method

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[2]Dean R&D, Edayathangudy G S Pillay Arts and Science College, Nagapattinam 611002.

Abstract

In the present study CeO_2 nanoparticles have been prepared by using Sol-Gel method. The CeO_2 nanoparticles obtained were characterized by UV–visible spectroscopy, XRD, DLS, ZP, FT-IR and TEM. The CeO_2-NPs formation was confirmed by UV–visible spectroscopy through color conversion due to surface plasma resonance band at 324 nm. The synthesized nanoparticles retained the cubic structure, which was confirmed by X-ray diffraction studies. DLS studies revealed that the average size of CeO_2-NPs was found to be around 45 nm. Zeta potential value for CeO_2-NPs obtained was -17.80 mV indicating the moderate stability of synthesized nanoparticles. TEM images showed that the CeO_2-NPs possessed spherical shape and particle size of 15 nm and FT-IR analyses were also confirmed to formation of CeO_2 nanoparticle. Furthermore, the biomedical properties of CeO_2-NPs were premeditated as antibacterial and free radical scavenging activity. The synthesized CeO_2-NPs significantly inhibited the growth of medically important pathogenic gram-positive bacteria (*Staphylococcus saprophyticus* and *Bacillus subtilis*) and gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeruginosa*). The report suggests that the synthesized CeO_2-NPs could have a high potential for use in the preparation of drugs used against various diseases and also promising candidate for many medical applications.

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Abstract-39

Photocatalytic Performance of Integrated CuO Nanoparticles Tested at Different Temperatures

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Abstract

CuO nanoparticles are synthesized by the Sol-gel method and are characterized by UV-visible spectroscopy; XRD, SEM, FTIR and anti-bacterial disk diffusion method are analyses. Here is an attempt to reduce and ensure a simple way to integrate CuO NPs at different temperatures using the precursor solution CuCl2 dihydrate. XRD diffraction analysis revealed that synthesized CuO nanoparticles are in monoclinic structure with the particle size decreased with increases of temperatures. The SEM analyses conformed the particles are tablet tube like spherical shaped was observed. Blue shift absorption peak of about 376nm was observed in UV spectra analysis. The present of functional groups were observed in FTIR spectra. The photocatalytic study illustrated enhancement catalytic activity of CuO nanoparticles on discoloration of MB dye at ambient conditions. The present study demonstrates expedient employment of Lantana Camara leaf extract as a fuel for the efficient synthesis of CuO nanoparticles through a green synthesis method to obtain significantly active photocatalytic.

Key Words:

CuO, Particle size, X-ray diffraction, SEM, FTIR, Photocatalytic activity**;**

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Abstract-40

Spectroscopic investigation on NLO property of 2-Aminofluorene using computational [HF and DFT] confinement

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Abstract

In this research work, the inducement of NLO property on the compound 2-Aminofluorene has been analyzed using computational calculations. The FT-IR, FT-Raman, FT-NMR and UV-Visible spectra have been recorded in specified region for molecular analysis. The optimized inducement of NLO activity by the molecular structural deformation due to the interaction between fluorene and amino group has been investigated. The supportive analyses such as Mulliken charge levels, first order and second order polarization, vibrational investigation, frontier molecular interactions, thermodynamic function (Gibbs energy) and VCD profile for proving NLO mechanism in the compound have been carried out. The chemical environment of the compound was simultaneously monitored by simulating and recording ^{1}H and ^{13}C NMR spectra. The isotropic and anisotropic chemical shift related to carbons and hydrogens after the formation of target compound have been carefully interpreted. The stabilization of orbitals by interchanging of energy between donor and acceptor was observed by NBO perturbation calculations.

Key words:

Aminofluorene, NLO activity, VCD, isotropic, NBO perturbation.

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Abstract-41

Vibrational, NMR and UV-Visible spectroscopic investigation, VCD and NLO studies on N-Cynomethyl-N-methyl-4-nitroaniline using computational calculations

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Abstract

In order to explore the unbelievable NLO property of prepared N-Cynomethyl-N-methyl-4-nitroaniline, the experimental and theoretical investigation has been made. The theoretical calculations were made using RHF and CAM-B3LYP methods at 6-311++G(d,p) basis set. The presence of C=N ligand in the compound which amalgamate the non-Centro symmetry primitive to improve the second harmonic generation (SHG) efficiency. The molecule has been examined in terms of the vibrational, electronic and optical properties. The entire molecular behavior was studied by their fundamental IR and Raman wavenumbers and was compared with the theoretical aspect. The molecular chirality has been studied by performing vibrational circular dichroism (circularly polarized infrared radiation). The Mulliken charge levels of the compound ensure the perturbation of atomic charges according to the ligand. The Gibbs free energy was evaluated at different temperature and from which the enhancement of chemical stability was stressed. The VCD spectrum was simulated and the optical dichroism of the compound has been analyzed.

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Abstract-42

Molecular structure investigation towards Pharmacodynamic activity and QSAR analysis on 8-chloroquinoline using Experimental and Computational Tools

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Abstract

The structural properties of 8- chloroquinoline compound related to molecular dynamic activity have been ornately interpreted in this methodical research work. The FT-IR, FT-Raman, NMR and UV-Visible spectral analysis has been carried out and the obtained results were validated using theoretical tools. The tautomerism of the compound has been monitored while analyzing the molecular structure regarding to describe unknown properties and applications. The displacement of chemical shift of core carbons in pyrimidine and Imidazole rings by the injection atom and the mechanism customized to induce chemical properties were interpreted. The electronic degeneracy pathway in the interaction orbitals was discussed by viewing the frontier molecular overlapping. The drug and biological activity of the present compound was interpreted, and the capability of suitable applications has been interpreted. The VCD spectrum for the measurement of toxicity level was simulated and the rate of masking was examined.

Key words:

8-chloroquinoline l, QSAR properties, Ligand efficiency, electronic degeneracy, Lipophilic Efficiency.

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Abstract-43

Pharmacodynamic investigation and QSAR analysis on Molecular structure of Tetrachlorophthalic acid using spectroscopy tools supported by quantum calculations

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Abstract

The molecular properties of Tetrachlorophthalic acid related to molecular dynamic activity have been elaborately studied in this systematic research work. The spectroscopic tools (FT-IR, FT-Raman, NMR and UV-Visible) and theoretical tools (HF and DFT) have been used to elucidate the molecular structure and study the pharmaceutical properties instantly. While analyzing the molecular structure useful results regarding unknown properties and applications were obtained. The calculated values; heats of formation, QSAR properties, Lipinski's parameters, Ligand efficiency (LE), Lipophilic Efficiency (LipE), were reported and discussed, to understand the biological activity of the Tetrachlorophthalic acid. The biological activity of the present compound was studied, and the capability of drug action has been interpreted. The VCD spectrum for the toxic study was simulated at stable conformer and the rate of masking was predicted.

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Abstract-44

Molecular spectroscopy investigation on Pharmacodynamic activity and biological property analysis on anti-mycobacterial drug 4-Aminosalicylic acid

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Abstract

The Pharmacodynamic activity was keenly observed by recording FT-IR, FT-Raman, UV-Visible and NMR spectra of 4-Aminosalicylic acid. The observed absorption and scattering spectral sequence were analyzed to predict the role of compositional parts in the compound activity. The unknown physicochemical properties were calculated and were correlated with the physical parameters. The drug activity of the compound was predicted by observing frontier molecular interaction profile. The electronic transitions among different energy levels of electronic structure were determined and hyperactive Polarizability causing the anti-micro bacterial activity was discussed. The exchange of chemical potential for creating drug potential by making transitions among non-bonding molecular orbitals has been examined. The QSAR properties were calculated and Lipinski's rules for drug likeness were reported and discussed to recognize the biological activity of the molecule. The VCD spectrum in different range of IR region for determining enantiomer ability was replicated at stable conformer and the hiding of toxicity was predicted.

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Abstract-45

Vibrational study, NBMO's, HOMO-LUMO, VCD investigation on Benzoyl peroxide using Quantum computational Calculations

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Abstract

The present compound is an antibiotic agent which mainly utilized with many drug combinations. the electron clouds are directly concentrated over the carbons of benzene rings and are directed from peroxide groups via the peroxide connected carbon of the top moiety of ring to create the wonderful drug property for the title compound. Due to the asymmetric charge orientation, the carbons of the peroxide groups become neutral whereas the electron cloud is remains concentrated on π- bonded 3O and 4O in order to maintain the chemical equilibrium. In addition to that, the strong dipole bonds (C=O) are created symmetrically on peroxide groups. The negative charge distribution is appeared on both sides of molecule and the depletion zone is centered at peroxide group due to which the strong drug property consistently emphasized.

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Abstract-46

Spectroscopic and QSAR analysis on Antibiotic drug; 2-Amino-4,6-Dimethyl pyrimidine using Quantum computational tools

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Abstract

The antibiotic activity of 2-Amino-4,6-Dimethyl pyrimidine has been analyzed using molecular spectroscopy tools. The biological activity was interpreted, and drug likeness was evaluated by calculating biological parameters. The activeness of the internal molecular parts was assessed by the assignment of fundamental modes of vibrations. The chromophores action for the inducement of the antibiotic activity of the compound was analyzed from the electronic excitation absorption peaks. The σ-bond, π-bond and δ-bond interaction lobes were identified and the exchange of energy between the orbitals was investigated from frontier molecular orbital profile. The asymmetrical charge distribution among different entities of the molecule for the perseverance of anti tuberculosis mechanism was recognized. The NMBO interaction profile was evaluated by the NBO calculation adapted with Gaussian and the exchange of maximum energy transaction among various functional groups for the incentive of antibiotic were determined. The second order Polarizability of the compound emphasized the consistency of the antibiotic activity of the molecule. The inhibition catalytic efficiency of the title molecule was fully tested by molecular docking study.

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Abstract-47

Molecular Vibrational Investigation [FT-IR, FT-RAMAN, UV–Visible and NMR] On Methyl Aminomethyl Anthracene by Using Computrized Quantum Calculations

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Abstract

The FT-IR, FT-Raman spectra of the Methyl aminomethyl anthracene was recorded and analyzed. The observed fundamental frequencies in finger print and functional group regions be assigned according to their individuality region. The computational calculations were carriedout by HF and DFT (B3LYP and B3PW91) methods with 6-31++G(d,p) and 6-311++G(d,p) basis sets and the corresponding results were tabulated. The present organo-metallic compound was made up of covalent and coordination covalent bonds. The modified vibrational pattern of the complex molecule associated with ligand group was analyzed. Furthermore, the 13C NMR and 1H NMR spectral data were calculated by using the gauge independent atomic orbital (GIAO) method with B3LYP/6-311++G(d,p) basis set and their spectra were simulated and the chemical shifts linked to TMS were compared. A study on the electronic and optical properties; absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies were carried out. The kubo gap of the present compound was calculated related to HOMO and LUMO energies which confirm the occurring of charge transformation between the base and ligand groups of the molecule.

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Abstract-48

NLO activity mechanism investigation on 4-methyl 5-nitrouracil using computational solvation tool

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Abstract

The semi organic crystal 4-Methyl 5-Nitrouracil was grown and its source of linear and non-linear optical properties was explored. The stability of the crystal structure was ensured by performing the theoretical calculations; HF and B3LYP methods with 6-311++G(d,p) level of basis set. The Mulliken charge profile, electronic, optical and hyper polarizability analyses have been carried out in order to evaluate nonlinear optical (NLO) performance of the crystal. The accurate optical electron transitions the UV-Visible are also calculated and there by the optical characteristics were studied. The injection of necessary molecular ligand group for the stimulus and tuning of NLO properties were investigated by performing fundamental vibrational of the molecules. The optical energy transformation surrounded by frontier molecular levels has been described by NMBO profile. The outer shell of different chemical environment monitored from the NMR spectra. The vibrational optical polarization characteristics with respect to molecular composition in the compound have been studied by VCD spectrum.

Keywords:

4-Methyl 5-Nitrouracil, hyper polarizability analyses, Mulliken charge.

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Abstract-49

Growth, Spectral Analysis and Characterization Of L-Histidine of Ammonium Chloride Nlo Crystal

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Abstract

Optically good crystal of l-Histidine of ammonium chloride were grown using the slow evaporation technique. The collected well grown crystals were re-crystallized to get crystal of good quality of size, powder X-ray diffraction pattern of the grown sample has been indexed for the material. The FTIR analysis verifies the functional group of the grown crystal. Optical absorption spectrum revealed the optical properties of the grown crystals. The NLO property of the crystal was examined. The Mulliken charge levels of the compound ensure the perturbation of atomic charges according to the ligand group. The molecular interaction of frontier orbitals emphasizes the modification of chemical properties of the compound through the reaction path. The enormous amount of NLO activity was induced by the l-Histidine of ammonium chloride. The Gibbs free energy was evaluated at different temperature and from which the enhancement of chemical stability was stressed. The VCD spectrum was stimulated and the optical dichroism of the compound has been analyzed.

Key words:
l-Histidine of ammonium chloride, perturbation, Gibbs free energy, VCD.

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Abstract-50

Molecular spectroscopy investigation on Pharmacodynamic activity and biological property analysis on anti-bacterial drug; Benzhydrylamine using computational tools

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Abstract

The spectroscopic tools (FT-IR, FT-Raman, NMR and UV-Visible) and theoretical tools (HF and DFT) have been used to illuminate the molecular structure and study the pharmaceutical properties directly. For analyzing these molecular structure results concerning unknown properties and applications were obtained. The change of chemical environment of the core carbons in hexagonal prototype in the molecule by the addition of acid groups and chlorine atoms has been clearly monitored and the corresponding customized chemical properties have interpreted. The electronic degeneracy in the orbitals was studied by screening the frontier molecular interactions. The involvement of non-bonding molecular orbitals has been examined by finding the magnitude of transitions among the orbitals are biological activity of the Benzhydrylamine. The biological activity of the present compound was studied, and the capability of drug action has been interpreted. The VCD spectrum for the toxic study was stimulated at stable conformer and the rate of masking was predicted.

Key words:

Benzhydrylamine, electronic degeneracy, molecular interactions.

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Abstract-51

Structural, spectral, linear and non-linear optical studies of 3-(3,4-dihydroxyphenyl)-L-Alanine

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Abstract

In this research work, the inducement of NLO property on the compound 3-(3,4-dihydroxyphenyl)-L-Alanine has been analyzed using computational calculations. The FT-IR, FT-Raman, FT-NMR and UV-Visible spectra have been recorded in specified region for molecular analysis. The optimized inducement of NLO activity by the molecular structural deformation due to the interaction between Alanine group has been investigated. The supportive analyses such as Mulliken charge levels, first order and second order polarization, vibrational investigation, frontier molecular interactions, thermodynamic function (Gibbs energy) and VCD profile for proving NLO mechanism in the compound have been carried out. The chemical environment of the compound was simultaneously monitored by simulating and recording ^{1}H and ^{13}C NMR spectra. The isotropic and anisotropic chemical shift related to carbons and hydrogens after the formation of target compound have been carefully interpreted. The stabilization of orbitals by interchanging of energy between donor and acceptor was observed by NBO perturbation calculations.

Key words:
3-(3,4-dihydroxyphenyl)-L-Alanine, NLO activity, VCD, Isotropic, NBO perturbation.

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Abstract-52

Electronic and Vibrational Spectroscopic (FT-IR and FT-Raman) investigation using ab initio (HF) and DFT (B3LYP and B3PW91) and HOMO/LUMO/MEP analysis on the structure of L-Serine Methyl Ester

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Abstract

The Vibrational spectroscopy (Fourier Transform Raman and Infrared spectra) of L-Serine Methyl Ester (LSMEHCL) have been recorded and the observed vibrational frequencies are assigned and tabulated. The Gaussian Hybird Computational calculations were determined by HF and DFT (B3LYP and B3PW91) methods with 6-31++ G(d,p) and 6-311++G(d,p) as basis sets and corresponding results were tabulated. The change of structure of amino acid due to the addition of subsequent substitutions of methyl, ethyl, carboxylic and hydroxyl chain is investigated. It plays a vital role in the production of different pharmaceutical and cosmetics industries. The 6-311+G(d,p) basis set and ^{13}C and ^{1}H nuclear magnetic resonance chemical shifts related to TMS were compared. A study on the optoelectronics properties: absorption wavelengths, excitation energy, oscillator strength, dipole moment and FMO were executed by the HF and DFT methods. UV-Visible spectrum of the present compound is recorded in the region is 200-400nm and the electronic properties HOMO and LUMO energies are deliberated by TD-DFT method. The Kubo gap of the present molecule was calculated, for the charge transformation between base and ligand. The stability of the molecule and charge delocalization has been analyzed using natural bond orbital (NBO).

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Abstract-53

Pharmacodynamic investigation on Organic structure and Molecular spectroscopic analysis of Ethambutol with computational support

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Abstract

The molecular properties of Ethambutol related to molecular dynamic activity have been elaborately studied in this systematic research work. The spectroscopic tools (FT-IR, FT-Raman, NMR and UV-Visible) and theoretical tools (HF and DFT) have been used to elucidate the molecular structure and study the pharmaceutical properties instantly. While analyzing the molecular structure useful results regarding unknown properties and applications were obtained. The change of chemical environment of the core carbons in chain pattern in the molecule by the injection of acid groups and OH-CH-NH-CH as been clearly monitored and the corresponding customized chemical properties have interpreted. The electronic degeneracy in the orbitals was studied by screening the frontier molecular interactions. The involvement of non-bonding molecular orbitals has been examined by finding the magnitude of transitions among the orbitals. The calculated values; heats of formation, QSAR properties, Lipinski's parameters, Ligand efficiency (LE), Lipophilic Efficiency (LipE), were reported and discussed, to understand the biological activity of the Tetrachlorophthalic acid. The biological activity of the present compound was studied, and the capability of drug action has been interpreted. The VCD spectrum for the toxic study was simulated at stable conformer and the rate of masking was predicted.

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Abstract-54

Molecular structure and Pharmacodynamic activity behavior investigation and QSAR analysis on Hypoxanthine using computational tools

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Abstract

The structural properties of Hypoxanthine compound related to molecular dynamic activity have been ornately interpreted in this methodical research work. The FT-IR, FT-Raman, NMR and UV-Visible spectral analysis has been carried out and the obtained results were validated using theoretical tools. The tautomerism of the compound has been monitored while analyzing the molecular structure regarding to describe unknown properties and applications. The displacement of chemical shift of core carbons in pyrimidine and Imidazole rings by the injection of =O atom and the mechanism customized to induce chemical properties were interpreted. The electronic degeneracy pathway in the interaction orbitals was discussed by viewing the frontier molecular overlapping. The involvement of CT-complex transitions in non-bonding molecular orbitals has been inspected. The QSAR properties, Ligand efficiency (LE), Lipophilic Efficiency (LipE), were calculated and reported for explaining biological activity of Hypoxanthine. The drug and biological activity of the present compound was interpreted, and the capability of suitable applications has been interpreted. The VCD spectrum for the measurement of toxicity level was simulated and the rate of masking was examined.

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Abstract-55

Spectroscopic investigation on physical and analytical chemistry Premoline by using the calculations

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Abstract

The Antibiotic activity was zealously observed by recording FT-IR, FT-Raman, UV-Visible and NMR spectra of Premoline (2-Imino-5-phenyl 4-oxazolioinone). The observed amalgamation and scattering spectral sequence were analyzed to compute the role of compositional parts in the compound activity. The unknown Predicted Properties be calculated and were interrelated with the physical parameters. The drug Stimulation of the compound was predicted by observing frontier molecular interaction profile. The electronic transitions among different energy levels of electronic arrangement were determined and hyperactive Polarizability causing the anti-micro bacterial activity was discussed. The exchange of chemical potential for creating drug budding by making transitions among non-bonding molecular orbitals has been examined. The QSAR properties were designed and Lipinski's rules for drug similarity were reported and discussed to recognize the biological activity of the molecule. The VCD spectrum in different range of IR region for determining enantiomer ability was replicated at stable conformer and the hiding of toxicity was predicted.

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Abstract-56

Preparation, Characterization and Spectroscopic Study on Sno_2 Nano powder

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Abstract

In this research work, pure and singe phase SnO_2 Nano powder is successfully prepared by simple sol-gel combustion route method. The photo luminescence and XRD measurements were made and their geometrical parameters are compared with calculated values by theoretical calculations. The FT-IR and FT-Raman spectra were recorded, and the fundamental frequencies were assigned. The optimized parameters and the frequencies were calculated using HF and DFT (LSDA, B3LYP and B3PW91) theory in bulk phase of SnO_2 and were compared with the Nano phase. The vibrational frequency pattern in nano phase would be realigned and the frequencies were shifted up to higher region of spectra when compared with bulk phase. The NMR and UV-Visible spectra were simulated and analyzed. Transmittance studies showed that the HOMO-LUMO band gap (Kubo gap) was reduced from 3.47 eV to 3.04 eV while it is heated upto 800°C. The Photoluminescence spectra of SnO_2 powder showed a peak shift towards lower energy side with the change of Kubo gap from 3.73 eV to 3.229 eV for as-prepared and heated up to 800°C.

Key words:

SnO_2 Nano powder, electronic and optical properties, nano phase approach.

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Abstract-57

FT-IR, FT-RAMAN, UV-VIS AND NMR Analyses on Chlorfenson Using Computational Calculations

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Abstract

In the present work, the recorded FT-IR/FT-Raman spectra of the Chlorfenson (4-Chorophenyl-4-chlorobenzenesulfonate) are analyzed. The observed vibrational frequencies are assigned and the computational calculations are carried out by DFT (LSDA, B3LYP and B3PW91) methods with 6-31++G(d,p) and 6-311++G(d,p) basis sets and the corresponding results are investigated with the UV/NMR data. The fluctuation of structure of Chlorobenzene sulfonate due to the substitution of C_6H_4Cl is investigated. The vibrational sequence pattern of the molecule related to the substitutions is intensely analyzed. Moreover, ^{13}C NMR and ^{1}H NMR chemical shifts are calculated by using the gauge independent atomic orbital (GIAO) technique with HF/B3LYP/B3PW91 methods on same basis set. A study on the electronic properties; absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies, are performed by HF and DFT methods. The calculated energy of Kubo gap (HOMO and LUMO) ensures that the charge transfer occurs within the molecule. Besides frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) is executed. NLO properties and Mulliken charges of the Chlorfenson is also calculated and interpreted. The thermodynamic properties (heat capacity, entropy, and enthalpy) of the title compound at different temperatures are calculated in gas phase.

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Abstract-58

Preparation, Characterization and Structure Prediction of In 2 sno$_3$ Using Spectroscopic (FT-IR, FT-RAMAN, NMR and UV-VISIBLE) study

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Abstract

In this work, pure and single phase In_2SnO_3 Nano powder is successfully prepared with the doping ratio of 80-20% (In_2O_3-Sn) by simple sol-gel combustion direction. The material is characterized by XRD measurements and their geometrical parameters are compared with calculated values. The FT-IR and NMR spectra are recorded in both bulk and Nano phase and FT- Raman spectrum is recorded in bulk phase and the fundamental frequencies are assigned. The optimized parameters and the frequencies are calculated using HF and DFT theory in bulk phase of In_2SnO_3 and are compared with its Nano phase. The vibrational frequency pattern in nano phase gets realigned and the frequencies are shifted up and down little bit to the region of spectra when compared with bulk phase. The UV-Visible spectrum is simulated and analyzed. The frontier molecular orbital analysis has been carried out and the values of the HOMO-LUMO band gap (Kubo gap) explore the optical and electronic characteristics of the In_2SnO_3. Structural studies by XRD showed the crystallite sizes of the particles. The atomic arrangement in the grain boundary seems to be somewhat different from regular periodic arrangement whereas inside the grain there is a good periodic arrangement of atoms.

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Abstract-59

Dielectric, Electrical Conductivity of Organic NLO Crystals - Picolinium Maleate (PM) - Novel Material

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Abstract

Organic crystals are important for materialistic applications such as frequency matching, phase matching, opto-electronic applications. The PM crystal is of second order NLO and as good NLO coefficient.

The XRD, dielectric, AFM, electrical conductivity, refractive influx is studied and reported.

The XRD study reveals the lattice parameters of the grown PM crystals and dielectric property analysis the PM crystals as the case how it performs in non-conducting way and AFM portrays the surface analysis and refractive influx specifies the velocity change and electrical conductivity graph portrays the V-I response and linearity of the graph.

Keywords:

PM, NLO, dielectric, electrical conductivity etc.,

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Abstract-60

Optimizing the physical properties of calcium nanoferrites to be suitable in many applications

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Abstract

The Calcium nano ferrite with composition $CaGd_xEr_yFe_{2-x-y}O_4$ (x = y = 0.0, x = 0.025, y = 0.05) was prepared by citrate gel auto combustion method. The prepared samples showed orthorhombic phase structure and the crystallite sizes were found in the range of 32.1–35.3 nm. Detailed observation via the Field Emission Scanning Electron Microscopy (FESEM) showed that the calcium ferrite nano-particles were spherical and capsule like formation shape. The hysteresis loop confirms the magnetic behavior of the investigated samples, which is then discussed on the basis of super exchange interactions. Magnetic parameters such as saturation magnetization, coercively, and retentivity were obtained. The $CaFe_2O_4$-type structure includes edge- and corner sharing BO_6 octahedral, constituting a very unique network similar to perovskite-related nanoparticles. This structural network leads to an improvement in the physical properties of the investigated samples.

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Abstract-61

NBO, Conformational, NLO, Homo-LUMO, NMR and Electronic Spectral Study on 1-Phenyl-1-Propanol by quantum Computational Methods

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Abstract

In this study, FT-IR, FT-Raman, NMR and UV spectra of 1-phenyl-1-propanol, an intermediate of anti- depressant drug Fluoxetine, has been investigated. The theoretical vibrational frequencies and optimized geometric parameters have been calculated by using HF and density functional theory with the hybrid methods B3LYP, B3PW91and 6-311+G(d,p)/6-311++G(d,p) basis sets. The theoretical vibrational frequencies have been found in good agreement with the corresponding experimental data.1H and13C NMR spectra were recorded and chemical shifts of the molecule were compared to TMS by using the Gauge-Independent Atomic Orbital (GIAO) method. A study on the electronic and optical properties, absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies are performed using HF and DFT methods. The thermodynamic properties (heat capacity, entropy and enthalpy) at different temperatures are also calculated. NBO analysis is carried out to picture the charge transfer between the localized bonds and lone pairs.

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Abstract-62

XRD, AFM, Refractive influx, Dielectric, Electrical Conductivity of Organic NLO Crystals Acetoacteanilide (AAC)

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Abstract

Organic crystals play a vital role such as frequency matching, phase matching, opto-electronic applications. The AAC crystal is of second order NLO with good non-linear coefficient. The XRD, dielectric, AFM, electrical conductivity, refractive influx is studied and reported. The XRD study reveals the lattice parameters of the grown AAC crystals and dielectric property analysis the AAC crystals as the case how it performs in non-conducting way and AFM portrays the surface analysis and refractive influx specifies the velocity change and electrical conductivity graph portrays the V-I response and linearity of the graph.

Keywords:

AAC, NLO, dielectric, electrical conductivity etc…

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Abstract-63

Spectroscopic [FT-IR and FT-Raman] and theoretical [UV-Visible and NMR] analysis on α-Methylstyrene by DFT calculations

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Abstract

In the present research work, the FT-IR, FT-Raman and ^{13}C ^{1}H NMR spectra of the α-Methylstyrene were recorded. The observed fundamental frequencies in finger print and functional group regions were assigned according to their uniqueness region. The Gaussian computational calculations are carried out by HF and DFT (B3LYP and B3PW91) methods with 6-31++G(d,p) and 6-311++G(d,p) basis sets and the corresponding results were tabulated. The impact of the presence of vinyl group in phenyl structure of the compound is investigated. The modified vibrational pattern of the molecule associated vinyl group was analyzed. Moreover, ^{13}C NMR and ^{1}H NMR were calculated by using the gauge independent atomic orbital (GIAO) method with B3LYP methods and the 6-311++G(d,p) basis set and their spectra were simulated and the chemical shifts linked to TMS were compared. A study on the electronic and optical properties; absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies were carried out. The kubo gap of the present compound was calculated related to HOMO and LUMO energies which confirm the occurring of charge transformation between the base and ligand. Besides frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) was performed. The NLO properties related to Polarizability and hyperpolarizability based on the finite-field approach were also discussed.

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Abstract-64

Spectroscopic Analysis, Aim, Nlo and VCD Investigations of Acetaldehyde Thiosemicarbazone Using Quantum Mechanical Simulations

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Abstract

The prepared Acetaldehyde thiosemicarbazone (ATSC) have been investigated by both the experimental and theoretical methods; through this work, the essentiality of elucidation of molecular fragments source linear and non-linear optical properties was explored. The stability of the structure and entire calculations have been performed on HF and B3LYP methods with 6-311++G(d,p) level of basis set. The Mulliken charge profile, electronic, optical and hyper polarizability analyses have been carried out in order to evaluate nonlinear optical (NLO) performance of the present compound. The exact optical location of the ATSC was determined by executing UV-Visible calculations on TDSCF method. The existence of the molecular group for the inducement and tuning of NLO properties were thoroughly investigated by performing fundamental vibrational investigation. The optical energy transformation among frontier molecular levels has been described in UV-Visible region. The Gibbs energy coefficient of thermodynamic functions was monitored in different temperature and it was found constant irrespective of temperatures. The appearance of different chemical environment of H and C was monitored from the ^{1}H and ^{13}C NMR spectra. The vibrational optical polarization characteristics with respect to molecular composition in the compound have been studied by VCD spectrum.

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Abstract-65

Spectroscopic (FT-IR/FT-Raman) and Computational (HF/DFT) investigation and HOMO/LUMO/MEP analysis on 2-Amino-4-chlorophenol

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Abstract

The spectra (FT-IR & FT-Raman) of the present compound; 2-Amino-4-chlorophenol (2A4CP) were recorded in the range of 4000-100 cm^{-1}. All the computational calculations were made in the ground state using the HF and DFT (B3LYP and B3PW91) methods with 6-31++G(d,p) and 6-311++G(d,p) basis sets. From potential energy surface calculation, there are two conformers, Rot-1 and Rot-2 for this molecule. The computational results detected that Rot-1 form is the most stable conformer. Making use of the recorded data, the complete vibrational assignments were made and analysis of the observed fundamental bands of molecule is carried out. The complete assignments were performed on the basis of the total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) method and PQS program. The shifting of the frequencies in the vibrational pattern of the title molecule due to the substitutions; NH_2 and Cl were deeply investigated by the vibrational analysis. Moreover, ^{13}C NMR and ^{1}H NMR chemical shifts were calculated by using the gauge independent atomic orbital (GIAO) method with HF/B3LYP/B3PW91 methods with 6-311++G(d,p). A study on the electronic properties, such as HOMO and LUMO energies, were performed by time-dependent DFT (TD-DFT) approach. Besides frontier molecular orbitals (FMO), molecular electrostatic potential (MEP) was performed. NLO properties and Mulliken charges of the 2A4CP were also calculated and interpreted.

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Abstract-66

Synthesis, Characterization and Photophysical Studies of Schiff base: The Intramolecular Charge-Transfer State Produced by Excited-State Intramolecular Proton Transfer

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Abstract

Synthesis of donor-π-acceptor dye (E)-2-((4-(10H-phenothiazin-10-yl) phenylimino) methyl) phenol (PSA) with spectral Characterization by FT-IR, ^{1}H NMR and ^{13}C NMR. The photophysical studies of PSA in different solvents were explored using steady state absorption, fluorescence and time resolved fluorescnec studies. The absorption, fluorescence and excitation spectrum were recorded in non-polar to high polar solvents. The absorption and emission maximum were red shift with increasing solvent polarity due to the intramolecular charge transfer (ICT). This positive solvatochromic shift in ESIPT keto fluorescence creates from the formation of an intramolecular charge-transfer (ICT) state after the ESIPT process.