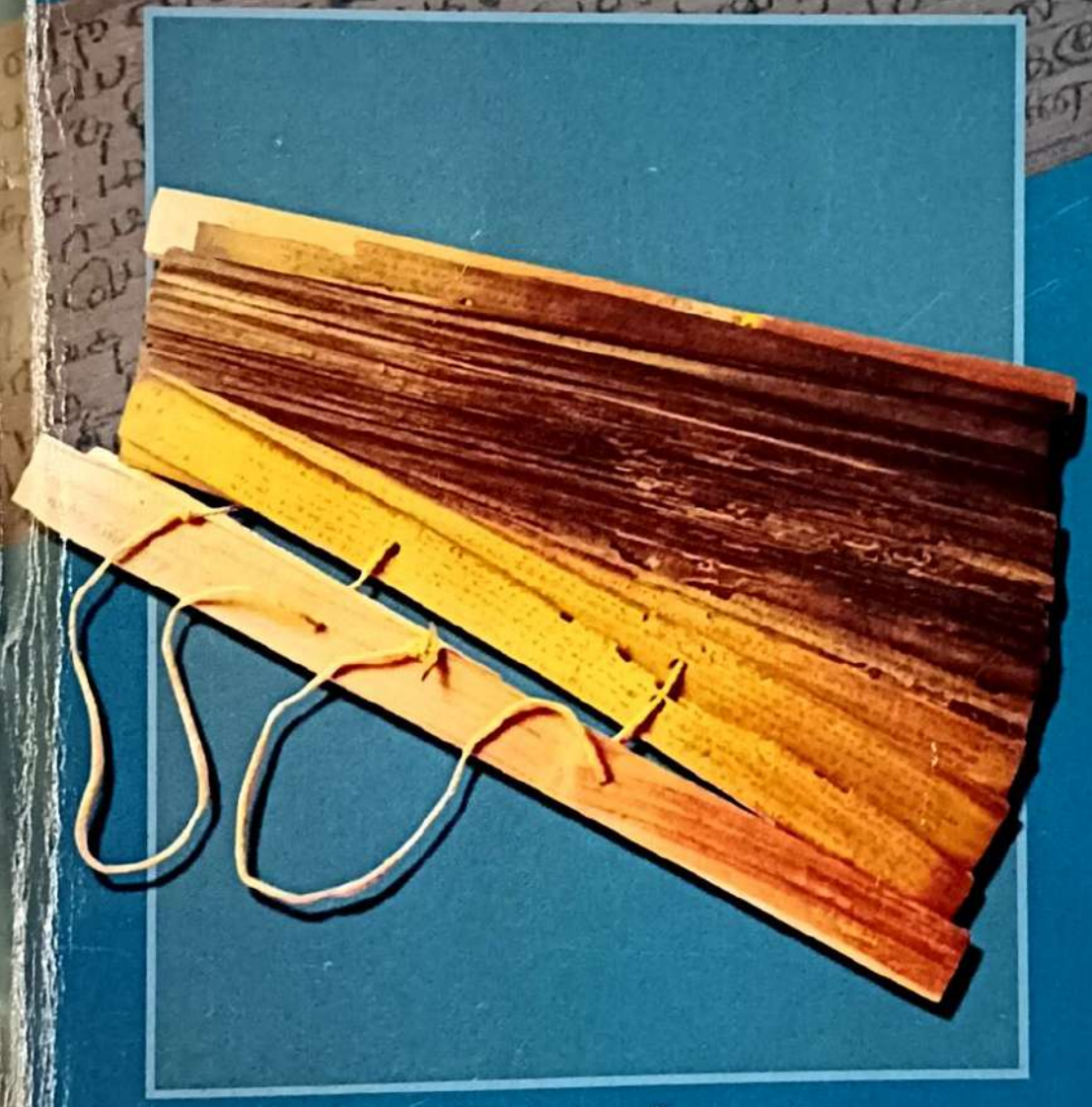

# வற்மக்கண்ணாடி

## ஐநூறு

சுவடிப் பதிப்பு நூல்

ம. பெரில் திரேஸ்

# வற்மக்கண்ணாடி ஐநூறு

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நாஞ்சில் கத்தோலிக்க கலை மற்றும் அறிவியல் கல்லூரி
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## CONTRIBUTED PAPERS

**OP-03**

# SYNTHESIS, MOLECULAR DOCKINGAND ANTIMYCOBACTERIAL ACTIVITY OF GREEN MEDIATED AG-CDONANOPARTICLES

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## ABSTRACT

The lack of an effective vaccine, combined with the rise of Mycobacterium tuberculosis (MTB) strains that are highly resistant to therapies, foreshadows a difficult future situation. This work focuses on the possibilities for biomedicine associated with the environmentally benign synthesis of Ag and Ag-CdO nanoparticles from natural materials produced from Sauropusandrogynus.Energy dispersive X-ray spectroscopy (EDX) and scanning electron microscopy (SEM) analyses were utilised to analyse the characteristics of the synthesised nanoparticles. In accordance with DFT studies, the Diethyl Phthalate found in Sauropusandrogynus Leaf extract plays a role for the leaf extract's ability to function as a reducing agent, converting $Ag^{+}$ ions into $Ag^{0}$. Using molecular docking studies, the synthetic compound's anti-tuberculosis activity was evaluated. An in vitro antimycobacterial investigation has been performed for the mycobacterial strain Mycobacterium smegmatis.

**Keywords**: Tuberculosis, Mycobacterium smegmatis, DFT, Nanoparticles, green synthesis

## INTRODUCTION

It is estimated by the World Health Organization (WHO), that two billion individuals are infected with MTB, of which eight million develop active tuberculosis and almost two million surrender to the disease annually.Doping CdO with metallic elements Ag has the ability to change its physical characteristics; as a dopant, it increases electrical conductivity, optical band gap, and n-type conductivity. This background led to the design of this study, which examined the effectiveness of Ag doped CdO produced by Sauropus leaf extract as a treatment against mycobacterium. Moreover, the identification of accomplished interactions between Ag-CdO NPs and their ability to inhibit the protein targets responsible for Tuberculosis is determined by computer-aided drug design techniques.

## SYNTHESIS OF SILVER NANOPARTICLES

To the dissolved 0.1 M AgNO3 solution, 10 ml of Sauropusandrogynus leaf extract was added and stirred continuously until the solution changed colour from colourless to brown. The decrease of $Ag^{+}$ to $Ag^{o}$ was confirmed through colour change, as well as the formation of Ag nanoparticles. Then, for two to three hours the reaction mixture was heated at 70°C. Following two centrifugations, the reaction mixture was cleaned using deionized water and ethanol. It was then dehydrated for the entire night at 80 °C in a hot oven.

## SYNTHESIS OF AG-CDO NANOPARTICLES

To synthesise cadmium acetate, 2% silver nitrate ($AgNO_3$) and 20 mL of Sauropusandrogynus leaf extract were used. 2% $AgNO_3$ solution diluted in 25 mL DI water was mixed with a 100 mL DI water solution containing cadmium acetate. To obtain 2% Ag-CdO, 20 mL of Sauropusandrogynus leaf extract was added dropwise to the precursor solution. The reaction mixture was incubated for 24 hours at 37 °C to allow the produced nanocomposite to fully develop. After being re-dispersed in ethanol and de-ionized water, the precipitate was centrifuged. Finally, the precipitate was calcined at 500°C for 3 hours to yield the required product.

## RESULTS AND DISCUSSIONS

### Scanning Electron Microscopy (SEM)

The spherical shape of CdO-free nanoparticles changes when CdO is added, resulting in a surface that differs significantly from the pure sample. Morphology of Ag-CdO revealed an aggregated spherical shape; these particles are typically spherical in shape. The agglomeration of the particle was observed owing to CdO nanoparticles' polarity and electrostatic attraction. The average Particle size of the Nano powder after the milling process was observed to be smaller than 100 nm. Fig. 1(a,b) displays SEM images of nanoparticles of Ag and Ag-CdO.

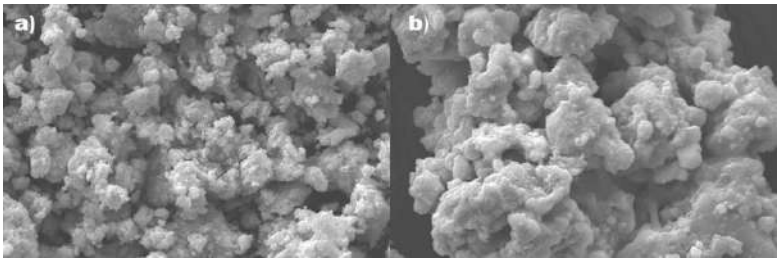

**Fig.1SEM images of a) Ag and b) Ag-CdO NP's.**

**Energy dispersive X-ray spectroscopy (EDX)**

From the fig.2 it is confirmed that Ag is present in the pure sample and that Ag, Cd, and O are present as dopants in the doped sample. Pure silver nanoparticle formation is illustrated by the Ag peak identified at 3 KeV. The presence of biological components in the plant extract used for bio reduction may be the cause of the other weak peak of Na.

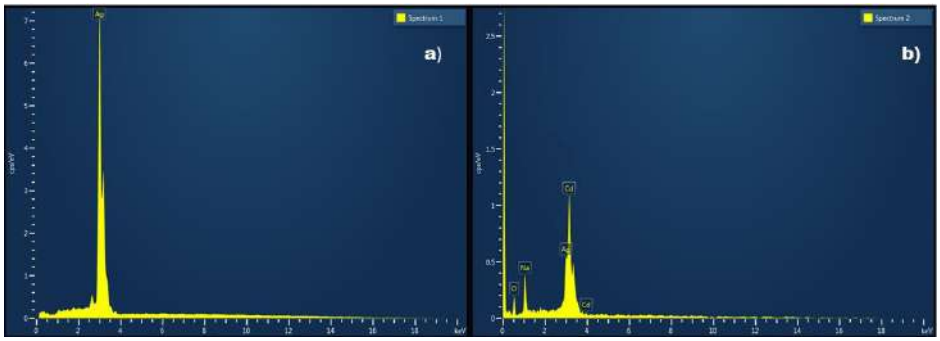


**Fig. 2EDX spectrum of a) Ag and b) Ag-CdO NP's**

**QUANTUM CHEMICAL STUDY**

DFT (density functional theory) analysis was conducted to investigate the reduction behaviour of Diethyl Phthalate (DP), a compound found in the Sauropusandrogynus leaf extract, which was identified through GCMS analysis. The optimized structure of DP is represented in fig.3. A decrease in the energy gap or ΔE value between HOMO-LUMO signifies that electrons can be extracted from the last occupied orbital of the molecule with only the least amount of energy. In order to enhance the reduction of silver nitrate ($AgNO_3$ to metal), this will bind to the surface of the metal halide and promote the reactivity of the molecule. Furthermore, ΔE offers insights into the stability of the complex that is produced on the surface of the metal halide.

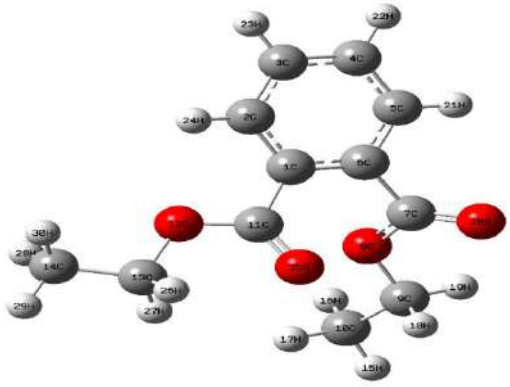

**Fig 3. Optimized molecular structure of Diethyl Phthalate**

**MOLECULAR DOCKING**

To determine the anti-tubercular activity of DP molecule, PDB: 5D6N is chosen. The binding affinity of the DP molecule is −5.3 kcal/mol. The molecule was docked deeply with the 5D6N binding pocket, making seven hydrogen bonds with the amino acids THR463, GLY424 and GLY463 which is shown in fig.4. The nitrite oxygen atom generates 3.18 A˚ and 3.26 A˚ bonds with THR463 and GLY424 residues, respectively. The carboxyl group bonded to the compound shows hydrophobic interactions with GLY463 and GLY424 with bond distances of 2.91 A˚ and 2.93 A˚ respectively, which further contribute to the stability of the compound. The results imply that DP may target protein 5D6N to exert antimycobacterial effectiveness against M.smegmatis species.

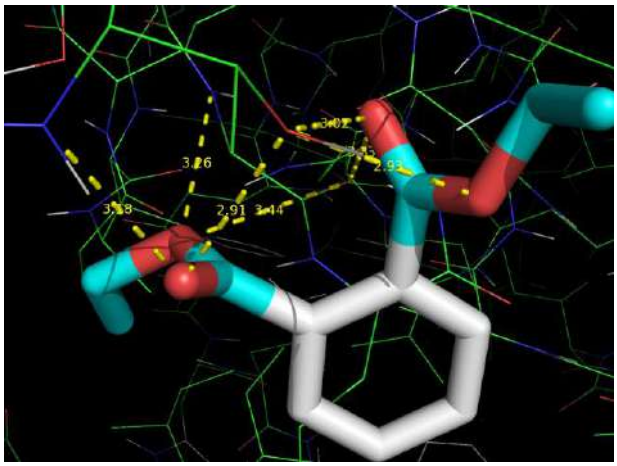


**Fig .4 Docking of target protein with Diethyl Phthalate**

**IN VITRO ANTI-MYCOBACTERIAL ACTIVITY**

It was observed that the nanosynthesized Ag-CdO exhibited significant activity against M.smegmatis, with inhibition zones measuring 19 mm and 21 mm at concentrations of 500 µg and 1000 µg, respectively while the Ag nanoparticles possessed no inhibition to the bacterial growth. This demonstrated the potential of nano-synthesized Ag-CdO as an effective antimicrobial agent. The inhibitory effect of the synthesized materials was further confirmed by the color change of the dye. The colour change in the Ag nanoparticles also did not show enhanced reduction of alamar blue compared to the medium control, indicating their limited activity against M.smegmatis.

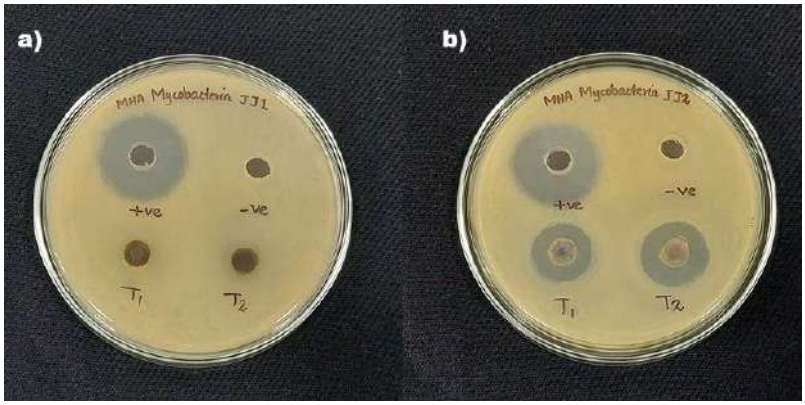


**Fig 5(a,b) Antimycobacterial activity of the synthesized NP's**

## CONCLUSION

The current work offers a simple and low-cost approach for producing Ag-CdO NPs in aqueous environments utilising of Sauropusandrogynus leaf extract. The DFT studies reveal that the Diethyl Phthalate presented in the leaf extract play a vital role in reducing $AgNO_3$ and also behave as a better stabilising agent. Furthermore, the work explores the anti-mycobacterial activity of biosynthesised Ag-CdO NPs and can be used as alternate therapeutic agent for the treatment of Tuberculosis.

# STRUCTURE BASED COMPUTATIONAL AND SPECTROSCOPICINVESTIGATIONS OF CYCLOPROPANE DERIVATIVES

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## ABSTRACT

Density Functional Theory (DFT) has emerged as a widely embraced quantum chemical method for all theoretical analyses and calculating diverse molecular properties across chemical, physical, and biological systems. In this study, B3LYP DFT calculations accurately predict the molecular geometries of 1-acetyl-2-(3-methoxy-4-propoxyphenyl)cyclopropane by optimizing the compound.The computed band gap energy of HOMO-LUMO reveals charge transfer and stability of the molecule. NCI interaction study reveals that it is having steric effect, Van der Waals force, and hydrogen bond. Using MTT assay, Cytotoxicity of the compound has been assessed and characterized for potentially toxic and harmful effects. Docking studieshelpedin identifying the ligand-target interactions and

binding affinity.By ligand-target interactions, the ligand interacts with different proteins to determine the effectiveness of compound against microbial pathogens. NMR spectroscopy reveals intricate details of molecular structure by analyzing local magnetic fields around atomic nuclei, essential in diverse fields like organic synthesis, drug development, and biochemistry.The theoretical Chemical shifts of $^{13}C$ and $^{1}H$ were determined by NMR spectra that is compared with recorded experimental data.

**Keywords**: DFT, charge transfer, NMR, chemical shift.

## INTRODUCTION:

Density functional theory (DFT) stands as a cornerstone in the realm of quantum mechanics, revolutionizing the understanding and predictive capabilities in studying the electronic structure and properties of atoms and molecules [1].Utilizing B3LYP as the basis set, the compound 1 acetyl-2-(3-methoxy-4-propoxyphenyl) cyclopropane (AMPC) was optimized and ΔE band gap energy obtained due to charge transfer in the molecules is determined. Molecular docking is used to predict the biological activity of the compound. Chemical shifts were predicted with theNMR spectral bands.

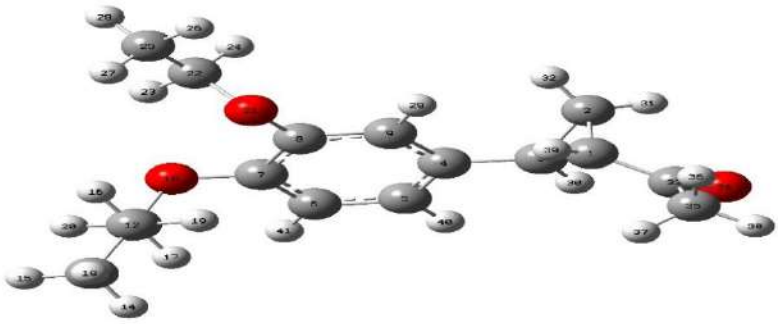
## COMPUTATIONAL DETAILS:

The optimized molecular configuration of the AMPC molecule was determined using gradient-corrected density functional theory (DFT)at the Becke-3-Lee–Yang–Parr (B3LYP) level employing the Gaussian 09 W program package with the 6-311++G (d,p) standard basis set [2]. The resulting ground state structure was visualized using the GaussView program.The AutoDock Vina Suite facilitated the determination of minimum binding energy, inhibition constants, and various parameters related to ligand-protein docking interactions.

## GEOMETRICAL PARAMETERS:

The electronic properties of a molecule are influenced through variations in bond lengths, bond angles, and dihedral angles along the compound's backbone. The shortest bond

length is observed between $C_6$-$H_{41}$ (1.0818Å) and the longest bond length is noted at $C_{12}$–$C_{13}$ (1.5318 Å). Specifically, the bond length of $C_{22}$ –$O_{21}$ (1.4421 Å) appears larger compared to the other C–O bonds, and the $C_6$–$C_7$–$O_{10}$ angle (125.40°) exceeds the other angles within the ring. This variance is due to distinctive environment of oxygen. The C33-O34 bond distance measures 1.2172 Å, lower than typical C-O bond lengths, supporting the presence of a double



bond

**Figure 1: Optimized structure of AMPC calculated at DFT level.**

**HOMO-LUMO:**

The excitation energies are commonly evaluated using the Frontier Molecular Orbitals (FMOs), namely the HOMOs and LUMOs, depicting the transition from the ground state to the first excited state through one-electron excitation.The HOMO is positioned over $C_{33}$=$O_{34}$ and C-C bonds of Cyclopropane and phenyl ring whereas, LUMO is delocalised over $C_7$-$O_{10}$, $C_8$-$O_{21}$ and C-C bonds of Phenyl and slightly on Cyclopropane ring structure. The LUMO–HOMO energy gap (3.962 eV)indicates molecule's stability.

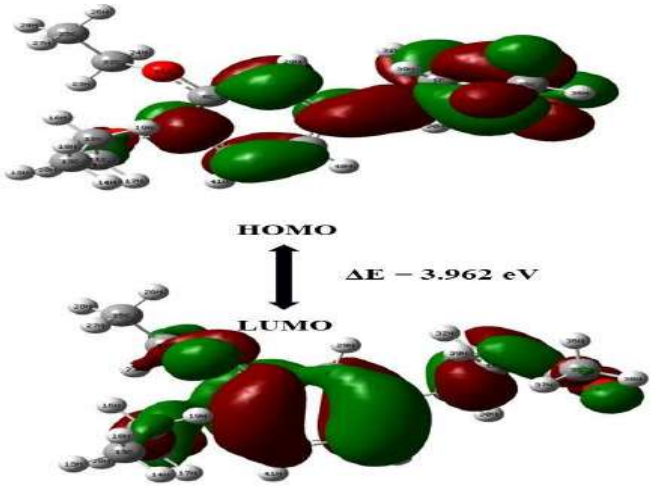



**Figure 2: FMO plot for AMPC**.

**REDUCED DENSITY GRADIENT (RDG) ANALYSIS:**

RDG is a topological technique to study noncovalent interactions (NCI) based on density of electron (r) and its first derivation. The red color at the isosurface's lower end shows strain in the phenyl ring, with non-bonding repulsion (0.01-0.02 a.u.) due to multicentric density interactions. Vanderwaals interaction (-0.01 a.u.) occurs around carbon atoms. In the molecule, Steric repulsion is found to be dominant.

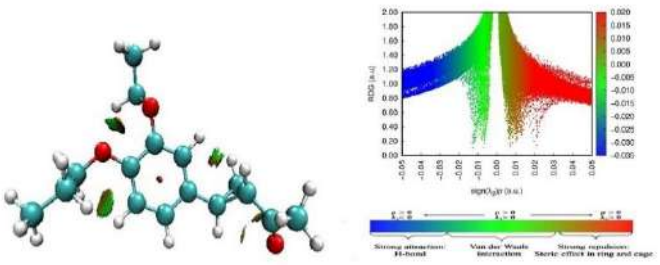


**Figure 3: Plots for RDG of AMPC.**

**MOLECULAR DOCKING:**

Molecular docking relies on structural drug design to analyze molecular interactions, predicting the binding affinity between receptors and ligands. The protein selected for docking investigation is 7asa with binding affinity -5.8 kcal/mol. This protein formed 5 bonds with amino acids UNL546, VAL536, GLN406 and GLY492.Specifically, UNL546 established bonds at distance of 3.53Å and 3.94Å from ligand atom $O_{21}$, while GLN406 and GLY492 forms bonds at distance 3.18 Å and 3.48 Å respectively from ligand atom $O_{34}$. These interactions prove7asa exhibited significant antimicrobial activity. This insight into Protein-Ligand interactions serves as valuable knowledge for the future design of antimicrobial drugs.

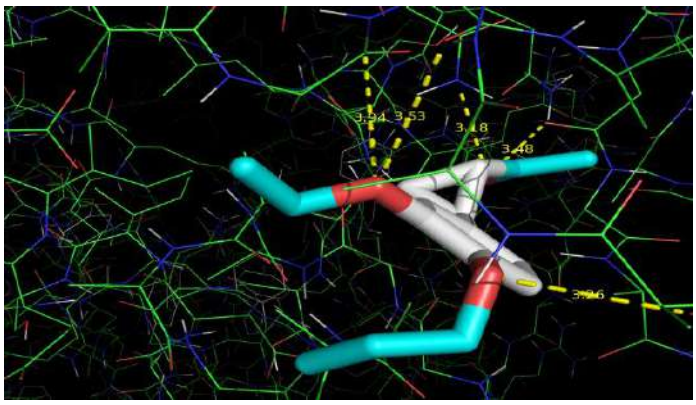



**Figure 4: Docking of AMPC with antimicrobial protein.**

**CYTOTOXICITY:**

Cytotoxicity is a term often used to describe a compound's capacity to induce changes in cellular behavior leading to cell death or a significant decrease in cell viability.Cytotoxic effect of the compound was evaluated on HeLa cells which were seeded in a 96-well plate and treated with varying concentrations (100, 150, 200 μM) for 48 hours.On treating the

HeLa cells with those concentrations, it resulted in cytotoxicityrates of 29.69%, 56.63%, 76.93% respectively. Changes in morphology of the treated HeLa cells have been observed when treated in a 24-well plate and higher concentrations resulted in increased cytotoxicity.

**NMR:**

Nuclear Magnetic Resonance (NMR) is a method used to analyze the structural and chemical properties of molecules. The GIAO (Gauge-independent Atomic Orbital) method is utilized to predict theoretical NMR spectra at B3LYP/6-311G(d,p) level.In this study, the theoretical chemical shift range for aromatic phenyl carbon atoms is 133.3-101.2 ppm, while the corresponding experimental chemical shift is between 132.73-110.42 ppm. The signals obtained at 1.7 δ and 1.6 δ refers to the methoxy group. The obtained NMR results effectively determine the rigidity of the molecule as the carbon atom positions are more accurately replicated compared to hydrogen atoms.

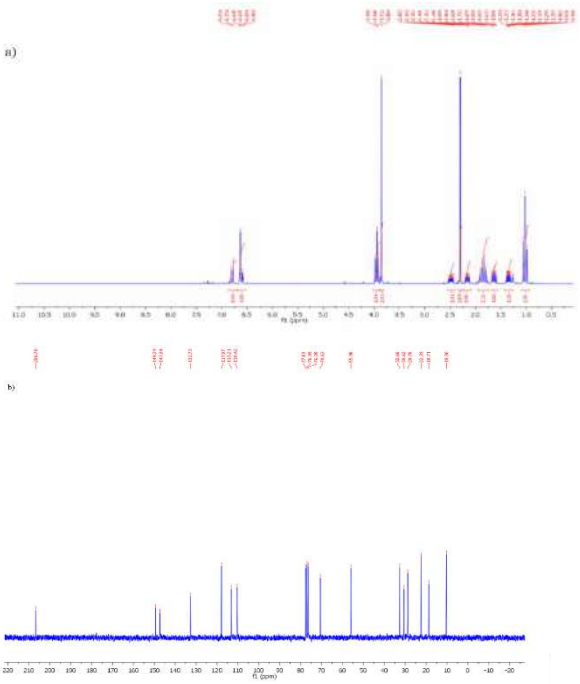


**Figure 6:$^{13}$C and $^{1}$H NMR spectra.**

**CONCLUSION:**

This study offers a thorough structural analysis of AMPC, integrating quantum chemical techniques. With a low HOMO-LUMO energy gap (E = 3.962 eV), the molecule shows potential for strong intramolecular charge transfer species, likely influencing its antimicrobial activity. Docking studies reveal that protein 7asa exhibits a binding affinity of -5.8 kcal/mol with the compound, indicating its antimicrobial activity. NMR analysis elucidates the molecule's rigidity. These studies confirms that the compound provides important role in antidote drug development.

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# DFT COMPUTATIONANDTOPOLOGICAL ANALYSIS OF5-(3,4 – DIMETHOXY PHENYL)-3-METHYL-4,5-DIHYDRO -1H-PYROZOLE -1-CARBALDEHYDE

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## ABSTRACT

Theoretical quantum chemical calculations of 5-(3,4-dimethoxy phenyl) -3- methyl-4,5-dihydro -1H-pyrozole-1-carbaldehydehave been carried out by density functional theory method. The optimizedgeometrical parameters were computationally obtained at the DFT/B3LYP level oftheory. The interpreted HOMO and LUMO energies indicate the chemical stability ofthe molecule.Molecular Electrostatic Potential was illustrated. The obtained results indicates that the compound possess good kinetic stability.

Key words: DFT, HOMO-LUMO, MEP,

## INTRODUCTION

Pyrozole and its derivative are gaining importance in medical and organic chemistry. They have displayed broad spectrum of pharmacological and biological activities such as anti-cancer, anti-viral and anti- inflammatory.Density Functional Theory is a popular method for defining the structural and electrostatics properties of atoms and molecules. In the present work 5-(3,4-dimethoxy phenyl) -3- methyl-4,5-dihydro -1H-pyrozole-1-carbaldehyde was optimized by DFT/B3LYP method with 6-31G(d, p). Geometry optimization such as bond length, bond angle, and dihedral angle has been carried out in the gas phase by B3LYP level

of DFT.The HOMO-LUMO energies the global reactivity parameters were calculated with the help of standard equation to investigate the reactivity and stability of the given molecule.

**COMPUTATIONAL DETAILS**

In this research, the computation of 5 -(3,4-dimethoxy phenyl) -3- methyl-4,5-dihydro -1H-pyrozole-1-carbaldehyde was optimized by the DFT method by using the Becke-3-Lee-Yang-Parr (B3LYP) level of theory with 6-31G(d,p) basis set that is implemented in Gaussian 09W program package. The HOMO-LUMO visualization was made using the Gauss view visualization program and molecular electrostatic

potential maps for identifying the potential region.Geometry optimization such as bond length, bond angle, and dihedral angle has been carried out in the gas phase by B3LYP level of DFT. Molecular electrostatic potential surface analysis used for predicts reactive sites and positive and negative regions of MEP are related to nucleophilic reactivity. The topology analysis ELF and LOL were tools for performing covalent bond analysis performed using multiwfn software.

**RESULTS AND DISCUSSION**

**Optimized Geometry:**

The optimized molecular geometry such as bond length and bond angles of given compound were stimulated at DFT/B3LYP level of theory with the B3LYP/6-31G (d,p) basis set.The optimized molecular structure is shown in figure 1.

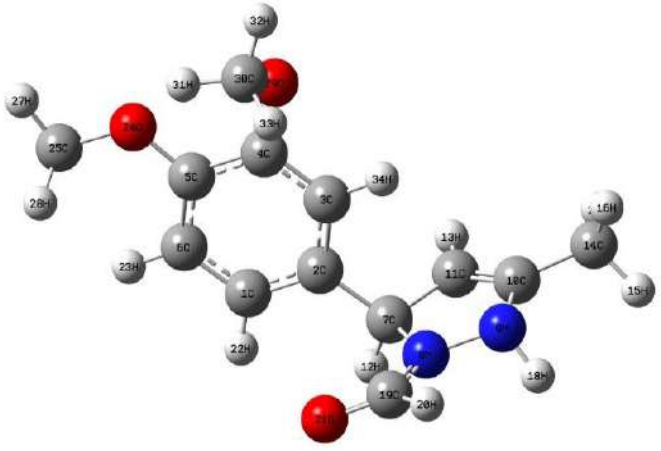

**Figure 1: optimized molecular structure of 5-(3,4 – dimethoxy phenyl)-3-methyl-4,5-dihydro -1H-pyrozole -1-carbaldehyde**

The C-C bond length of the phenyl ring range is 1.3743Å -1.3976Å. ($C_{10}$-$C_{11}$) bond lengths are lesser than the other C-C bond length because the presence of the hydrogen atom is attached to the carbon atom($C_{14}$-$H_{15}$) and ($C_{14}$-$H_{16}$) are approximately in the same bond length. The calculated bond length of ($C_4$-$O_{29}$) is 1.3801Å. The bond length differences in the (C-O) groups are due to different environments of oxygen. The shorting ($C_7$-$N_8$) bond length by 0.075 Å is mainly due to the hyper conjugate interaction between the phenyl ring and strong electron donating groupThe phenyl ring is connected to the pyrozole ring.

**FRONTIER MOLECULAR ORBITAL ANALYSIS**

Molecular HOMO and LUMO have been compute used in Gaussian 09 software program. The graphical representation of HOMO-LUMO is shown in figure 2.

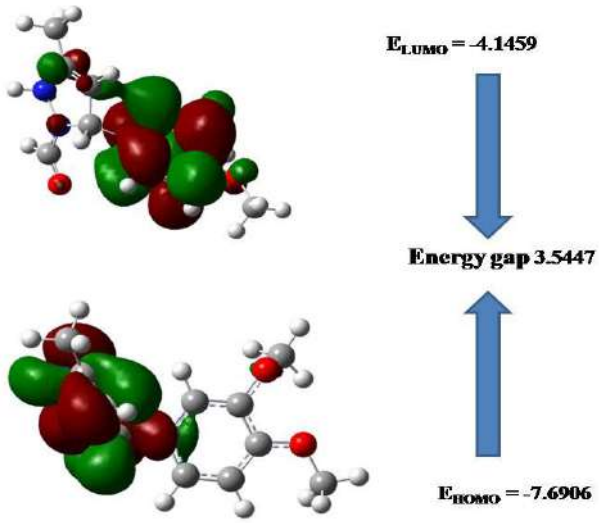


**Figure 2: HOMO-LUMO orbitals of 5-(3,4 – dimethoxy phenyl)-3-methyl-4,5-dihydro-1H-pyrozole -1-carbaldehyde**

The energy of the HOMO is directly related to the ionization potential. LUMO energy is directly related to the electron affinity. The energy gap calculated by B3LYP/6-311G (d,p) calculation method is shown below.

HOMO Energy =-7.6906 a.u

LUMO Energy =-4.1459 a.u

Energy gap =3.5447 a.u

This small energy gap confirms the conjugated compound with high chemical reactivity as well as polarizability. LUMO is mainly located on the phenyl group and HOMO

is mainly located on the pyrozole and carbaldehyde group. The energy difference between the HOMO and LUMO is obtained as 3.5447ev which indicates the high stability of the molecule.

**MOLECULAR ELECTROSTATIC POTENTIAL (MEP)**

In order to understand the relative polarity the molecular electrostatic potential surface (MEP) of the molecular complex has been determined by B3LYP/6-31 G(d,p) method. In our molecule the blue region is near the methoxy group it is indicating to the nucleophilic reactivity of the molecule. The negative potential is near the pyrozole ring it is indicate the electrophilic reactivity of the title molecule. MEP of the compound value range from $-8.762e^{-2}$ to $8.762e^{2}$ Molecular electrostatic potential of 5-(3,4 – dimethoxy phenyl)-3-methyl-4,5-dihydro -1H-pyrozole -1-carbaldehyde is shown in figure 3.

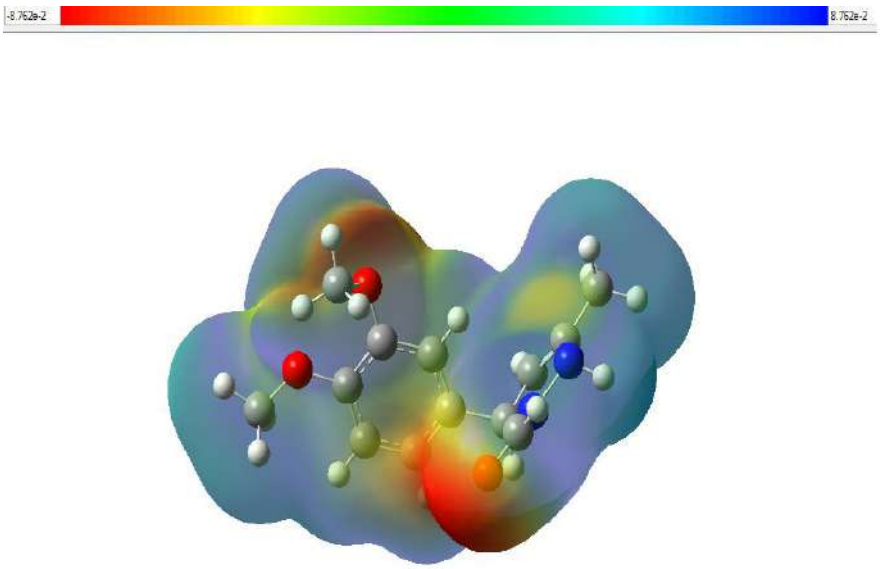

**Figure 3: molecular electrostatic potential**

**TOPOLOGY ANALYSIS**

**ELF and LOL**

Color shade map of the ELF and LOL for the title molecule are presented in figure 4 and figure 5. From figure high ELF regions are seen around hydrogen atom indicate the presence of highly localized bonding and nonbonding electrons. The blue region around few carbon atom show the delocalized electron cloud around it.The covalent regions are seen between hydrogen and nitrogen atoms indicated by red color with high LOL value the electron depletion region between valence shell and inner shell shown by blue circles around the carbon and oxygen nuclei .

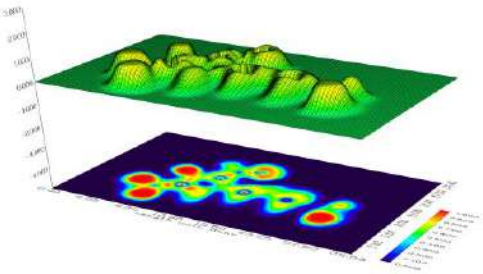

**Figure 4:Electron Localization function of the molecule**

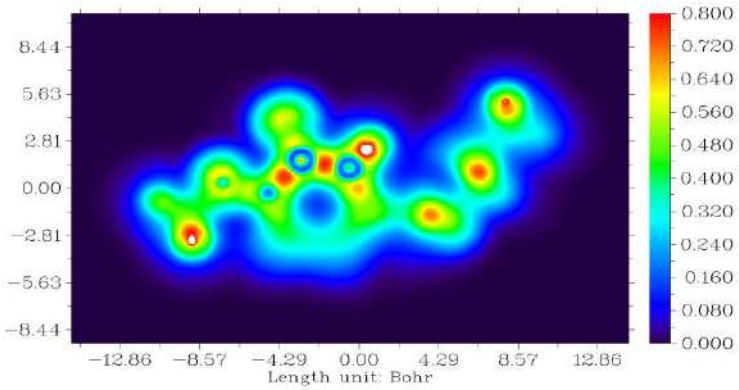


**Figure 5: Localized Orbital Locator of the molecule**

## CONCLUSION

In the present work 5-(3,4 – dimethoxy phenyl)-3-methyl-4,5-dihydro -1H-pyrozole -1-carbaldehyde was optimized by the DFT methods using the basis set B3LYP/6-311++G(d,p). The value of HOMO-LUMO energy gap is 3.5447 eV which is affect the chemical stability of the molecule. The MEP was used to calculate the reactivity sites such as nucleophilic and electrophilic reactivities.The chemical and electronic behaviour of the title compound ispredicted using the Electron localization function (ELF) andLocalized Orbital Locator (LOL) map.

# SYNTHESIS, STRUCTURAL, OPTICAL, AND MORPHOLOGICAL PROPERTIES OF ND-DOPED TITANIUM DIOXIDE NANOCOMPOSITES.

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## ABSTRACT

This study presents a comprehensive investigation into the synthesis, structural characterization, optical properties, and morphological analysis of neodymium (Nd)-doped $TiO_2$ nanocomposites. Synthesis of Nd- doped $TiO_2$ nanocomposites (NCPs) by the usage of *Annona muricata* extract. Structural characterization is performed using X-ray diffraction (XRD) and electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDX) to determine crystalline structure, phase purity, chemical bonds, particle size, morphology, and elemental composition. Optical properties are investigated through UV-visible spectroscopy to elucidate bandgap energy, optical transitions, and luminescent properties induced by Nd doping.The XRD pattern shows a crystallite structure with an Fm3m group space and particle size of about 23 nm. The FESEM images displayed that

NCPs have uniform distribution with nano rod morphology. The synergistic understanding of these properties facilitates the exploration of Nd-doped $TiO_2$ nanocomposites in various applications.

**Keywords:** Green synthesis, Nano composites, UV, FESEM

## 1.INTRODUCTION

In recent years, the development of advanced nanocomposite materials has garnered significant attention due to their unique properties and potential applications in various fields, including biomedicine. Among these materials, neodymium (Nd)-doped titanium dioxide ($TiO_2$) nanocomposites have emerged as promising candidates for a wide range of biological applications. The combination of $TiO_2$, a well-known semiconductor material with excellent biocompatibility, and Nd dopants, known for their unique optical and magnetic properties, offers a synergistic platform for addressing challenges in biomedicine [1,2].

The introduction of Nd dopants into $TiO_2$ nanocomposites introduces new functionalities and enhances their performance for biological applications. The incorporation of Nd ions can modify the optical, electronic, and magnetic properties of $TiO_2$, thereby expanding its potential utility in biological systems. These tailored properties enable the design of nanocomposites with enhanced capabilities for imaging, sensing, drug delivery, and therapeutic interventions.

Moreover, Nd-doped $TiO_2$ nanocomposites exhibit improved photocatalytic activity under visible light, making them suitable for applications such as photodynamic therapy and environmental remediation. The ability to harness light energy for controlled release of therapeutic agents or targeted destruction of pathogens highlights the versatility and potential impact of these nanocomposites in biomedical settings. Furthermore, the biocompatibility and stability of Nd-doped $TiO_2$ nanocomposites make them suitable for interfacing with biological systems, including cells, tissues, and organs. Their low cytotoxicity and compatibility with physiological environments pave the way for various biomedical applications, ranging from bioimaging and biosensing to tissue engineering and regenerative medicine [3-5].

## 2.MATERIALS AND METHODS

### 2.1 Materials

Annona muricata extract serves as a natural reducing and stabilizing agent in the synthesis process. titanium(IV) isopropoxide (TTIP), neodymium chloride ($NdCl_3$), Were purchased from Sigma Aldrich chemicals Pvt Ltd.

### 2.2 Methods

Titanium (IV) isopropoxide (TTIP) is used as a precursor for $TiO_2$ nanoparticles. In a typical synthesis, TTIP is hydrolyzed in the presence of water or a hydrolyzing agent to form $TiO_2$ nuclei. The reaction is often carried out under controlled conditions, such as temperature and pH, to control the size, morphology, and crystalline structure of the nanoparticles. The *Annona muricata* extract may be added to the reaction mixture to serve as a capping agent or stabilizer for the nanoparticles. The $NdCl_3$ precursor is dissolved in a 20 ml of water and added to the reaction mixture containing the $TiO_2$ nanoparticles. The reaction may be conducted under reflux or at elevated temperatures to ensure uniform doping of the nanoparticles with Nd ions. For additional purification of nano composites the sample was washed and centrifuged to remove excess reactants and impurities. The nano composites dried at 500 degree Celsius temperatures to enhance their crystallinity and stability.

## 3. RESULTS AND DISCUSSION

### 3.1 X-Ray Diffraction Analysis

XRD Pattern of undoped and neodymium doped $TiO_2$ nanoparticles. Broad peaks which are present in the patterns testify the nanocrystalline anatase structure of prepared samples. The average size of crystallites is in the range of 20 to 23 nm respectively. The doping of titanium dioxide with neodymium caused an increase in the crystallites sizes. In the XRD patterns of doped $TiO_2$ a broad and very weak peak at 35.9° of 2Θ range is observed. This peak is the strongest reflex from the hexagonal $Nd_2O_3$-structure. The difference in ion radiuses (1.13 nm for $Nd3^+$and 0.64 nm for $Ti4^+$) suggests that the neodymium ion is unable to effectively incorporate into the crystal lattice position of $TiO_2$. Therefore, it is more reasonable to assume that Nd-containing particles are localized at the surface of $TiO_2$ nanocrystals [6].

### 3.2 UV-Absorbance Analysis

UV-Vis absorption spectroscopy was employed to examine the optical characteristics

of both pure $TiO_2$ and Nd-doped $TiO_2$ nanoparticles. As the nanoparticle size decreased to the nanoscale, the optical properties of the prepared nanoparticles became increasingly pronounced.The absorption values for Pure $TiO_2$ and Nd-doped $TiO_2$ nanoparticles were measured at 356 nm, 340 nm, 328 nm, respectively. Notably, all absorption peaks were observed within the visible region (> 400 nm), attributed to exciton recombination at room temperature. With an increase in the doping concentration of Nd in $TiO_2$, a red shift in the absorption peaks towards higher wavelengths was observed. This shift signifies a decrease in the bandgap (Eg) of the material, potentially induced by strain and defects in the crystal lattice of $TiO_2$ nanoparticles. Such transitions occur as electrons move from the conduction band to the valence band [7].

**3.3 Scanning Electron Microscope and field Emission Scanning Electron Microscope Analysis**

The size and morphology of the nanoparticles were assessed through SEM analysis. SEM images as depicted in Fig. 1, both pure $TiO_2$ and Nd-doped $TiO_2$ nanoparticles exhibited heterogeneous morphologies characterized by non-uniform distribution and irregular arrangement. The particle sizes of $TiO_2$ nanoparticles appeared agglomerated. However, upon Nd doping, a reduction in agglomeration was observed, consequently inhibiting particle size growth. The FESEM images unveiled a tendency towards simple aggregation of Nano rod -like particles with decreasing particle sizes [8].

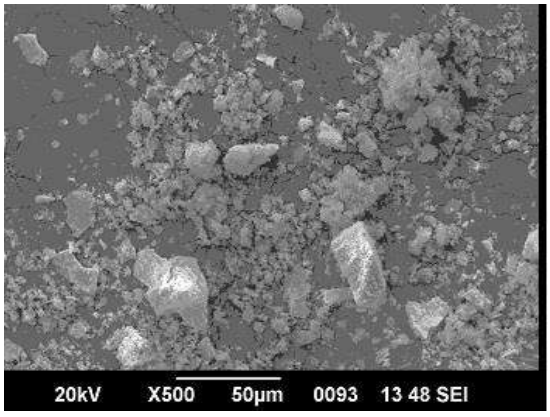


Figure:1a

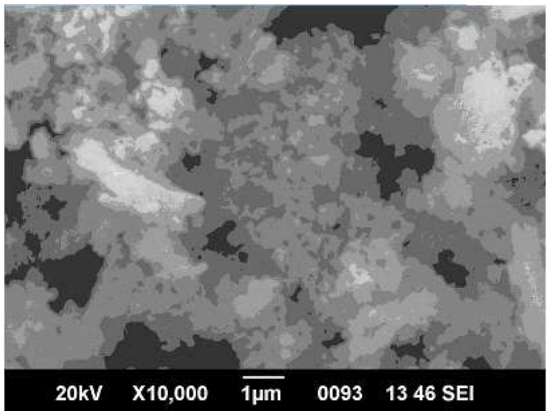


Figure:1b

**Figure 1 a,b shows SEM images of pure and doped $TiO_2$ NC**

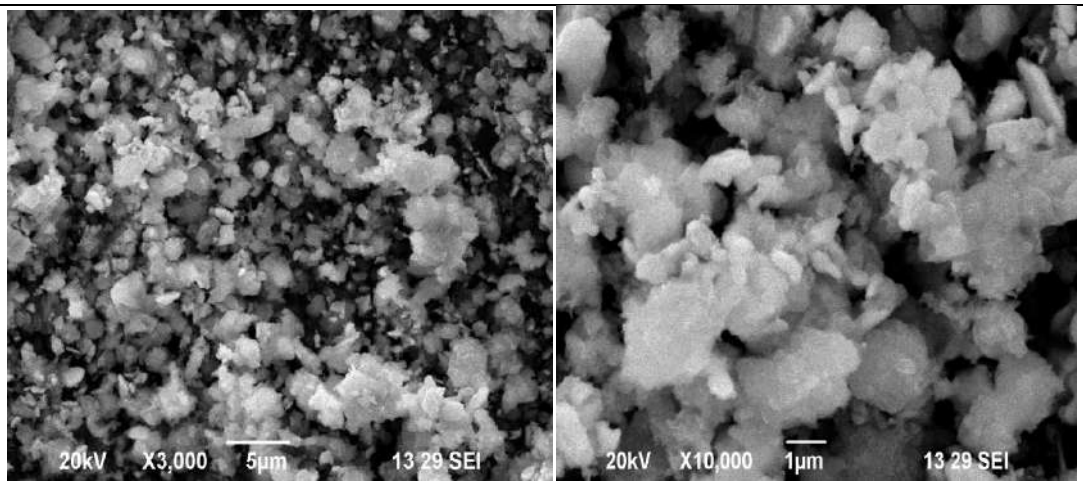


**Figure:2a** **Figure:2b**

**Figure 2a,b shows FE-SEM images of pure and doped $TiO_2$ NCs**

### 3.4 Elemental Dispersive spectra Analysis

The contents and chemical composition of the nanoparticles were analyzed using EDS spectra. Fig. 2 (a,b) displays the EDS spectra of pure $TiO_2$ and Nd-doped $TiO_2$ nanoparticles. The presence of titanium (Ti), neodymium (Nd), and oxygen (O) elements in the samples was confirmed by the EDS spectrum. Additionally, the presence of carbon (C) and copper (Cu) in the EDS spectrum can be attributed to the Cu grid used for sample preparation. The atomic percentages of Nd in the samples were calculated to be approximately 0.1%, indicating the successful incorporation of Nd ions into the $TiO_2$ nanoparticles.

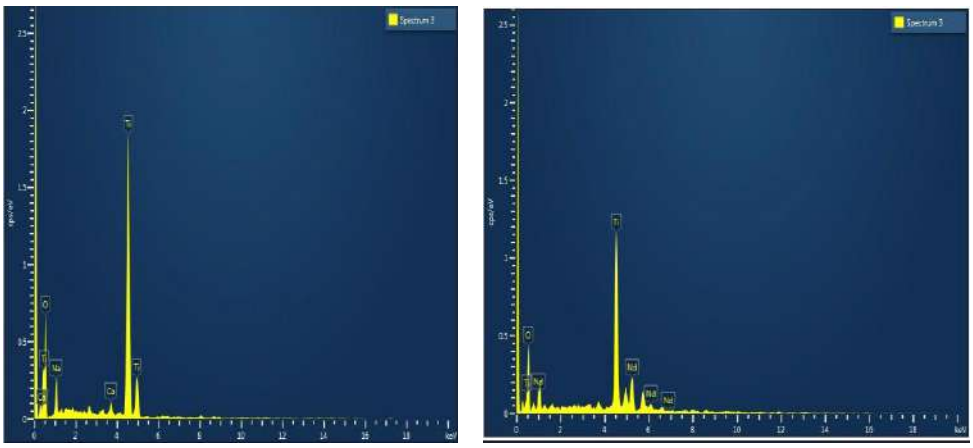

**Figure:2a** **Figure:2b**

**Figure 2a,b shows EDS Spectra of pure and doped $TiO_2$ NCs**

### 4. CONCLUSION

In this present work, Nd- doped $TiO_2$ nanocomposites (NCPs) are successfully

synthesized by green synthesis method using Annona muricata leaf extract. The powdered XRD patterns of the samples showed that the synthesized materials belonged to the nanocrystalline anatase structure and its average crystallite size was found to be in the nanometer range. SEM images displayed that the nanoparticles are free from agglomeration and the presence of composition elements like titanium (Ti), neodymium (Nd), and oxygen (O) were confirmed by EDAX analysis. The optical study reveals that the energy band gap of synthesized nanoparticles shows enhancement results towards optical properties and it makes the candidate suitable for biomedical application.

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TiO2 nanoparticles by sol-gel method for antibacterial and photocatalytic activity. Materials Science in Semiconductor Processing, 83, 70-82.

# SPECTROSCOPIC CHARACTERIZATIONS DFT STUDIESAND TOPOLOGY ANALYSIS OF 1- ACETYL-2(4 BENZOLOXY) -3 METHOXY PHENYL CYCLOPROPANE

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## ABSTRACT

A through spectroscopic investigation has been conducted in instruction to comprehend the structural

behaviour of the compound 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane. Thequantum chemical calculations have been carried out using DFT level of theory. An explicit surface analysis on the title compound was carried out theoretically using the wavefunction analyses multiwfn software, in order to study the reactivity of the compound. The input wavefunction files were generated by Gaussian 09W software using B3LYP/6-311++G (d, p) as the basis set. The topological analyses of the electron localization function (ELF) and the localized orbital locator (LOL) were completed using Multiwfn program.In general, a large ELF or LOL value in a region indicates high localization of electrons, due to the presence of a covalent bond, a lone pair of electrons, or a nuclear shell in that region.Topological parameters at bond critical points (BCP) have been evaluated by 'Quantum theory of atoms in molecules. Studies on docking have been done to forecast antiandrogenic and anti-metastasis properties against various pathogens.

**Keywords:** DFT, ELF, LOL, BCP

## 1.INTRODUCTION:

The organic Compounds like paracetamol, Aspirin contain acetyl moieties.[1] The compound with structural 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane correspond to have been shown to have strong anticancer effects among these possible anticancer medicines.[2] The optimizedgeometrical structure of the title compound was obtained usingGaussian 09W program with B3LYP/6-311++G(d,p) as the basis set.The topology analyses were made on the basis ofELF (electron localization function) andLOL (localized orbital locator) (Jacobsen, 2008) maps obtained frommultiwfn a wavefunction analyzes.The RDG isosurface of ABMC molecule is plotted by using Multiwfn software.As of late density functional theory (DFT) has become a dominant tool in theexamination of molecular structure. Various reports are accessible in the literature concerningthe structures and DFT studies.

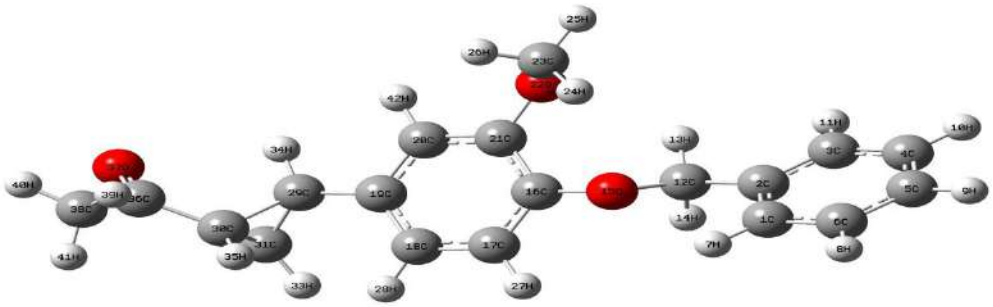
## 2.COMPUTATIONAL METHODS:

Calculation of structural parametersof the title compound in the ground state werecarried out using Gaussian 09 program packageby usingDFT method. Initially, the geometryoptimization and calculationof other parameters were performed at DFT level using 6-31G(d,p) basis set.The describe the topology analysis ELF, LOL and AIM in H bond examine with atoms. AIM calculated using multiwfn software in

the BCPS of Laplacian of electron density.

**3.OPTIMIZED GEOMETRY**

The geometrical parameter can be calculated by B3LYP/6311++ G (d, p) basic set-in focused Bond length, Bond angle, Dihedral value, integrated by optimized geometry in the Figure 1.These variations are likely due to intermolecular interactions in the molecule crystalline state.The intra molecule interacted by methoxy group have bond length $C_{23} – O_{22}$ (1.4364 Å) the ring larger than C – O bond length $C_{21}$ -$O_{22}$ (1.3757Å). The higher value of bond Length than $C_{36} – C_{38}$ (1.5145Å) other C – C bond length in presence of highly electron negative Methyl group. The dihedral angle $C_1 – C_2 – C_{12}$ -$O_{15}$ indicated by 4 benzoyloxy group in($C_6H_5CH_2O$) and $C_{17} –C_{18}$ of the phenyl ring being (31.1399).

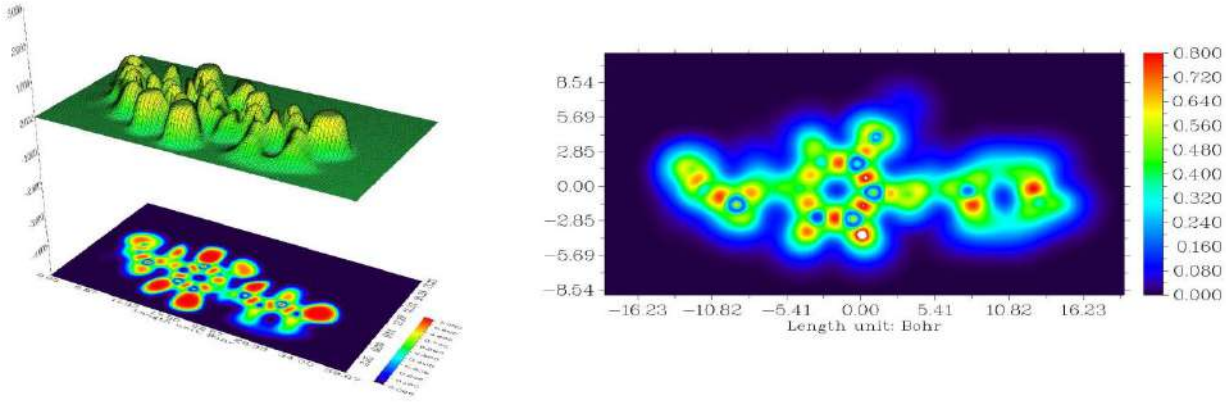


**Figures 1:** Optimized molecular structure of 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane

## 3.TOPOLOGY ANALYSIS:

### ELF-LOL

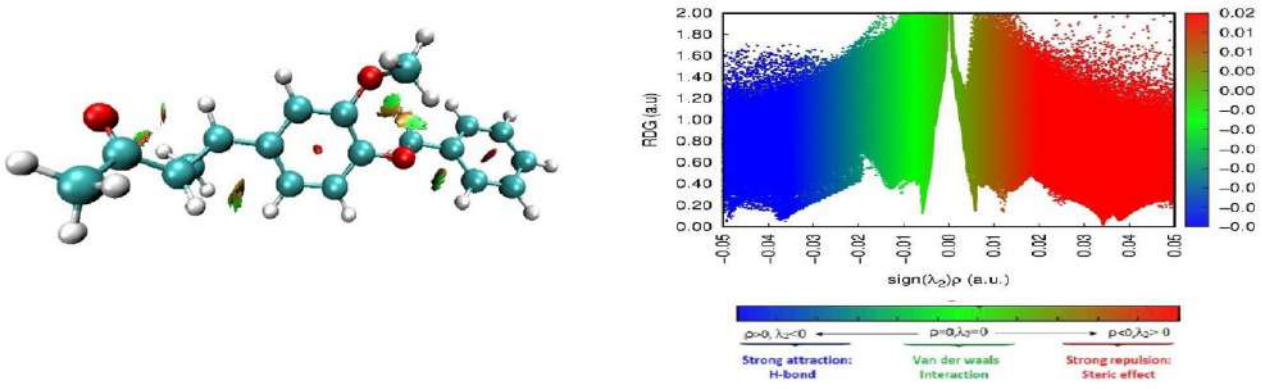
Topological analysis includes the localized orbital locator analysis (LOL) and the electron localization function (ELF) showing Figure 2. The high localization of electron occurrence of a covalent bond in ELF and LOL region around the hydrogen atoms implying the presence of highly localized bond and non-bond electrons. The blue region around carbon atom bond and non-bondingelectron.




**Figures 2:** Colour filled map of 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane

**RDG-AIM**

The electronic and chemical properties of ABMC have been explained using topologyanalysis. The Gaussian output has been taken through DFT/B3LYP/6-311++G(d,p) and utilizedin Multiwfn program for topology analysis. Reduced density gradient (RDG) is an extension of AIM analysis to explain non-covalent weak interactions. The weak interactions of AMBC exhibit considerable correlation with an electron density ρ. Now, interaction energy specifies at H-bonding of $O_{15}…H_{67,}$ $O_{15}…H_{7O}$, $O_{22}…H_{83}$, $O_{22}…H_{90}$, $O_{37}…H_{62}$ occur in temperate of nature are break because of weak interactions Generally, Hence the molecule surrounded by green area shows a wide green surface in the intermolecular spaces, presence of the van der Waals interaction between corresponding to the − 0.005 a. u to 0.002 a. u.The methoxy group and the ring hydrogen interact through Van der Waals forces.The reduced density gradient domain structure of ABMC with the scatter graph andcolor bar has been shown in Figure 3



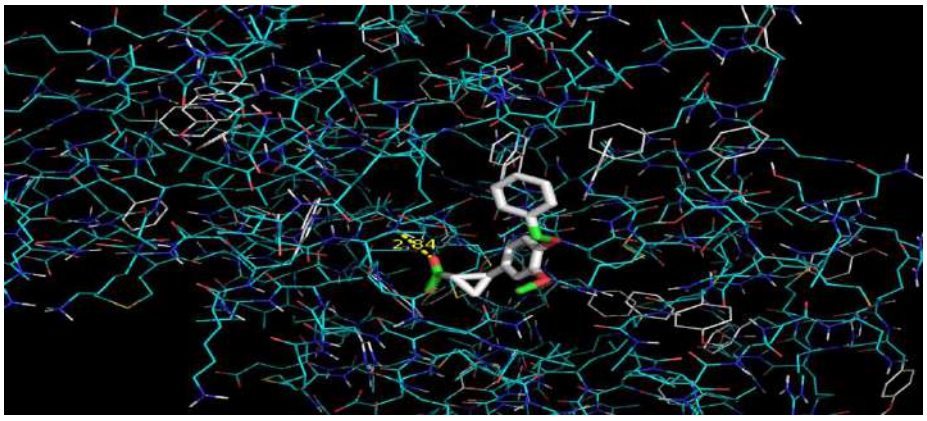

**Figures 3:** Reduced Density scatter plot and structure of plot of 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane

**4. MOLECULAR DOCKING**

A computational technique called “Molecular docking” is used to predict the protein ligand complex is

binding site and binding energy.For docking study high resolution fine molecular structure of anticancer Al proteins a (PDB ID: 1E3G) are taken. The 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane molecule was docked see the figure 4 forming one interaction with amino acid LIG (1) and LYS (808) and the binding affinity -7.4 kcal/mol.

Figure 4:Molecular docking of 1 -acetyl- 2(4 benzyloxy)- 3 methoxy phenyl cyclopropane compound with antiandrogenic Protein




**5. CONCLUSION**

In this present investigation, quantum mechanical computation (DFT studies) was carried out to calculate optimized geometry and topology analyses. The purpose of the molecular docking simulation was to forecast the compound affinity and potential orientation within the receptors active site.This confirms is a biomedical active compound.

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# Topological analysis on identification of an anticancer activity of 1-(p-toluenesulfonyl) imidazole

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## 1. INTRODUCTION

Imidazole derivative is an aromatic hetro cyclic compound that is used for many applications in the biological and medical fields[1]. The imidazole is an important synthetic precursor in the field of drug discovery [2-4]. The antibacterial, antifungal, antiprotozoal, antihelminthic, anti-HIV, antimicrobial, anti-convulsant, antitubercular, medications activities of imidazole derivative have already been reported [5-9]. The present work deals topological analysis such as AIM, ELF, LOL and RDG analysis in order t understand the interactions present in the molecule.

## 2. COMPUTATIONAL DETAILS

All the calculationswere performedby using Becke's three-parameter exchange functional in combinationwith the Lee–Yang–Parr correlation functional (B3LYP) method with split-valence polarized 6-311++G(d,p) basis set as implemented in Gaussian09W program package [7].The vibrational modes of the calculated wavenumbers are aided by the animation option of GAUSSVIEW program, which gives a visual presentation of the vibrational modes.

## 3. ELECTRON LOCALIZATION FUNCTION (ELF)

Electron localization is an important parameter to explain the aromaticity of a molecule, the nature of chemical bonding in transition metal complexes [40] and most importantly it directly reveals the Pauli exchange repulsion effect by measuring the excess of local kinetic energy due to Pauli repulsion which has several applications in VSEPR theory [41]. This leads to a deformation of the ELF distribution around the oxygen atom of the carbonyl group asobserved in Fig. 1. By examining ELF values of oxygen along with the carboxylic acid group, values are lower (represented by blue).The electrons in the bonds between the carbon-carbon atomsshowed localization (represented by red region) in comparison to the electrons in the bonds between carbon-hydrogen (represented by green region).

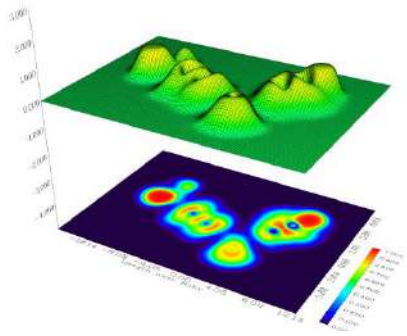

**Figure 1.2D plot electron localization function isosurfaces with projection for 1-(p-toluenesulfonyl)imidazole**

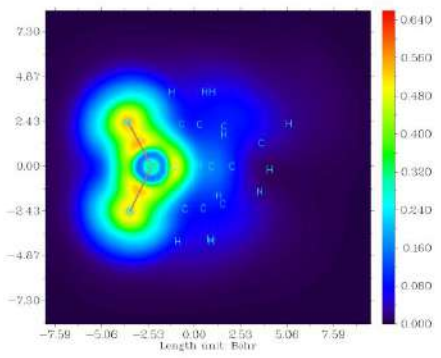


**Figure 2. Relief map with projection of localized orbital locator of 1-(p-toluenesulfonyl)imidazole**

### *4. LOCALIZED ORBITAL LOCATOR (LOL)*

Molecular orbitals which are concentrated in a limited spatial region constitute the localized molecular orbitals. Fig. 2 shows its localized orbital locator (LOL) distribution under 6-311G (d,p) basis set. For the title compound, the blue colour corresponds to low values of LOL some of carbon and hydrogen and S atoms present in the positive region and it indicates a blue in colour. The blue represents the region with the low end of LOL value of other lowest attraction atoms that are surrounded by yellow region.

### *5. AIM ANALYSIS*

Atoms in molecule(AIM) is a powerful method to gather knowledge about the chemical bonding and hydrogen bondings in the molecular system. In the 26PDC molecule, the electron density is maximum for C22-H25 (0.4309), C21-C22 (0.4302) bond and these bonds have a greater negative value of $\nabla^2\rho$ showing its covalent nature. In ellipticity the $C_2$-$C_3$ atom shows higher value than others and it indicates the nonstability of the bond.

### *6.REDUCED DENSITY GRADIENT (RDG) ANALYSIS*

The Reduced Density Gradient(RDG) is a fundamental dimensionless quantity coming from the density and its first derivative:

$$RDG(r) = \frac{1}{2(3\pi r^2)^{1/2}} \frac{|\nabla \rho(r)|}{\rho(r)^{4/3}} \qquad \text{……..(4.2)}$$

The real space weak interaction is based on electron density and RDG analysis developed by Johnson et al. [46]. From Figure 3 and 4 the weak interaction is identified by analyzing the below electron density values. The plot of RDG vs r provides the presence of interaction strength. The $\lambda 2$ sign is used to differentiate the bonding ($\lambda 2 < 0$) interactions from non- bonding ($\lambda 2 > 0$) interaction. The Multiwfn and VMD software analyze the interaction of strength in the molecular system, in which blue color indicates stronger attraction and red indicates repulsion. From shown, the red color represents the ring system which is responsible for the steric effect. In this molecule, the steric effect is more which is represented in red color in the RDG scatter plot.

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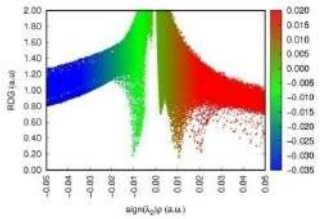
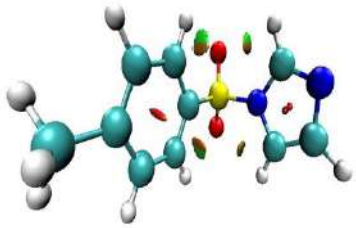
|  |  |
| **Figure 3. Plots of the RDG versus the electron density ρ multiplied by the sign of λ2 for 1-(p-toluenesulfonyl)imidazole** | **Figure 4. Plots of the RDG versus the electron density interaction** |

## 7.CONCLUSION

The Aim, ELF, LOL and RDG analysis of the title compound 5-Chloro Salicylaldehyde were determined using the basic set of DFT / B3LYP / 6-311 ++ G (d, p). Molecular orbital composition and their chemical bonding contributions are studied by Total partial and overlap population density-of-states. ELF,and LOL were used to examine the electron distribution and reactive sites on the surface of the title compound.

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# STRUCTURAL AND THERMOGRAVIMETRIC ANALYSIS OF CALCIUM COBALITE FOR THERMOELCTRIC APPLICATIONS


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**ABSTRACT**

Energy is the basic need for all living beings. The world's need for energy is causing a drastic escalation of social and political unrest. More than 60% of energy is lost via worldwide in the form of heat. In order to lower the consumption of fossil fuels, reduce the greenhouse gases especially $CO_2$ and to enhance the environmental well being an alternative source of energy with low toxicity and high efficiency has to be introduced. Challenges to develop alternative energy sources are increasing. Technologies that can convert waste heat into electrical energy by using Seebeck effect plays key role in current days. Materials that can directly and reversibly convert thermal energy into electrical energy are known as thermoelectric materials (TE). Good TE should have high Seebeck coefficient, high electrical conductivity and low thermal conductivity. Oxides are featured by their chemical versality, structural and compositional tailoring. Oxides are low cost and ecofriendly. Calcium Cobalite is the most prominent material with high efficiency and known for its electronic and magnetic properties. Calcium Cobalite is prepared by using simple solid-state reaction method by taking 3:4 ratio of Cobalt oxide and Calcium Carbonate as starting materials. They were mixed and ball milled at 400rpm for 1 hr in ethanol medium. The ball milled powders were dried at 150 ˚C and dried in agetatemortar. Thermal analysis was used to monitor the thermal decomposition of CCO powders. The weight loss percentage is calculated from the TG graph. The samples were annealed at 600 ˚C and 900 ˚C. The structural and morphological parameters were characterized using XRD and SEM analysis and compared with the previous reports. The presence of $Co_3O_4$ phases is also noted along with $Ca_3CO_4O_9$. The intensity and crystallinity increase with increasing annealing temperature. The particle size and structural parameters were determined by XRD and SEM analysis.

***Keywords: Annealing, Calcium Cobalite, Thermoelctrics, Thermogravimetric***

**INTRODUCTION**

The world currently faces numerous challenges in energy consumption. The world's demand for energy has been drastically increased. On the other side there is huge wastage of energy loss. 60%of energy lost worldwide are in the form of heat energy. Much of energy will still produce unstable heat in the vehicle exhaust or on the cooling system. 40% of fuel energy in vehicle is wasted as exhaust gas, 30% is dissipated in the engine coolant, 5% is lost as radiation and friction and only 25% is usable for vehicle mobility and accessories Challenges to develop alternative technologies that can convert waste heat in to electricity plays a key role in current days. It can reduce our dependent on fossil fuels and reduce greenhouse gas emission

[1]. Materials that can directly or reversibly convert thermal energy into electrical energy have aroused interest in current days. Materials that possess such properties are called thermoelectric materials. The need of developing high efficiency TE materials for waste heat recovery is urgent and will bring vast economic and environmental benefits [2].Home heating, automotive exhaust and industrial process can generate an enormous amount of unused waste heat that could be converted into electricity by using thermoelectric materials. The need of developing high efficiency thermoelectric materials for waste heat recovery is urgent and will bring vast economic and environment benefits [3].

The first-generation TE materials were highly toxic and mainly Lead based materials. Currently, high thermal and electrical stability of oxides has influenced the research towards them. Oxide TE mainly involves p-type $CaMnO_3$, ZnO, $SrTiO_3$, $Ca_3Co_4O_9$. This article involves the fabrication and structural analysis of$Ca_3Co_4O_9$ [4]. A good thermoelectric material, that can perform such conversion mechanism should have certain unique properties. The conversion efficiency of the thermoelectric materials is related to the quantity called figure of merit (ZT), defined as

$$ZT = \frac{S^2 \sigma T}{k} \qquad (1.1)$$ where,

$S \rightarrow$ Seebeck coefficient ($\mu V/K$)

$\sigma \rightarrow$ Electrical conductivity ($\Omega^{-1}cm^{-1}$)

$k \rightarrow$ Thermal conductivity ($Wm^{-1}k^{-1}$)

$T \rightarrow$ Temperature (K)

$S^2\sigma \rightarrow$ Power factor

The complex parameter relationship makes the approach of increasing ZT difficult. Generalizing all the properties, it can be stated that a good thermoelectric material should possess a 'phonon-glass-electron-crystal (PGEC) 'model. This model describes the properties of thermoelectric materials. This stated that an ideal thermoelectric material should have the combination of glass like thermal conductivity and crystal-like electrical properties. Glasses exhibit low lattice thermal conductivities. In glass, thermal conductivity is viewed as a random walk of energy through lattice rather than rapid transport via phonons and leads to the concept of minimum thermal conductivity. However, they make poor thermoelectrics because they lack the needed electron-crystal properties. Good thermoelctrics are therefore crystalline materials that manage to scatter phonons without significantly disrupting the electrical conductivity.[5].

**CALCIUM COBALTITE**

$Ca_3Co_4O_9$(CCO) is a p-type semiconducting material well known for its electronic, magnetic and electro

optic properties. In the family of Cobaltite, CCO has gained a special place due to its misfit layered structure. Fig.1.1. Structure of$Ca_3Co_4O_9$. Its crystal structure consists of two different CdI2 – type monoclinic structures. The middle layer consists of Ca and O. The others

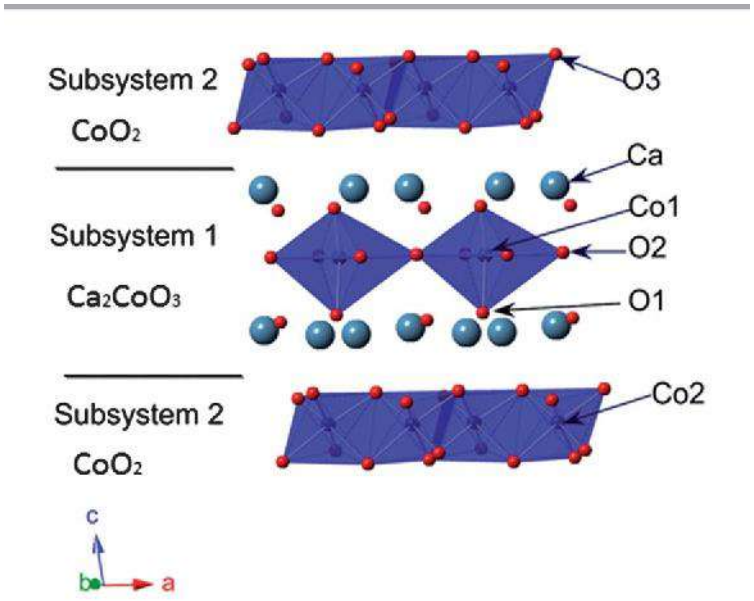



**Figure .1.Structure of CCO**

contain Ca and O. The substructure has the composition of $Ca_3Co_4O_9$and is usually referred to as rock salt structure [6].

**EXPERIMENTAL PROCEDURE:**

Large-grained $Ca_3Co_4O_9$powders are prepared using solid state reaction by taking Cobalt oxide ($Co_3O_4$) and Calcium Carbonate ($CaCO_3$) as starting materials. The Ca:Co molar ratio was 3:4. This process was carried out in a high-energy planetary ball milling equipment, using ethanol as a medium. The HEBM was performed at a constant speed of 400 rpm for 30 minutes. After ball milling the remaining ethanol was evaporated and the prepared powder was calcined at 100˚C for 1hour. Finally, it was grounded manually in agate mortar for half an hour and was annealed at 600 ˚C and at 900˚C for two hours [7].

**CHARACTERIZATION OF $Ca_3Co_4O_9$POWDERS:**

The crystal structure of the obtained powders was analysed by X-ray powder diffraction. The XRD patterns shows results received between 10 and 60˚. Morphology and particle size of the products were investigated using Scanning Electron Microscopy. Weight loss were calculated using TG analysis.

**RESULTS AND DISCUSSION**

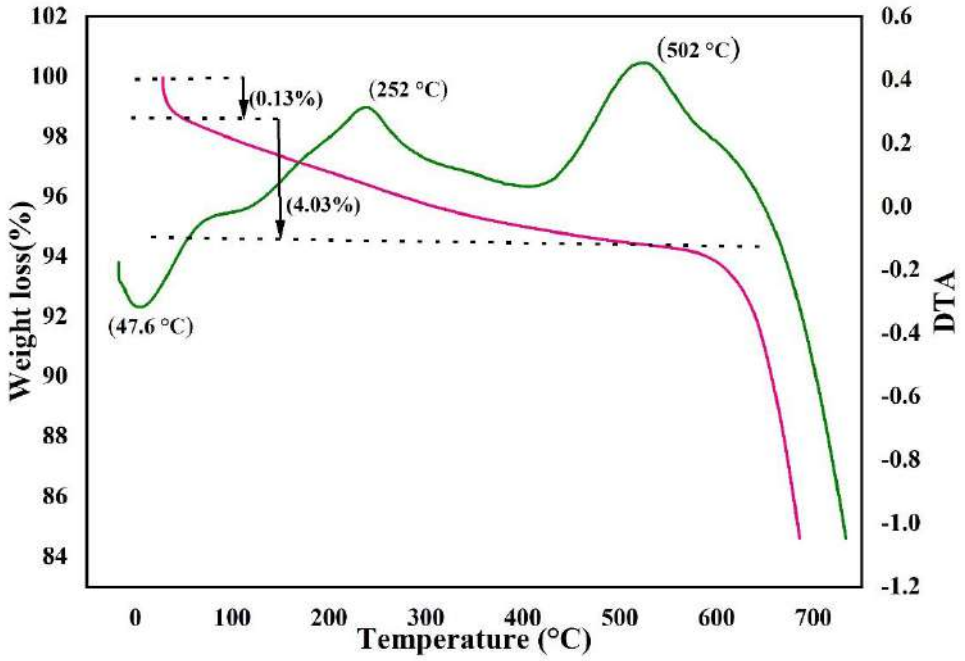


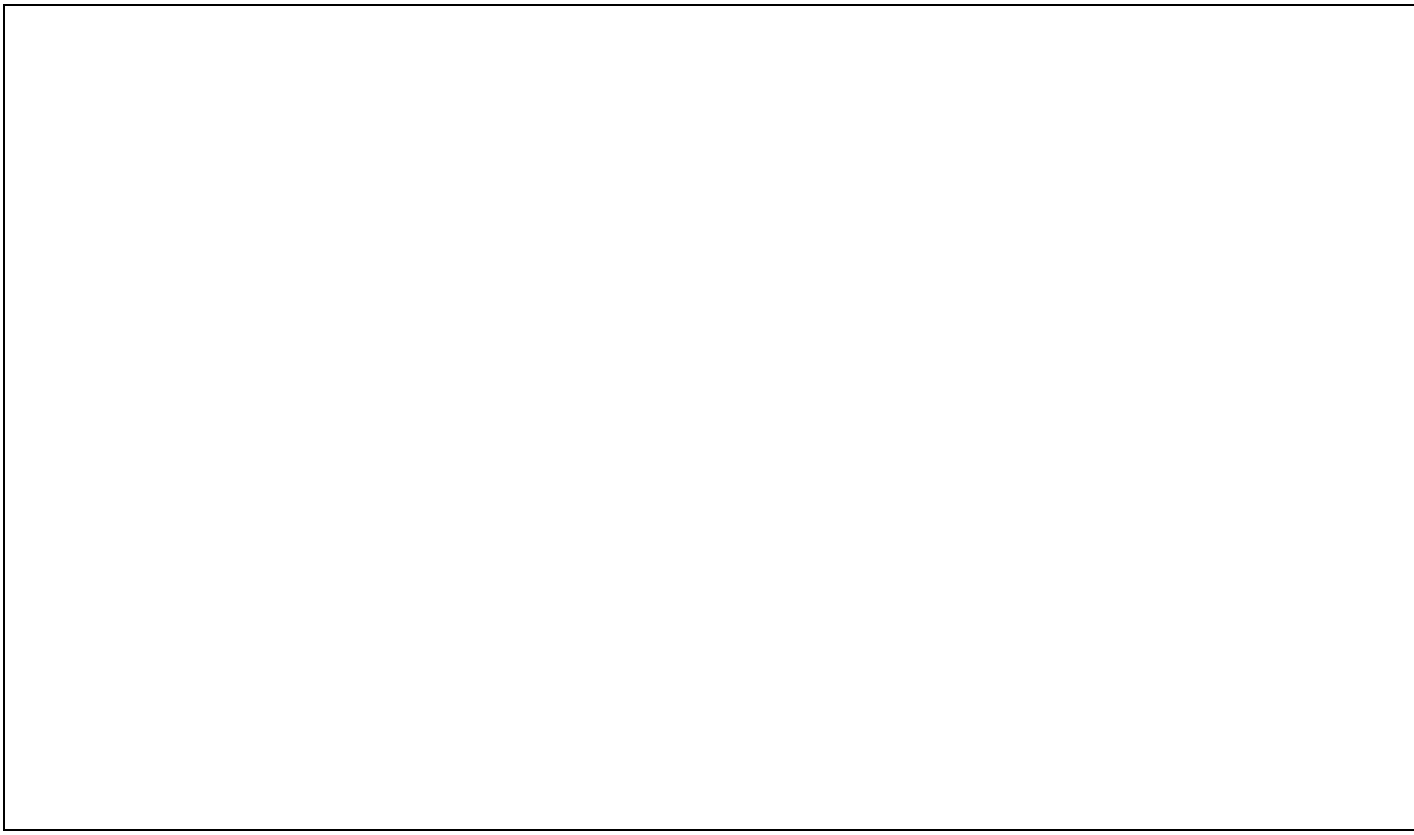

**Figure 2. TG and DTA analysis of CCO**

**TG ANALYSISS:**

Differential analysis performed on the as-prepared sample is displayed in Figure 2. TGA is an important tool to determine the stable product formation and decomposition steps. The evolution of heat flow as a function of temperature together with its derivate were shown. Three well differenced peak can be observed in the differential curve. The first endothermic curve appearing at 47.6 ˚C and other two exothermic peak appearing at 252 ˚C and 502˚ C. The third peak being more intense than the other two indicating the crystallization of the$Ca_3Co_4$. An abrupt weight loss is observed from 200 ˚C To 600 ˚C simultaneously with the exothermic peak at 502 ˚C indicates the decomposition of carbonates [8,9].

**XRD ANALYSIS:**

Figure 3 display the XRD patterns of as-prepared $Ca_3Co_4O_9$ powder and the samples annealed at 600˚C and 900 ˚C. As it can been seen that, all the three samples contain pure phases of $Ca_3Co_4O_9$ with embedded $Co_3O_4$. As seen that the sample annealed at 900 ˚C shows almost pre phase. As the annealing temperature is increased the secondary phases gets reduced and the enhancement of major phases can be noticed. The results obtained were in accordance with the ICDD CARD NO:23-0110 [10].



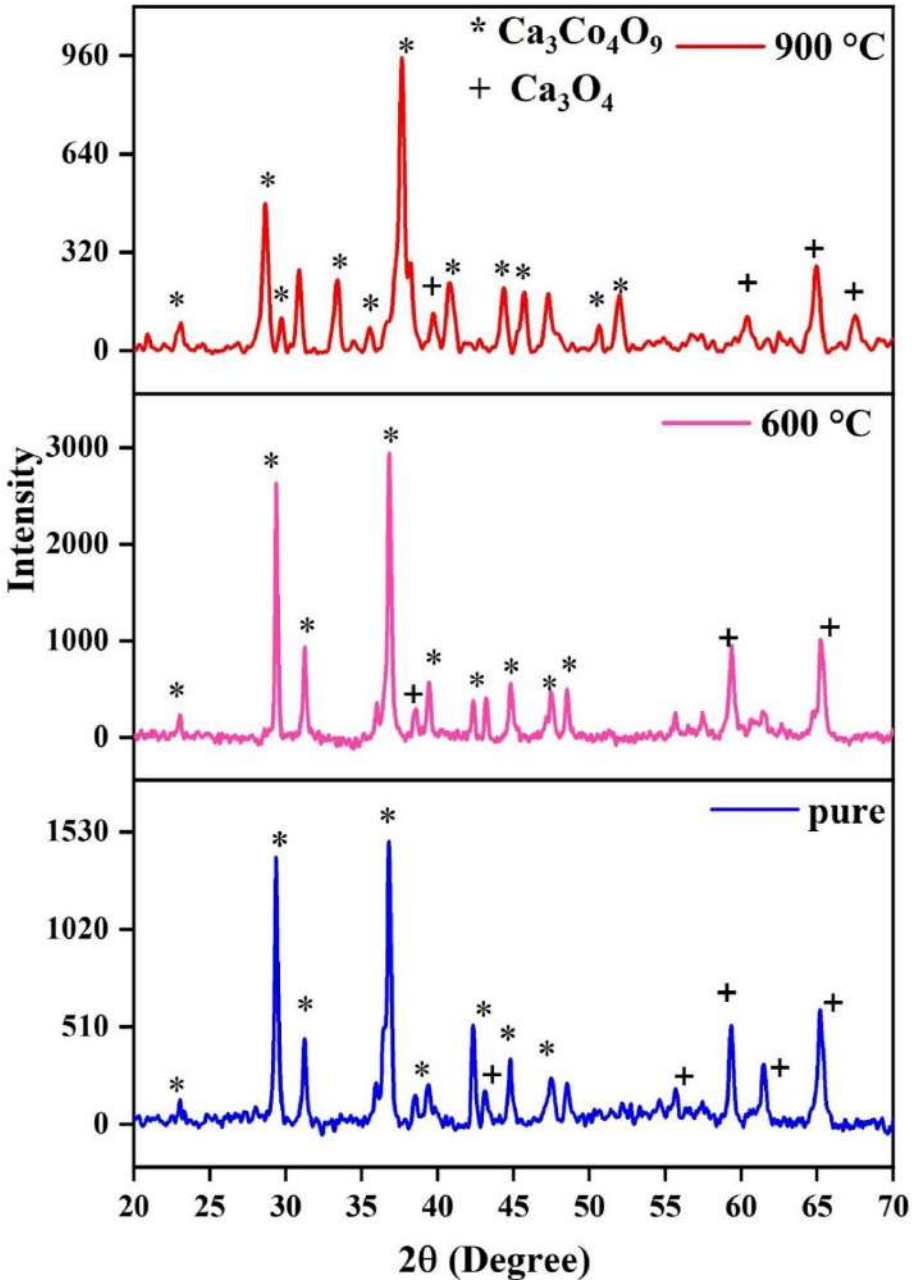



**Figure.3. XRD pattern of 1)as prepared CCO 2)annealed at 600 ˚C 3)annealed at 900˚ C**

**SEM ANALYSIS**

Figure 4 depicts results of SEM studies of pure and annealed samples. The images reveals that the annealing temperature has an effect on the particle size and morphology of these particles. The distribution of particle size is quite homogenous and normally distributed. The morphology of the powder has changed slightly with increasing the average particle size and some agglomerations were observed between fine particles. The plate-like shaped particles increased on annealing, which is due to the grain growth [11]. Further it reveals the presence of microporous sphere like morphology with agglomerated assembled spheres indicating a

good connectivity among grains. The particle size is determined to be 1.002 μm ,0.857μm and 1.105 μm for the as prepared and samples annealed at 600 ˚C and 900 ˚C respectively .

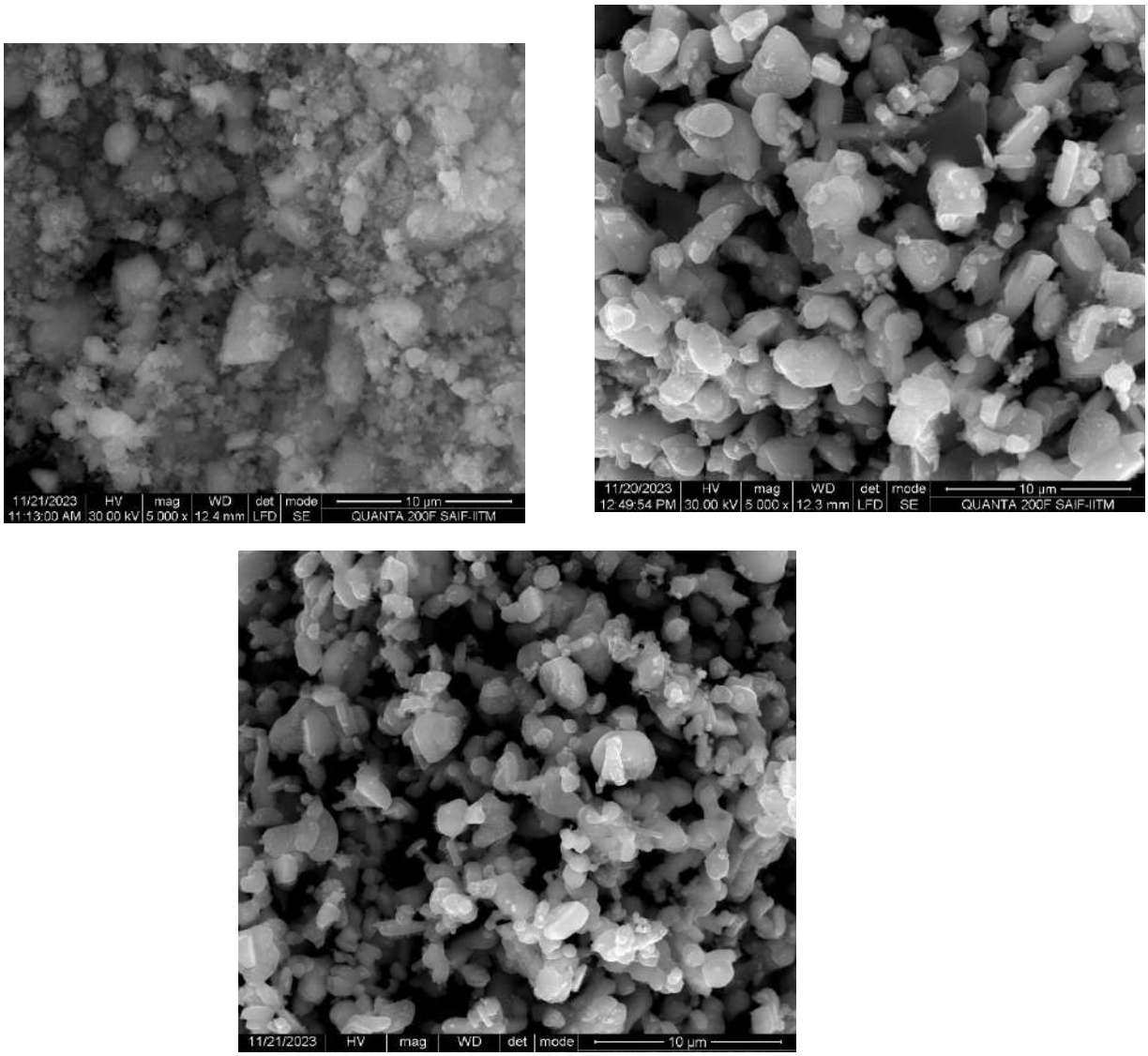



**Figure .4.SEM analysis of 1) as prepared 2)annealed at 600 ˚C 3)annealed at 900˚ C**

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# COMPUTATIONAL, FRONTIER MOLECULAR ORBITAL ANALYSIS TOPOLOGICAL INVESTIGATIONS AND MOLECULAR DOCKING STUDIES OF CAFFEIC ACID USING DFT APPROACH

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**ABSTRACT**

Caffeic acid (3,4-dihydroxycinnamic acid) is a polyphenol produced through the secondary metabolism of vegetables, including olives, coffee beans, fruits, potatoes, carrots and propolis, and constitutes the main hydroxycinnamic acid found in the diet of humans. In this study, the DFT-B3LYP 6-311++G(d,p) basis set was used to optimise the Molecular geometry of the Caffeic acid and the structural parameters were identified. The intra- and inter-molecular interactions were calculated from the NBO analysis. The lower HOMO-LUMO energy gap value accounts for the biological activity of the molecule. The topological analysis was utilised to evaluate the title compound's reactive sites and electron distribution. The molecular docking investigations verified the bioactivity of the title compound.

Keywords: DFT, NBO, HOMO-LUMO, MEP, Molecular Docking.

## 1. Introduction

The spread of bacterial infection is a significant offensive threat to human life on this planet. Moreover, the biocompatibility of the synthesized antibiotic has an equivalent rank to assure their safe clinical translations [1]. Phenolic chemicals are naturally occurring secondary metabolites found in nearly all plant components, including plant-based dietary items. The predominant subclass of phenolic chemicals is hydroxycinnamic acid [2]. The present work mainly focused to analyse the topological activity and docking ability of 3,4-dihydroxycinnamic acid (Caffeic acid) against the antibacterial proteins. DFT was used to investigate the compound's geometrical optimization, electronic, topological, and biological aspects. The charge transport inside the structure was determined using a HOMO/LUMO study [3]. Docking studies proves the antibacterial potential of the title compound.

## 2. Computational Details

The Gaussian 09W software package was employed to do the computational calculations utilising B3LYP correction with the 6-311G++ (d, p) basis set. The molecular structure was visualised with the help of Gauss View 5.0.8 software. Donor-acceptor interactions in natural bond orbitals (NBO) have been

determined using a secondary order Fock matrix, by employing NBO version 3.1 which is launched in the Gaussian 09W package. Multiwfn 3.7 software was employed to carry out AIM, Electron Localization Function (ELF), Localized Orbital Locator (LOL), fukui and Non-Covalent Interaction (NCI) analysis. Open Babel, Py Rx and Pymol softwares were used to perform the molecular docking studies.

## 3. Results and discussion

### 3.1. Optimized geometry

Molecular geometry provides important information about the overall structure of the molecule, as well as critical geometric characteristics including bond lengths, bond angles, torsional angles, and individual atom positions. Figure 1 shows the optimized structure of the title compound. In the title compound, the increase in the bond length of the C–C atoms is due to the impact of neighbouring hydrogen atoms. The decrease in bond length of C–O atoms shows the presence of double bond within the carbon and oxygen atoms. The bond angle values shows that the oxygen being more electronegative than carbon atom.

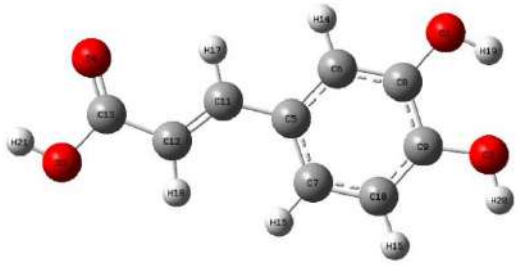

Figure 1. Optimized structure of the title compound

### 3.2. NBO Analysis

Natural bond orbital (NBO) evaluation is a strong tool in computational chemistry that may determine a molecule's precise Lewis structure. In the title compound, the hyper-conjugative interactions of π(C5 – C7)→ π*(C6 – C8), π(C5 – C7) → π*(C9 – C10), π(C5 – C7) → π*(C11 – C12), π(C6 – C8) → π*(C9 – C10), π(C9 – C10) → π*(C6 – C8), π(C11 – C12) → π*(O4 – C13) are found to be 19.72, 21.10, 17.94, and 21.67 kcal/mol, respectively. Also, the stabilisation of the compound is greatly aided by the interlinkage of the electron lone pair on the oxygen atoms. It is evident by the hyper-conjugative interactions of LP(2) O3 →π*(O4 – C13), LP(1) O1→ σ *(C8 – C9), LP(2) O4→ σ *(C12 – C13) and LP(2) O2→ π*(C9– C10).

### 3.3. Frontier molecular orbital analysis

The FMOs idea based on HOMO and LUMO is one of the best chemical stability theories

available. HOMO is the maximum occupied molecular orbital whereas, LUMO is the minimum occupied molecular orbital. The energy of the LUMO and HOMO molecules, along with their energy gap, indicate the molecule's chemical function and stability. The global reactivity parameters were also calculated and tabulated in Table 1. Figure 2 shows the HOMO-LUMO analysis of the title compound.

**Table 1. Global Reactivity descriptors of Caffeic Acid**

| Molecular Properties | Mathematical Description | Energy(eV) |
|---|---|---|
| $E_{HOMO}$ | Energy of HOMO | -8.5358 |
| $E_{LUMO}$ | Energy of LUMO | -5.8095 |
| Energy Gap | $\Delta E_g = E_{HOMO} - E_{LUMO}$ | 2.7262 |
| Ionization Potential ($I_P$) | $IP = -E_{HOMO}$ | 8.5358 |
| Electron Affinity ($E_A$) | $EA = -E_{LUMO}$ | 5.8095 |
| Electronegativity ($\chi$) | $\chi = -1/2(E_{LUMO} + E_{HOMO})$ | 7.1726 |
| Chemical potential ($\mu$) | $\mu = 1/2(E_{LUMO} + E_{HOMO})$ | -7.1726 |
| Global Hardness ($\eta$) | $\eta = 1/2(E_{LUMO} - E_{HOMO})$ | 1.3631 |
| Softness (S) | $S = 1/2\eta$ | 0.3668 |
| Electrophilicity index ($\omega$) | $\omega = \mu^2/2\eta$ | 18.8709 |

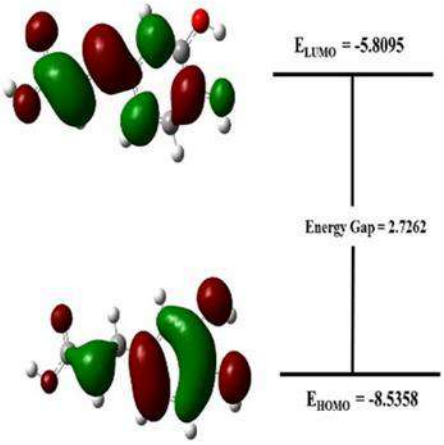


**Figure 2. HOMO-LUMO plot of Caffeic Acid**

### 3.4. Molecular electrostatic potential

Molecular electrostatic potential (MEP) is used for site prediction and electrophilic/nucleophilic reactivity prediction [4]. The title compound's colour code ranges from −7.872e−2 to +7.872e−2. Oxygen atoms are more electronegative in the title compound as indicated by the red colour and is prone to the electrophilic attack. Similarly, the blue colour regions indicate the nucleophilic attack. The title molecule's interactions and active sites indicate the compound's biological activity. The MEP plot is shown in Figure 3 (a).

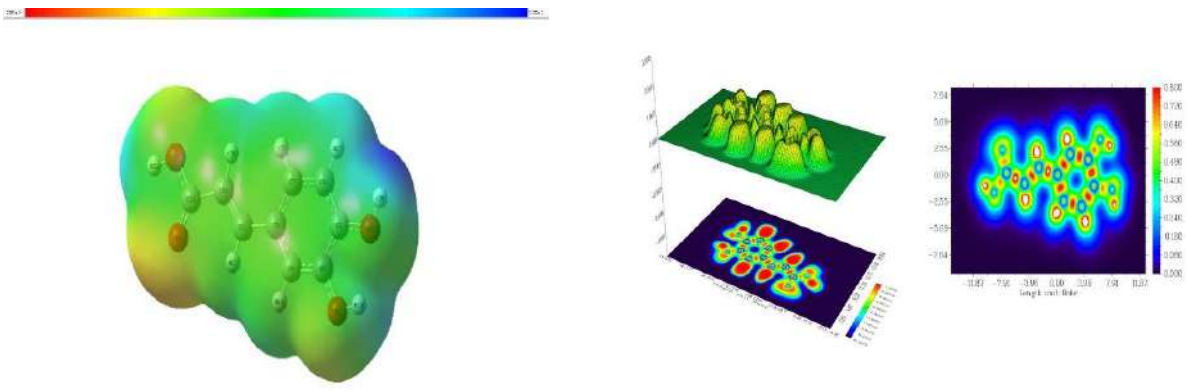

Figure 3. MEP and ELF-LOL of Caffeic Acid

### 3.5. ELF-LOL Analysis

The ELF and LOL maps were utilised to carry out surface analysis based on covalent bonding. Colour codes represent ELF values as red for high, yellow to green for medium, and blue for low. LOL merely displays the gradient of localized orbitals, and is utilised when localized orbits overlap. The reds and oranges hues, critical locations, trajectories, chemical bonds, and chemically relevant regions near hydrogen atoms in the ELF map depicts localised bonding or non-bonding electrons. Figure 3 (b) shows the ELF and LOL images of the title compound.

### 3.6. Non covalent interaction (NCI) analysis

The NCI plot is calculated by plotting the RDG (reduced density gradient) against the sign of λ2 (eigenvalues of the electron density of the Hessian matrix) multiplied by the density, ρ. The nature of interaction is predicted from (sign λ2)ρ value [5]. For the title compound, the red coloured interactions in the RDG isosurface map depicts the steric influence. Similarly, the blue and green colour interactions show the hydrogen bonding and Vander Waals effect respectively. Figure 4 depicts the RDG graph of the title compound. RDG isosurfaces exhibit a red spike indicating steric repulsion. The existence of the combined red and green peaks suggests a modest non-covalent interaction between the bonds.

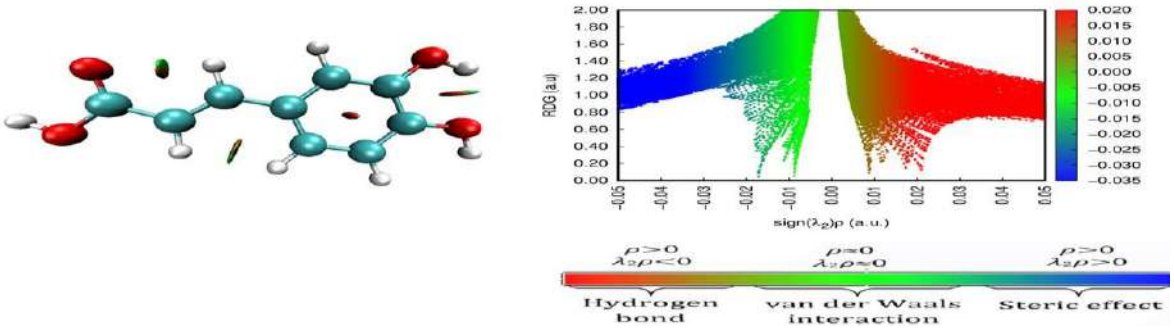


Figure 4. NCI Analysis of Caffeic Acid

### 3.7. Molecular Docking

Docking is a computational molecular modelling technique used to forecast how an enzyme will interact with ligands, or tiny molecules. The interaction of the protein-ligand complex and binding energy is predicted via molecular docking. Figure 5 shows the docking studies of the title compound. The docking parameters are tabulated in table 2. The title compound is docked with the antibacterial proteins 1JIL. The

protein ligand binding affinity is calculated as -7.1 kcal/mol. From the obtained outcomes, the title compound exhibits good antibacterial activity.

**Table 2. Docking parameters of Caffeic Acid**

| Protein (PDB:ID) | Binding residues | Bond distances (Å) | Binding energy (kcal/mol) |
|---|---|---|---|
| 1JIL | ASN124 | 2.18 | -7.1 |
| | THR75 | 3.08 | |
| | GLN196 | 3.05 | |

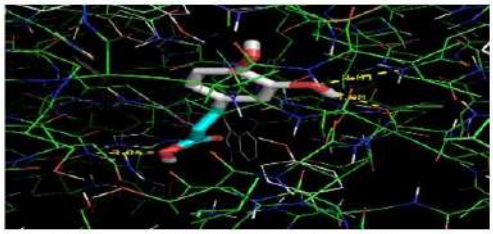

**Figure 5. Antibacterial activity of Caffeic Acid**

## 4. Conclusion

Using the quantum chemical computations, the structural, vibrational and topological characteristics of the compound was studied. The HOMO-LUMO energy gap is calculated as 2.7262 eV which also accounts for the biological activity of the molecule. The steric repulsion, weak and strong attractions of the title compound were investigated using the NCI method. MEP and the topological analysis were utilised to evaluate the title compound's reactive sites and electron distribution. From the docking results, the title compound exhibits good antibacterial activity.

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# Spectroscopic profiling, Topology Analysis, and Charge Transfer Excitation of5-Chloro-2-Pyridinol

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**Abstract**

Nonlinear optics plays a crucial role in the field of photonics and optoelectronics. The study of the vibrational spectra of substituted pyridine attracts the attention of many spectroscopists due to their wide application in pharmacology and agro-chemistry. This study provides a complete vibrational spectroscopic investigation on the molecule to give a detailed assignment of the fundamental bands in FTIR and FT Raman spectra on the basis of calculated PED and electronic analysis under both theoretical and experimental background. Comparing the bond length $C_2$-$C_3$ ($1.401A^0$) with $C_5$-$C_6$ ($1.387A^0$) in 5-Chloro-2-pyridinol is increased due to the influence of OH group in the $C_2$ position. The stability and different types of hydrogen bonds inside the molecule are explained by natural bond orbital analysis (NBO). The chemical stability of the molecule is predicted by the HOMO and LUMO energies. RDG analysis is used to identify weak interactions of the studied molecule based on electron density. The Fukui function identified the chemical reactivity sites. The first hyperpolarizability which is an important parameter for future studies of nonlinear optics (NLO) was calculated to check the potential of the molecule to be an NLO material.

**Keywords**: DFT, RDG, NLO,

https://doi.org/10.3390/molecules26113289.

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# Structural and Functional Analysis of Pure and Mg Doped Calcium Oxide Nanoparticles Using Co- precipitation Method

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## ABSTRACT

The present study involves synthesis and structural analysis of pure and Mg doped Calcium Oxide nano particles. The prepared nanoparticles were characterized by X-ray powder Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The structure, crystallite size,lattice parameters and microstrain of the prepared samples were studied using XRD analysis. The XRD spectra indicated cubic structure for both pure and doped samples. The crystallite size of pure and Mg doped calcium oxide nanoparticles were calculated as 39nm and 45nm respectively. The microstrain present in the pure and Mg doped CaO samples were calculated to be around 0.04 and 0.03 respectively. The presence of functional groups and metal oxide formation was confirmed using FTIR analysis. The band corresponding to calcium

oxide formation in are found around 873 $cm^{-1}$.

**Keywords**: CaO nanoparticles, Co-precipitation XRD, FTIR

# DENSITY FUNCTIONAL THEORY, FMO CALCULATIONS AND TOPOLOGICAL ANALYSIS OF WARFARIN TITANIUM

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## ABSTRACT

In this work, we reported the topology analysis of the Warfarin Titanium by theoretical and quantum chemical calculation. The structure of the compound was optimized and the structural characteristics were determined by density functional theory (DFT) using B3LYP method with LANL2DZ basis sets. The FMO analysis indicates the density of delocalized electrons within the molecule. The interpreted HOMO and LUMO energies indicate the chemical stability, distribution of energy and energetic behavior of the compound. The chemical reactivity sites have been revealed by Molecular Electrostatic Potential (MEP) analysis. MEP were used to recognize the nucleophilic and electrophilic regions of the molecule, adding information on reactivity. The chemical implication of the molecule was explained using ELF, LOL with contour

map. ELF andLOL maps generated reveals the charge distribution on the surface. ELF describes the electron pair density, on the other hand LOL describes the orbital gradient-induced maximum overlap of localized orbitals. The interactions such as Vander Waals, hydrogen bonds, and steric effects are detected using RDG, a topological technique. Based on the electron density, weak interaction of the molecule was identified and visualized by using VMD tool.

**Key words:** DFT, MEP, ELF, LOL, RDG

# OPTIMIZED GEOMETRY, FRONTIER MOLECULAR ORBITALS AND TOPOLOGICAL ANALYSIS OF WARFARIN INDIUM BY DFT METHOD

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## ABSTRACT

A systematic spectroscopic investigation of Warfarin Indium was performed by utilizing Density Functional Theory approaches at B3LYP level using Gaussian 09w software package. The B3LYP/LANL2DZ computations were used to optimize the structure of the molecule. FMO analysis shows the higher reactivity of the molecule. The chemical stability of the molecule is predicted by Highest Occupied Molecular orbital (HOMO) and Lowest Unoccupied Molecular orbital(LUMO) analysis. While the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. The molecular electrostatic potential (MEP) is related to the electronic density and is a very useful descriptor for

determining sites for electrophilic attack and nucleophilic reactions as well as hydrogen-bonding interactions.By using the Multiwave function software, the topological analysis of ELF and LOL were performed.ELF is used for determining the probability of electron pair localisation. LOL is used to describe molecular bonds, reactivities and chemical structures.Based on electron density, weak interactions of the molecule are identified with the aid of RDG analysis.Additionally, it provides the most significant interaction data, such as Van der Waals, hydrogen bond, and steric relationships within the molecule.

**Key words:** DFT, MEP, HOMO LUMO, ELF, LOL

## GROWTH AND UV CHARACTERIZATION OF PURE AND L-THREONINE DOPED SINGLE CRYSTAL

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### ABSTRACT

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields. L-Threonine was doped into the $MgSO_4.7H_2O$ solution in different molar ratios and single crystals were grown by the slow evaporation method at room temperature . Good quality transparent Crystals were harvested within 25 days . These crystals were subjected to X-ray diffraction and found their latticeparameters. The Crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystals belongs to monoclinic system. The crystals were characterised to find the band gap using UV spectrum.

**Keyword:**$MgSO_4$, L-threonine, Slow evaporation, UV

## SYNTHESIS AND CHARACTERISATION OF CADMIUM IONS DOPED MAGNESIUM OXIDE NANOPARTICLES

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## ABSTRACT

Magnesium Oxide nanoparticles show favourable properties leading to their use in many industrial applications. A systematic synthesis and study of pure and Cadmium Chloride doped MgO nano particle has been undergone by the simple co-precipitation method. The structure analysis and the functional group analysis is done using XRD and FTIR analysis. The optical property of the sample is studied using UV-VIS Spectroscopy


**Keywords**:MgO Nanoparticles, FTIR, XRD, UV-VIS, Co-precipitation.


# STRUCTURAL AND FUNCTIONAL ANALYSIS OF PURE AND ZN DOPED CALCIUM OXIDE NANOPARTICLES USING CO-PRECIPITATION METHOD


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## ABSTRACT

In the present study, pure and Zn doped Calcium Oxide nano particles were prepard by co-precipitation method. The prepared samples were characterized by X-ray powder Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) for structural and functional analysis. The structure, crystallite size,lattice parameters and microstrain of the prepared samples were studied using XRD analysis. The XRD spectra indicated cubic structure for both pure and Zn doped CaOnanoparticles.The crystallite size of pure and Mg doped calcium oxide nanoparticles were calculated as 39nm and 44nm respectively. The microstrain present in the pure and Mg doped CaO samples were calculated to be around 0.04 and 0.6 respectively. The presence of functional groups and metal oxide formation was confirmed using FTIR analysis. The band corresponding to calcium oxide formation are

found around 873 $cm^{-1}$.

**Keywords**: CaO nanoparticles, XRD, Co-precipitation

# STRUCTURAL AND FUNCTIONAL ANALYSIS OFPURE AND MG DOPED ZINC OXIDE NANOPARTICLES USING CO-PRECIPITATION METHOD

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## ABSTRACT

The study involves synthesis and structural analysis of Pure and Mg doped Zinc Oxide nano particles. The structural and functional characterization of the prepared nanoparticles weredone by X-ray powder Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The structure, crystallite size,lattice parameters and microstrain of the prepared samples were studied using XRD analysis. The XRD spectra indicated hexagonal wurtize structure for both pure and Zn doped CaOnanoparticles.The crystallite size of pure and Mg doped calcium oxide nanoparticles were calculated as 46 nm and 50nm respectively. The microstrain present in the pure and Mg doped CaO samples were calculated to be around 0.02 and 0.01 respectively. The presence of functional groups and metal oxide formation was

confirmed using FTIR analysis. The band corresponding to calcium oxide formation in are found around 473 $cm^{-1}$.

**Keywords**: ZnO nanoparticles, XRD, Co-precipitation

# A STUDY ON MOLECULAR STRUCTURE, HOMO-LUMO AND TOPOLOGICAL ANALYSIS OF WARFARIN GALLIUM BY DFT TECHNIQUES

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## ABSTRACT

The structure of the compound Warfarin Gallium was optimized and the structural characteristics were determined by density functional theory (DFT) using B3LYP method with 6-31G(d, p) and 6-311++G(d, p) basis sets. The optimized geometric parameters, bond lengths and bond angles were calculated. The electronic properties, such as HOMO and LUMO energies were studied. In addition, $E_{HOMO}$, $E_{LUMO}$, energy gap, ionization potential, global hardness, softness and electrophilicity index were calculated to explore the reactivity,

stability and bio activity of the title compound. Furthermore, the topological analysis including electron localization function (ELF) and local orbital locator (LOL), were performed by using Multiwfn, a multifunctional wave function analysis tool. The Molecular Electrostatic Potential (MEP) map was generated in order to spot the electrophilic and nucleophilic sites in the title compound. It provides a visual representation of the molecule's relative polarity. It demonstrates the degree of reactivity by the colours of the regions under electrophilic and nucleophilic assault. The RDG was performed using Multiwfn and the visual molecular dynamics (VMD) application, a topological tool that exposes non covalent interactions such as van der Waals, steric effects and hydrogen bonds.

**Keywords:** DFT, Warfarin Gallium, HOMO-LUMO, ELF, LOL

# GROWTH AND FTIR CHARACTERIZATION OF PURE AND L-THREONINE DOPED SINGLE CRYSTAL

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## ABSTRACT

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields. L-Threonine was doped into the $MgSO_4.7H_2O$ solution in different molar ratios and single crystals were grown by the slow evaporation method at room temperature . Good quality transparent Crystals were harvested within 25 days . These crystals were subjected to X-ray diffraction and found their latticeparameters. The Crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystals belongs to monoclinic system. The crystals were characterised FTIR Spectrum.

**Keyword:**$MgSO_4$, L-threonine, Slow evaporation, FTIR

# THE STUDY OF CONCENTRATED SOLAR-THERMAL POWER

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## ABSTRACT

This study explores Concentrated Solar-Thermal Power (CSP), evaluating its technologies, recent advancements, economic viability, environmental impact, and policy implications. It examines parabolic troughs, solar power towers, and dish systems assessing their efficiency and scalability. Advances in materials, design, and thermal energy storage are studied for enhanced efficiency. Economic considerations, including the levelized cost of electricity, are compared with other energy sources. Environmental sustainability is analysed through life cycle assessments, and the role of CSP in climate change mitigation is examined. The analysis concludes with insights into policy frameworks, government incentives, and successful CSP projects, offering a comprehensive understanding of the current state and future prospects of concentrated solar-thermal power.

Keywords: CSP, Environmental Sustainability.

# GROWTH AND PHOTO LUMINESCENCE CHARACTERIZATION OF PURE AND L-THREONINE DOPED SINGLE CRYSTAL

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## ABSTRACT

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields. L-Threonine was doped into the $MgSO_4.7H_2O$ solution in different molar ratios and single crystals were grown by the slow evaporation method at room temperature . Good quality transparent Crystals were harvested within 25 days. These crystals were subjected to X-ray diffraction and found their latticeparameters. The Crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystals belongs to monoclinic system. The crystals were characterised by Photo Luminescence.

**Keyword:**$MgSO_4$, L-threonine, Slow evaporation, Photo luminescence.

# THE STUDY OF SOLAR ACTIVITY BY KODAIKANAL SOLAR OBSERVATORY

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**ABSTRACT**

This study looks at how the Sun behaves, focusing on things like sunspots, solar flares, and other solar activities. The Kodaikanal Solar Observatory carefully watches these events and analyzes them. By doing this, they help us understand how the Sun affects our weather in space and on Earth. This study helps scientists predict and prepare for space weather events that could affect our technology and climate. The work done by the observatory is important because it helps us understand more about the Sun and its effects on our planet.

**Keywords: Solar activity, Space weather.**

# THE STUDY OF DYNAMICS OF SUN USING SOLARDYNAMICS OBSERVATORY

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**ABSTRACT**

The Solar Dynamics Observatory (SDO) is a cornerstone mission for understanding the dynamics of the Sun and its influence on space weather. Launched in 2010 by NASA, SDO employs advanced instruments to capture high-resolution images and spectra of the Sun across multiple wavelengths. By observing the Sun continuously, SDO provides crucial data on solar phenomena such as solar flares, coronal mass ejections, and magnetic field dynamics. These observations help scientists better comprehend solar activity's impact on Earth's magnetosphere, ionosphere, and technological infrastructure, enhancing our ability to predict and mitigate space weather events. SDO's unprecedented data have revolutionized solar physics, enabling breakthroughs in solar modelling, space weather forecasting, and understanding of fundamental solar processes. Its contributions are vital for safeguarding satellites, astronauts, and terrestrial technology, while also advancing our comprehension of the Sun's fundamental role in shaping the solar system.

Keywords: SDO, Space weather, Magnetic field

# GROWTH AND STRUCTURAL STUDIES ON MIXED $MgSO_4.7H_2O$ AND $ZnSO_4.7H_2O$ SINGLE CRYSTALS IN THE RATIO 1:1

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**ABSTRACT**

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields.Zinc Sulphate were mixed into the $MgSO_4.7H_2O$ solution in different molar ratio 1:1 and single crystals were grown by the slow evaporation method at room temperature. Good quality transparent crystals were harvested within 25 days. These crystals were subjected to X-ray diffraction and found their lattice parameters. The crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystal belongs to monoclinic system. The values are a=10.5792, b=10.5712 and c=9.9900. The grown crystals were characterized UV and FTIR spectrum.

**Key Words:** Slow evaporation, XRD

# GROWTH AND STRUCTURAL STUDIES ON MIXED $MgSO_4.7H_2O$AND KCl SINGLE CRYSTALS IN THE RATIO 1:1

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**ABSTRACT**

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields. Potassium Chloride were mixed into the $MgSO_4.7H_2O$ solution in different molar ratio 1:1 and single crystals were grown by the slow evaporation method at room temperature. Good quality transparent crystals were harvested within 15 days. These crystals were subjected to X-ray diffraction and found their lattice parameters. The crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystal belongs to monoclinic system. The values are a=9.1505, b=9.6874 and c=11.2933.The grown crystals were characterized UV and FTIR spectrum.

**Key Words:** Slow evaporation, XRD

# GROWTH AND STRUCTURAL STUDIES ON MIXED $MgSO_4.7H_2O$ AND KCl SINGLE CRYSTALS IN THE RATIO 2:2

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**ABSTRACT**

$MgSO_4.7H_2O$ is a hydrogen bonded crystal having wide application in various fields.

Potassium Chloride were mixed into the $MgSO_4.7H_2O$ solution in different molar ratio 2:2 and single crystals were grown by the slow evaporation method at room temperature. Good quality transparent crystals were harvested within 21 days. These crystals were subjected to X-ray diffraction and found their lattice parameters. The crystalline nature and purity of grown crystals are confirmed by X-ray diffraction pattern. It reveals that the grown crystal belongs to monoclinic system. The values are a=9.8845,b=10.6498 and c=10.095.The grown crystals were characterized UV and FTIR spectrum.

**Key Words:** Slow evaporation, XRD

# SYNTHESIS AND CHARACTERIZATION OF CALCIUM IONS DOPED MAGNESIUM OXIDE NANOPARTICLES

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## ABSTRACT

In the last few decades, there has been a trend involving the use of nanoscale fillers in a variety of applications. Magnesium Oxide is one of the promising materials which has unique properties of which made it suitable candidate for the use in the wide range of application. In the present work pure and Calcium Nitrate doped MgO nanoparticles are prepared by simple co-precipitation

method. The highly crystalline phase of MgO nanoparticles are confirmed by the XRD and FTIR studies. The Optical property of the synthesized samples was analysed using the UV-VIS Spectroscopy.

**Keywords:**MgO Nanoparticles/, XRD, FTIR, UV- VIS , Co-precipitation.

## ANALYSIS OF SOLAR MAGNETIC FIELD BY UDAIPUR

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### ABSTRACT

Udaipur Solar Observatory(USO) is Asia's largest Solar Observatory. Udaipur

Solar Observatory has become the project center to develop Solar physics in India. The Observatory comprises a range of telescope that provide excellent quality of Solar observations. Utilizing a variety of telescopes, USO is known for its Solar observations, which include high resolution Solar Chromospheric, magnetic field, velocity and spectral observations, for studies pertaining to solar flares, mass ejections, and the evolution of solar active regions. The observatory is adding a new instrument by the name of "Solar Vector Magnetograph" to its store-house. This instrument will play an important role in the future research program by determining the magnetic field of the active regions.

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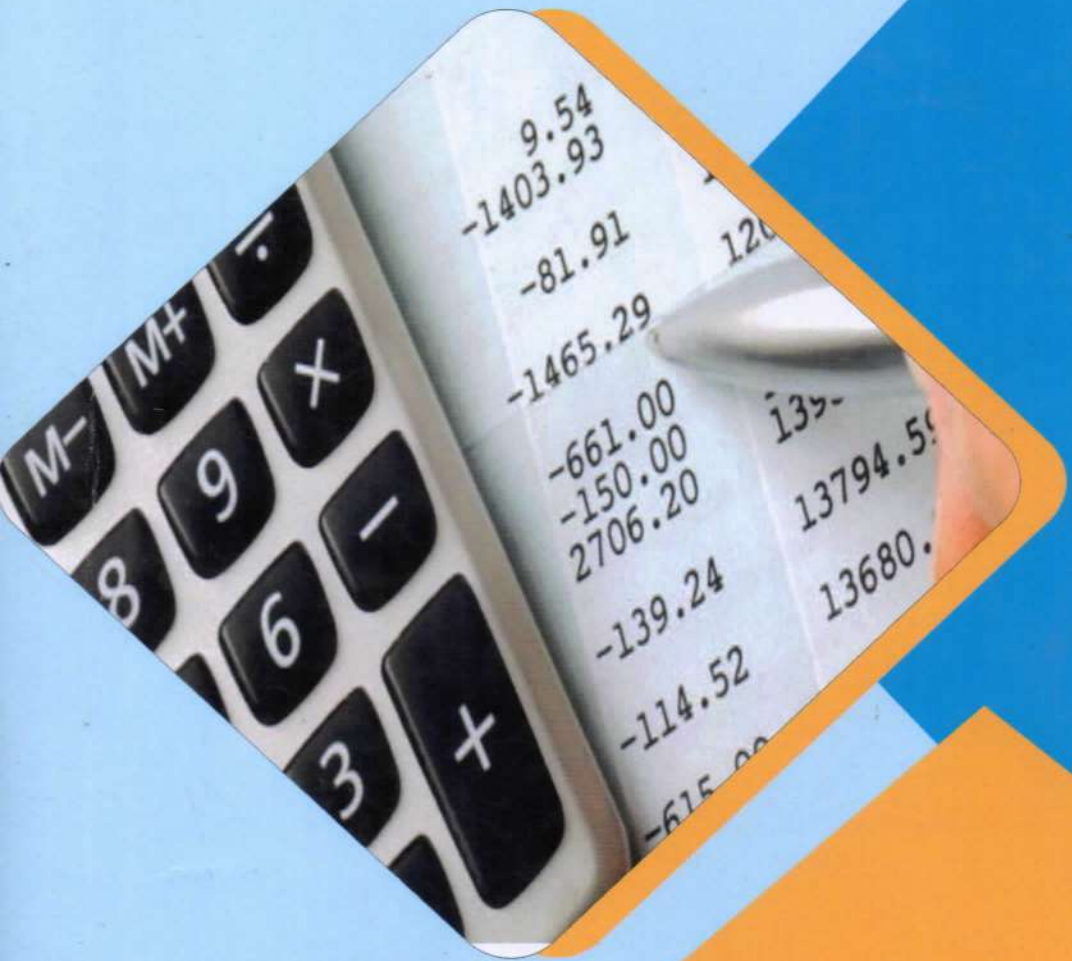


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