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Spectroscopic investigations on the orientation of 1,4-dibromonaphthalene on silver nanoparticles

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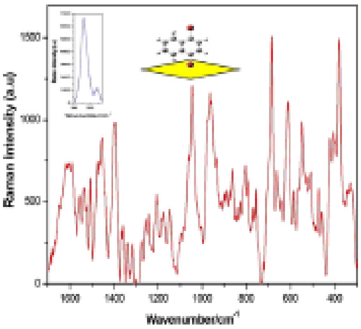
HIGHLIGHTS

- Silver nanoparticles were synthesized by solution combustion method.
- Prepared silver nanoparticles are fcc structure with SPR at 380 nm.
- nRs and SERS studies were performed for 1,4-DBrN.
- Higher enhancement observed for C–H out-of-plane and C–Br stretching modes.
- Orientation of 1,4-DBrN on silver nanoparticles is 'stand-on'.

GRAPHICAL ABSTRACT



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ABSTRACT

Silver nanoparticles (Ag NPs) have been prepared by solution combustion method with glycine as fuel. Silver nanoparticles were characterized by X-Ray Diffraction (XRD), High Resolution Transmission Electron Microscopy (HRTEM) and UV–visible spectroscopy. The prepared silver nanoparticles exhibit cubic crystalline structure with grain size of 59 nm. HRTEM image shows that the silver nanoparticles have strain and four-fold symmetry formed by twinning in the crystal structure. The optical adsorption spectrum shows that the surface plasmon resonance peak of silver is observed at 380 nm. The orientation of 1,4-dibromonaphthlaene (1,4-DBrN) on silver nanoparticles has been inferred from nRs and SERS spectral features. The absence of a C–H stretching vibrations, the observed high intense C–H out-of-plane bending modes and high intense C–Br stretching vibration suggest that the 1,4-DBrN molecule may be adsorbed in a 'stand-on' orientation to the surface.

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Introduction

Naphthalene derivatives have a wide range of applications in biology, pharmacology and material science. They are present in different families of plants, which have been used in diverse cultures such as colorants for cosmetics, fabrics, foods, and for medicinal purposes, including antitumor, anti-inflammatory and antimicrobial agent's medicine of diseases, especially cancer [1].

1,4-Dibromonaphthalene (1,4-DBrN) has become increasing important as a triplet excitation acceptor with useful phosphorescent properties. It is also useful as a precursor for other 1,4-dibromonaphthalene derivatives such as enzyme-inhibitory, antifungal, antibacterial, anticancer, antiproliferative, antiviral, trypanocidal, antiplatelet, anti-inflammatory, antiallergic, antimalarial, phenols, amines, aryl ethers, alkyl ethers and organ metallic's [2,3]. The treatment of 1-bromonaphthalene with bromine in dichloromethane at −30 °C yielded the formation of 1,4-dibromonaphthalene in excellent yield (91%).

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Orientation of 1,4-dimethoxy-3–bromomethylanthracence-9,10-dione on silver nanoparticles: SERS studies

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HIGHLIGHTS

- Silver nanoparticles were synthesized by solution combustion method.
- Prepared silver nanoparticles are fcc structure with SPR at 380 nm.
- nRs and SERS studies were performed for DMBMAQ.
- Higher enhancement observed for C—H out-of-plane modes.
- Orientation of DMBMAD on silver nanoparticles is 'stand-on'.

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ABSTRACT

Silver nanoparticles (Ag NPs) are prepared by solution combustion method with glycine as fuel. Silver nanoparticles are characterized by UV–visible spectroscopy, X-ray Diffraction (XRD) and High Resolution Transmission Electron Microscopy (HRTEM). The optical adsorption spectrum shows that the surface plasmon resonance peak of silver is observed at 380 nm. The prepared silver nanoparticles exhibit cubic crystalline structure with grain size of 59 nm. HRTEM image shows that the silver nanoparticles have strain and fivefold symmetry is formed by twinning in the crystal structure. Surface-enhanced Raman scattering (SERS) of 1,4-dimethoxy-3-bromomethyl-9,10anthraquinone dione (DMBMAD) adsorbed on silver nanoparticles has been investigated. The orientation of DMBMAD on silver nanoparticles has been inferred from nRs and SERS spectral features. The observed spectral feature corroborated that DMBMAD would absorb on silver surface with 'stand-on' orientation through the high intensity of C—H out-of-plane bending mode, C—Br stretching, ring stretching and C=O. In present case we used the DMBMAD and Ag NPs as component molecules for energy gap analysis, whereas DMBMAD serve as donor and Ag NPs as acceptor. The calculated HOMO and LUMO energy gap shows that charge transfer occur within molecule and Ag NPs.

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1. Introduction

Anthraquinone (AQ) is the most important quinone derivative of athracene. Plants containing anthraquninoes have been used for millennia as dyestuffs and purgatives. Though quinones are found in plants and in a few animals, they usually are prepared by oxidation of aromatic amines, polyhydric phenols, and polynuclear hydrocarbons. Anthraquinone derivatives have various biomedical characteristics (bioactivities) and have the wide application for medicines, pesticides, etc. [1,2].They are used principally in photographic dye chemicals, in medicines, as an antioxidant, in paints, varnishes, motor fuels, oils, pigments and in organic inhibitor. They play a vital role in paper industry as a catalyst to increase the pulp production yield and to improve the fiber strength through reduction reaction of cellulose to carboxylic acid [3,4].

Metal nanoparticles have widely used in the field of medicine, materials science, chemistry, physics, environmental science and biotechnology. Coinage metals such as gold, silver and copper have been used for the synthesis of stable nanoparticles, which are useful in photography, catalysis, biological labeling, photonics, optoelectronics and SERS detection [5]. They have captured much interest due to their optical, electronic, magnetic and chemical properties. Among the metal nanoparticles, silver nanoparticles have received considerable interest because of unique properties such as good conductivity, chemical stability, catalysis and antimicrobial activity [6]. Silver nanoparticles are widely used in textiles, cosmetics, sprays, plastics and paints owing to their antimicrobial activity

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Surface Enhanced Raman Spectroscopic investigations of 2-bromo-3-methylamino-1,4-naphthoquinone on silver nanoparticles

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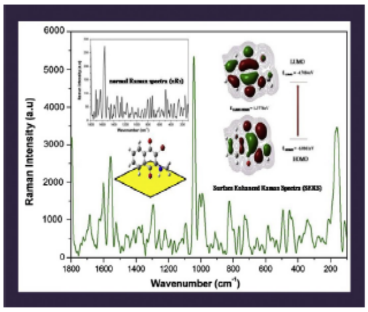
HIGHLIGHTS

- Silver nanoparticles were synthesized by solution combustion method using citric acid as fuel.
- Prepared silver nanoparticles are fcc structure.
- nRs and SERS studies were performed for BMANQ molecule.
- Higher enhancement observed for C=O and C—Br stretching modes.
- Orientation of BMANQ molecule on silver nanoparticles is 'stand-on'.

GRAPHICAL ABSTRACT



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Surface Enhanced Raman scattering

ABSTRACT

Surface Enhanced Raman Spectroscopic technique has been employed to investigate the orientation of 2-bromo-3-methylamino-1,4-naphthoquinone (BMANQ) on silver nanoparticles. Silver nanoparticles have been prepared by solution combustion method with citric acid as fuel. Silver nanoparticles were characterized by X-ray Diffraction (XRD), High Resolution Transmission Electron Microscopy (HRTEM) and Scanning Electron Microscopy (SEM). XRD and morphological results confirmed the nanocrystalline nature of the prepared silver nanoparticles. The observed intense C=O stretching, C—Br stretching and NH_2 vibration suggests that the BMANQ molecule may be adsorbed in a 'stand-on' orientation to the silver surface. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy show that charge transfer occurs within the molecule.

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Introduction

Surface Enhanced Raman Spectroscopic (SERS) has been of interest in the fields of Physics, Chemistry, Surface Science, Nanoscience, and Biomedical Science. SERS is a high sensitivity spectrum without damage to samples. It has high potential in providing some useful information about the nature, orientation of adsorbed molecular species and the adsorbate–metal interaction mechanism [1]. SERS technology has been well established for obtaining detailed information of molecules adsorbed on the surfaces of silver, gold or other noble metals, such as the adsorption configuration of molecules and the interaction mechanism of the molecules with the surfaces of substrates [2–7]. SERS is widely used to explain in sequence, the performance of biomolecules adsorbed at the metal surfaces, orientation of adsorbed species

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