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RECENT TRENDS IN BASIC SCIENCE RESEARCHES (RTBSR: 2017)

Under the aegis of
University Grants Commission (NERO)

Organized by
Department of Physics and Chemistry
Srikishan Sarda College, Hailakandi,
Assam, 788151

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Vibrational spectra of the linear triatomic molecule OCS using Lie algebra

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Abstract

The aim of this work is to study the highly excited vibrational states of Carbonyl sulfide (OCS) in exact vibron model. Considering the $U(4)\otimes U(4)$ spectrum generating algebra, the standard Hamiltonian is constructed by the linear combination of Casimir operators. The vibron number for each bond is calculated from the harmonic frequency and the anharmonicity constant. The algebraic interaction parameters are evaluated from the least square fit against an experimental data. Using the vibron numbers and the algebraic interaction parameters 25 vibrational

Key Words: Vibron model, linear triatomic molecule, Carbonyl sulfide.

1. Introduction

Carbonyl sulfide is an organic compound with the linear formula OCS. It is a colourless flammable gas with an unpleasant odor. It is a linear molecule consisting of a carbonyl group double bonded to a sulfur atom. Carbonyl sulfide can be considered to be intermediate between carbon dioxide and carbon disulfide, both of which are valence isoelectronic with it. Carbonyl sulfide is the most abundant sulfur compound naturally present in the atmosphere, at 0.5±0.05 ppb, because it is emitted from oceans, volcanoes and deep sea vents. As such, it is a significant compound in the global cycle. All these properties of OCS are enough to draw the attention of scientific community to work on it. A small work is reported here, which calculate the infrared vibrational spectra of OCS using Lie algebra.

Molecular spectroscopy is an area of science which studies the spectra of molecule and provides information regarding different molecular aspect. With the introduction of various detection techniques [1-3], there is a progress in the field of molecular spectroscopy. The progress of molecular spectroscopy is not only due to the introduction of sophisticated experimental techniques, but also the introduction of the effect of anharmonicity, resonance, resonance perturbation etc. The introduction of all these effects has changed the theoretical field of molecular spectroscopy, to a more attractive and interesting one [4, 9]. When it is to deal with the modern spectroscopy, the most important thing that one need is that, a formulation, which is able to discuss simultaneously the structure of levels beyond the harmonic limit and the corresponding dynamics. Generally there are three conventional methods to interpret these experimental results obtained by different detection techniques. These are -1) The Dunham like expression of energy levels in terms of ro vibrational quantum numbers, 2) the solution of Schrodinger equation with potential obtained either by appropriate modified ab initio calculation or by more phenomenological method and 3) the vibron model formulated in lie algebraic method . In Dunham approach the infrared energy levels in the ground electronic state can be expressed in the wave number unit with an error below 10 cm^{-1}. This is almost the

Microwave-Assisted Synthesis of Gold Nanoparticles Stabilised By Poly Ethylene Glycol and Their Catalytic Activities

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Abstract

We report a facile and rapid one-pot microwave (MW) assisted synthesis of gold nanoparticles. Gold salt is reduced to gold nanoparticles by poly ethylene glycol (PEG) under the action of microwave irradiation. Colour of the mixture solution turns purple red in few second. Synthesised nanoparticles were characterised by ultraviolet–visible (UV-Vis), transmission electron microscopic (TEM) Fourier transform infra-red spectroscopy (FTIR) and photoluminscence. The photocatalytic activity of gold nanoparticles was investigated by monitoring the photochemical reduction of 2, 4, 6 trinitrophenol in the presence of excess $NaBH_4$.

Key words: Gold nanoparticles, poly ethylene glycol, catalytic activity, picric acid.

1. Introduction

A catalyst is something which makes a chemical reaction more rapid .Enzymes in our body is a common example of a naturally occurring catalysts which speeds up several bio-chemical reaction in our body. In the fields f synthetics chemically and chemical engineering catalysis has greatest contribution such as in oil refining industries, plastics and petrochemicals industries. Action of catalysis is lie on reactivity and reactivity can be enhanced by increasing the surface area of substrate. If something has more surface area there more places for other chemicals agent to bind, interact and react[1].As The use of nanoparticles results in a large contact area between the nanoparticles and surrounding phase as nanoparticles have large surface to volume ratio[2].That is the reason nanoparticles often have exhibits good catalytic activity including oxidation of hydrocarbons ,C-C coupling ,hydrogenation –dehydrogenation and redox [3].Now a day's gold nanoparticles become an attractive choice of research because of their unique physicochemical properties[4].Gold is usually inert but Haruta er al.[5] showed that gold nanoparticles shows effective catalytic activity and is dramatically influenced by the size and shape of it. Use of gold nanoparticles as catalytic agent is also preferable due to the fact that it is easy to synthesis in different size and shape and can be easily functionalised using different functional group [6]. Gold nanoparticles can be synthesized in a range of shapes and sizes. So far various shaped gold nanoparticles have been reported in the literature such as nanorods, nanotriangles, nanoboots, nanotubes, nanoflower, and nano stars etc [7-10]. Most of the above polyshaped GNPs have synthesized via wet chemical methods using reagent such as sodium citrate, cetyltrimethyle ammonium bromide(CTAB) ,tetra octyle ammonium bromide (TOAB),ascorbic acid , sodium borohydride [11,12]. Key factors of synthesis of gold nanoparticles are the precursor concentration, reducing agent, stirring and temperature. The biological response can be altered using capping agents such as polyethylene glycol (PEG). Further it is known that functionalizing AuNPs with PEG increases stability, both in vivo and in vitro [13]. In this work, we have demonstrated a one-pot process using microwave (MW) irradiation synthesize of isotropic gold nanoparticles from $HAuCl_4$ using poly ethelyne glycol (PEG) which act as both reducing

Silver and their Core-shell Nanoparticles as Novel Antibacterial Agents

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Abstract

Silver have been in used since ancient time in the form of silver, silver nitrate, silver sulfadiazine for the treatment of wound, bacterial infections. But due to the emergence of antibiotics, the use of silver had been declined. At the beginning of 1990s, the problems of certain strains of bacteria became so life-threatening that silver has made a remarkable comeback as a supplemental or alternative medicine. Currently, advances in nanotechnology have produced novel horizons in nanomedicine by enabling synthesis of nanoparticles that could be assembled into complex structure like core-shell. These cores – shell structures are also finding potential applications in diverse fields ranging from silver based dressing, silver coated medical devices etc.

1. Introduction

Nanotechnology is an interdisciplinary branch of science that is related to Physics, Chemistry, Biology and Medicine and involves materials having dimensions in the order of 100 nm or less. It finds useful applications in various fields of science and technology [1-2]. Recently, nanomedicine is emerging as the fastest growing filed in the medical research in which the physiochemical properties of nanoparticles are being used to develop NPs based targeted drug carriers, rapid pathogen detection and bio-molecular sensing as well as nanoparticle-based cancer therapies [2].

Nanoparticles are defined as the clusters of atoms in the range of 1-100 nm, which possess defined optical, chemical and mechanical properties and are extremely promising for their antibacterial activity [1-2]. Theses optical as well as antibacterial properties are believed to be due to their larger surface to volume ratio which makes them unique unlike their own bulk materials. Moreover, scaling down of the particle size makes them efficient tools with improved biocompatibility. This feature makes them superior and indispensable in many areas of human activity and also excellent candidates for biomedical applications in variety of biological processes that occur at nanometer level.

Different types of metal NPs like silver, gold, copper, zinc, titanium has been extensively studied for their antibacterial properties but AgNPs has proved to be the most promising material for antimicrobial properties against both types of Gram-negative and Gram-positive bacteria, viruses along with some eukaryotic micro-organisms.

Silver had been widely used for many different purposes since ancient times, for example in fabrication of jewelry, coins, dental alloy etc. The metal has a history of extensive use as medicine since more than 7,000 years in preventing many diseases, healing of wounds, in preservation of drinking water, preventing the food spoilage without even though the exact mechanism of action was not known [1-3]. Some of the examples are: the introduction of silver coins in milk in the prevention of various diseases and retarding the fermentation process by reducing lactic acid bacteria. It is believe that

CONTENTS