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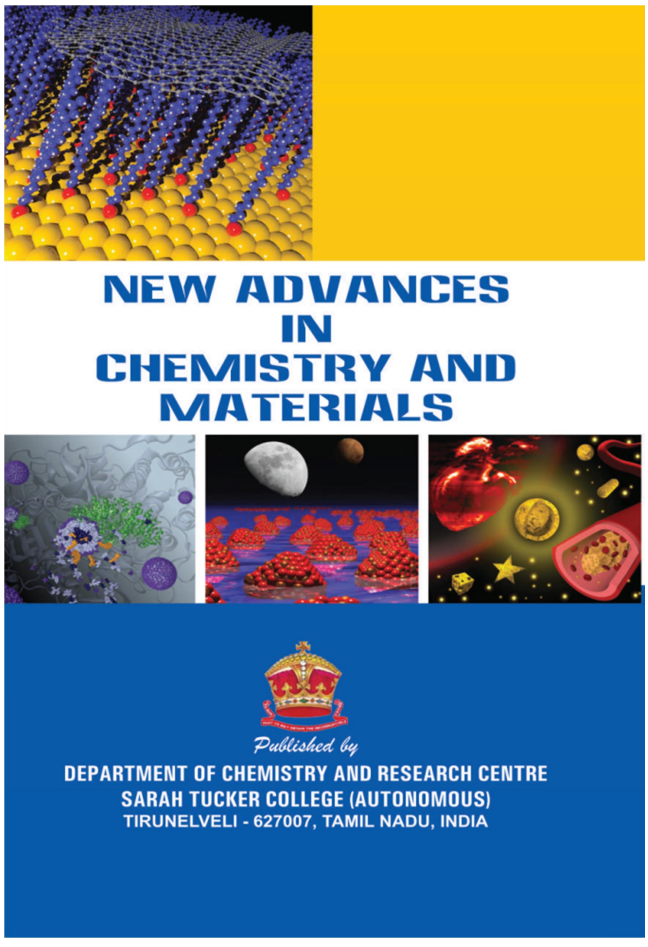

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Dr. V. Rama

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A STUDY ON VIBRATIONAL FREQUENCIES OF MOCLOBEMIDE BY DENSITY FUNCTIONAL THEORY

I. Antony Danish[†] *and J. Winfred Jebaraj*[‡]

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ABSTRACT

Moclobemide is an important drug widely used for the treatment of depressive disorders and less extensively studied for anxiety disorders. It is classified as a reversible inhibitor of mono-amine oxidase-A. It is a benzamide derivative of morpholine. The structural features of this drug may play a vital role in its activity. Hence, it was felt worthwhile to investigate the geometry and the physical properties of the titled compound. The vibrational frequencies was determined and analysed by B3LYP/DFT level by utilizing the basis set 6-31G.

Key words: *Vibrational frequencies, Moclobemide.*

1. Introduction

Moclobemide is a reversible inhibitor of mono-amine oxidase-A [MOA-A] and it is an important drug used extensively in the treatment of depressive disorders and less extensively studied in anxiety disorders [1]. Moclobemide has been reported to have a lower propensity for producing drug interactions than the first generation of irreversible, nonselective inhibitors of *monamine oxidase* [2]. Moclobemide is reported be a highly selective and reversible MAO-A inhibitor with less side effects, when compared with tricyclics [3, 4]. Further, Moclobemide has been chosen to be better than the heterocyclic depressants because of its negligible antichlinergic and antihistaminic actions [5]. It is also reported to be tested for prophylactic treatment of migraine [6]. Moclobemide has been also tested for its anti-ulcer and anti-oxidant activity in rats and it was found to be a potent anti-ulcer agent because it inhibits toxic oxidant radicals and because of its activation of anti-oxidant mechanisms [7]. It increases the levels of norephinepherine, dopamine and in specific serotonin [8, 9].Structurally, moclobemide is a benzamide derivative of morpholine [10].

It plays an important role as a drug with neuroprotective properties. The structural features of this drug may play a vital role in its activity. Gaussian 09 program is used for the calculation [11].

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A DFT STUDY: MOCLOBEMIDE

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ABSTRACT

Moclobemide is an important drug used in the treatment of depression disorders. It's structure is non planar. Gaussian 09 programme is used to determine the structural properties. DFT/B3LYP/6-31 G basis set is used to run the calculation.

Key words: *Bond angle, Bond distance, Mulliken charges, Dipole moment, quadrupole moment, Total energy and Electrostatic potential, Moclobemide.*

1. Introduction

Moclobemide is a reversible inhibitor of mono-amine oxidase-A and it is an important drug used extensively in the treatment of depressive disorders. Moclobemide plays an important role as a drug with neuroprotective properties. It is a benzamide derivative of morpholine. Owing to its drug activity, it was felt worthwhile to investigate the geometry and the physical properties of the target molecule. The geometry and physical properties like bond angle, bond distance, Mulliken charges, Dipole moment, Total energy and Electrostatic potential were determined and analyzed by Density Functional Theory (DFT) utilizing the basis set 6-31G. The skeleton of the optimized molecule is non-polar. The molecular electrostatic potential surface has been used to understand the activity of the molecule.

2. Quantum chemical calculation

In the theoretical calculation of a molecule. Geometry optimization is one of the most important process. Beeks's three parameter hybrid exchange functional [1] with Lee – Yang – Parr correlation functional (B3LYP). [2] and of the DFT [3] and 6-31G basis set was chosen for this calculation. Gaussian 09 Program [4] was used to perform the calculation.

3. Results and discussion

3.1 Bond distance, Bond angle and Mullikan charges

The spatial co-ordinates of the drug moclobemide were downloaded

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Study on the Interaction of a Schiff base metal complex with DNA by Spectroscopic and Electrochemical techniques

*P. Jeslin Kanaga Inba**[1] *and M.A. Neelakantan*[2]

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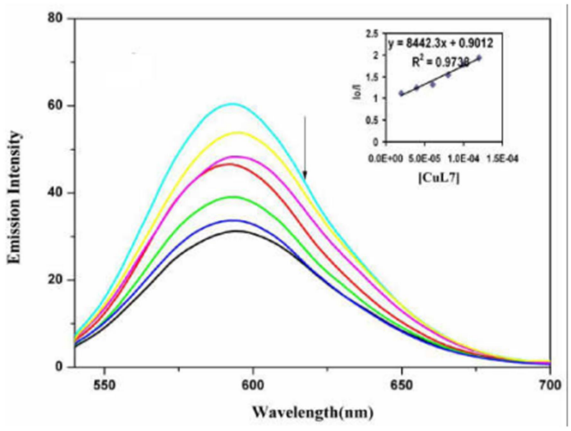
Abstract

This study was designed to examine the interaction of a Schiff base metal complex with calf thymus deoxyribonucleic acid (CT DNA) by UV/Vis in combination with fluorescence spectroscopy and cyclic voltammetric techniques. By the analysis of UV/Vis spectrum, it was observed that upon binding to CT DNA the Schiff base metal complex could slide into the base pairs through intercalative binding. Moreover, the binding constant value indicated that the Schiff base metal complex had a high affinity with CT DNA. At the same time, fluorescence spectra suggested that there is an existence of only one independent class of binding sites for the metal complex on DNA. The binding constants between the Schiff base metal complex and CT DNA were calculated based on fluorescence quenching data. The cyclic voltammetric studies suggest that copper complex binds intercalatively to CT DNA. The apparent binding constant values suggest moderate intercalative binding modes between the complex and DNA.



Introduction

DNA plays an important role in the life process since it contains all the genetic information for the cellular function. However, DNA molecules

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Eco-Friendly Biosynthesis of Silver Nanoparticles Using Wild Strain and its Biological Evolution of Antibacterial Activities

M. Sheik Muhideen Badhusha[a], *M.M. Abdul Kader Mohideen*[b], *J. Shakina*[c]

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Abstract

Biological synthesis of silver nanoparticles (Ag NPS) by *Lactobacillus strain*. The synthesized silver nanoparticles were characterized by UV- visible spectroscopy and Atomic Force Microscopy (AFM). The formation of silver nanoparticles was confirmed by the presence of an absorption peak at 420 nm using UV-visible spectrophotometer. The AFM images shows that silver nanoparticle is a spherical in shape and a diameter between 5 and 40 nm. Silver nanoparticles show excellent antibacterial activity against diseases causing bacterial pathogens.

Keywords: Silver Nanoparticles, Biosynthesis, Atomic Force Microscopy Antibacterial activity,

1. Introduction

Historically, silver compounds and ions have been extensively used for both hygienic and healing purposes [1].However, over time, the use of silver compounds and ions has faded as an anti-infection agent due to the advent of antibiotics and other disinfectants and the poorly understood mechanisms of their toxic effects. Most recently, renewed interest has arisen in manufactured silver nanomaterials because of their unusually enhanced physicochemical and biological properties activities compared to the bulk parent materials[2].

Due to the outbreak of the infectious diseases caused by different pathogenic bacteria and the development of antibiotic resistance the pharmaceutical companies and the researchers are searching for new antibacterial agents. In the present scenario, nanoscale materials have

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Synthesis and Characterization of Pungai oil based Biodegradable Thermosetting Polymers

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Abstract

A thermosetting polymer from Pungai oil has been investigated. The biodegradable oligomeric fumarated resin was prepared by the *in situ* hydroxylation followed by the fumaration of Pungai oil using controlled reaction conditions. Three new polymeric materials were prepared by varying the concentration of the co-monomers methyl methacrylate (MMA) and butyl methacrylate (BMA). The new polymeric materials exhibited tensile stress-strain behavior ranging from soft rubbers through ductile to relatively brittle plastics.

These synthesized polymers were characterized using differential thermal analysis (DTA) and thermo gravimetric analysis (TGA) and its mechanical properties like tensile strength, percentage elongation and hardness were also studied. Hydrolytic test, chemical resistance test and soil burial test were carried out to determine the biodegradability of the synthesized polymer. The synthesized Pungai oil based polymers expressed greater mechanical properties compare to that of commercially available rubbery materials and conventional plastics. In future, this Pungai oil based polymers may serve as a replacement in many applications.

Key words: biodegradable, soft rubbers, plastics, mechanical properties, thermo gravimetric analysis.

1. Introduction

Polymers and polymeric materials exhibit excellent mechanical properties, high corrosion résistance, dimensional stability and low assembly costs. Traditionally, polymers and polymeric composites have been derived from petroleum; however, as the application for polymeric materials increase, finding alternative sources of these materials has become critical (Anastas *et al.,* 2013). The challenge to replace petroleum-based materials with plant-derived renewable sources implies the application of well-established reactions to the production of compounds that produce materials with competitive performance (Ronda *et al*., 2011). Cellulose, starch, proteins and natural oils have all been examined as possible polymeric feedstocks. (Ronda *et al.,* 2013).

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Dr. M. Kamalutheen[1] and Dr. I. Antony Danish[2]

Abstract: In the present educational system, teachers have a demanding task in planning and implementing successful classroom science instruction for concept learning. It requires several kinds of knowledge like content knowledge, pedagogy knowledge, and knowledge of inquiry. Around the globe, the workshops or orientation courses conducted have been usually too short and occasional to foster a change in teachers' classroom practice. The challenges towards teaching chemistry could be met by helping the colleges and other educational institutions by treating teachers as equal partners in decision making. Moreover, teachers should play a greater role in providing important decision makers at all levels of the educational system. A leadership in science can be defined as the ability of a person to bring about changes among teachers and teaching.

The "Pedagogy" is a term that is used as a synonym for teaching. In reality, pedagogy describes the relational values, the personal engagement, the pedagogical climate, the total life-worlds and especially the normal life with students at College, at home, and in the community. The main idea of pedagogy is to differentiate between what is appropriate and what is less appropriate for students. Further, it also involves with the various ways of teaching and giving assistance to students and young people. In short, developing pedagogy might mean for teachers, it becomes immediately apparent that it entails considerably more than accumulating, "a bag of teaching tricks". In this article, the authors suggest the chemistry educators with some valuable insights into classroom practice.

Keywords: *Technical Skills, Conceptual Skills, Interpersonal Skills; Self-learning Skills, Pedagogy, Chemistry.*

Introduction

Chemistry is an essential branch of science for many aspects of our daily lives. Understanding Chemistry would give us the opportunity to make sense of, and explain the world around us. It develops basic knowledge of how to live in this world, to deal with the issues of daily life etc. Examples are, how food changes when we cook it?, how cleaning agents work and which cleaner to choose for which purpose. As a subject taught in class room, chemistry may enlighten the students about their responsibility in using energy resources, guaranteeing sufficient and healthy nutrition, securing sustainability in drinking water supply, framing sustainable industrial development, or dealing with the challenges of climate change [1-4].

In the present educational system, teachers have a demanding task in planning and implementing successful classroom science instruction for concept learning. It requires several kinds of knowledge like content knowledge, pedagogy knowledge, and knowledge of inquiry. Around the globe, the workshops or orientation courses conducted have been usually too short and occasional to foster a change in teachers'

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2 Assistant Professor, Department of Chemistry, Sadakathullah Appa College (Autonomous), Rahmath Nagar, Tirunelveli, India.

Challenges and Role of Teachers in the 21st Century

P. Jeslin Kanaga Inba[1] *& J. Jemi Merlin Rani*[2]

Introduction

"Teaching is not a service, profession or a job. It is a pillar of the society"

Teachers have crucial role to play in preparing young people not only to face the future with confidence but to build it with purpose and responsibility. The new challenges facing education are to contribute to development, to help people understand and to some extent come to terms with the phenomenon of globalization, and to foster social cohesion. The challenges of the coming century to eliminate poverty and ensure sustainable development and lasting peace will fall to today's young people. Educating the young to meet these challenges has become a priority objective for every society. The young generation is entering a world which is changing in all spheres: scientific and technological, political, economic, social and cultural. The outlines of the 'knowledge-based' society of the future are forming. The status of education is changing. 21st century teaching carries with it a complicated mix of challenges and opportunities. Challenges include the issues of teacher turnover, accountability, changing student populations and student expectations, mounting budget pressures, and intense demand to build students' 21st century skills. Teaching is getting more and more complex and challenging these days because the patience level of students is decreasing while rudeness, argumentation, disobedience and short temper is on the rise. It is due to modern age competition, stress, availability of alternate sources of knowledge like internet or violence shown in movies, TV series etc.

The role of teacher is changing so fast that no amount of pre-service or in-service teacher education can probably cope with the expectations of the society. The scope of education is far and wide and cannot really limit it to a specific field or trade. Education is the most powerful weapon which you can use to change the world. It was the teacher who was inculcating the long lasting values and carrying the responsibility of preserving our culture. Today, when we see the turmoil and disruption around us, education can not only be used as a weapon but also as a most effective medium to channelize today's vibrant and enthusiastic youth.

We have forgotten that the teacher is the real sculptor of our future generation. Education that does not review and rethink its content and processes, soon loses its relevance. From the individual point of view, the fundamental function of education should be to stimulate learning, to enhance thinking, to develop personality, to provide avenues for self expression and to liberate human potentialities. This report considers the situation of the teachers. It considers the emerging challenges for teachers and teaching posed by the introduction into education of the new information and communication technologies. In this article, we have discussed some of the challenges faced by the teacher and also the role of a teacher.

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The Pedagogy of Teaching Chemistry in the Current Educational Scenario

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Challenges of Virtual Reality in Education

Dr. M. Mohamed Sathik[1], M. Sheik Mansoor[2] and K.A. Mohamed Riyazudeen[3]

Abstract: This paper mainly focuses on the effects and use of virtual reality in education and then an analysis the challenges of VR in education. At the end it is concluded that adoption of virtual reality can be used as an addition to traditional education system.

Keywords: Virtual Reality, Education, Immersive, Illusion, 3-D Stimulus, Simulation, Head Mounts, Graphics.

Introduction

Virtual reality, as a concept has been around for over forty year. It is an illusion of reality created by the computer system. Virtual reality system is characterized by high degrees of immersion, believability and interaction. It's main goal is to make user believe, as much as possible, that he/she is actually in the computer operated environment. Virtual reality system has the potential to create systematic human testing, training and treatment environments which allow control of complex, immersive dynamic 3-D stimulus presentations. Virtual reality system is capable of simulating events which are normal, abnormal, dangerous or unforeseen. They create scenes and situations in which human mind can participate, interact and exist. Virtual reality is a promising technology which is applicable in various domains like education, training, medicine, health care and entertainment industry. This paper focuses on virtual reality effect in education.

S.W.O.T analysis of virtual reality systems

Opportunities

- Tele-presence and Tele-conferencing
- Medicine and surgery science, education and training
- Entertainment and games
- Military
- Heritage and archaeology
- Fiction and fine arts
- Music
- Manufacturing and urban design

Threats

- Awareness is limited and these are unrealistic
- expectation
- Technical and cultural challenges
- Addiction to virtual reality
- False sense of security
- Cost issues

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Virtual Reality in Teaching and Learning

R. Spurgen Ratheash[1], M.H. Ibrahim[2] and Dr. M. Mohamed Sathik[3]

Abstract: The Virtual Reality (VR) has much attention in higher education for the past few years. It provides visual, aural and tactile stimuli of a virtual world generated in real time. When using VR systems the user is involved in a new interactive environment which is made available by artificial electronic and electromechanical devices. Therefore, the efficiency of the subjective sensation of presence depends on the human-computer interface and the fidelity of the virtual interactions made available. One of the current lines of research aims to increment of the sensation of presence in the virtual world thus diminishing the influence of the real world in the synthetic experience. This paper explains Virtual Reality technology and application of Virtual Reality in science and engineering areas. It also discuss about interactive virtual environment for science, engineering undergraduates and postgraduates teaching and learning.

Keywords: *Chemical Laboratory, Electrical Engineering, Nanotechnology*

Introduction

Technology is an influential factor in education. A new generation of engineering students is entering higher education with significant computing knowledge, and with higher expectations. So that academic institutes will introduce them to appropriate technologies for their successful transformation into industry. Academic institutions are challenged by these new technological requirements and must adopt appropriate strategies to meet the innovative educational demand. Virtual Reality is also largely used in military training, automotive and aerospace design and medical training.

However, engineering education is predominantly descriptive and complex. The application of virtual reality to such teaching has great prospects for new style [1]. The recognised technique in engineering education is the use of laboratory demonstrations to enhance the student's practical knowledge. Laboratories are designed to improve the student ability to investigate and solve engineering problems with appropriate levels of independent thought and creativity and also to demonstrate suitable levels of reporting technical information [2]. Industry relies on distinctive skills to innovate and compete. Thus, it is essential for educational institutes to prepare for emerging technology in both infrastructures and policies.

Chemical Laboratory

The benefits offered by VR are the increased impact of the simulation provided by total immersion in the experience, and the intuitive interface that allows students to interact with the simulation in a more natural manner. To evaluate the former benefit, consider the difference between visiting a chemical lab and inspecting and

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However, engineering education is predominantly descriptive and complex. The application of virtual reality to such teaching has great prospects for new style [1]. The recognised technique in engineering education is the use of laboratory demonstrations to enhance the student's practical knowledge. Laboratories are designed to improve the student ability to investigate and solve engineering problems with appropriate levels of independent thought and creativity and also to demonstrate suitable levels of reporting technical information [2]. Industry relies on distinctive skills to innovate and compete. Thus, it is essential for educational institutes to prepare for emerging technology in both infrastructures and policies.

Chemical Laboratory

The benefits offered by VR are the increased impact of the simulation provided by total immersion in the experience, and the intuitive interface that allows students to interact with the simulation in a more natural manner. To evaluate the former benefit, consider the difference between visiting a chemical lab and inspecting and

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Challenges of Virtual Reality in Education

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Abstract: This paper mainly focuses on the effects and use of virtual reality in education and then an analysis the challenges of VR in education. At the end it is concluded that adoption of virtual reality can be used as an addition to traditional education system.

Keywords: Virtual Reality, Education, Immersive, Illusion, 3-D Stimulus, Simulation, Head Mounts, Graphics.

Introduction

Virtual reality, as a concept has been around for over forty year. It is an illusion of reality created by the computer system. Virtual reality system is characterized by high degrees of immersion, believability and interaction. It's main goal is to make user believe, as much as possible, that he/she is actually in the computer operated environment. Virtual reality system has the potential to create systematic human testing, training and treatment environments which allow control of complex, immersive dynamic 3-D stimulus presentations. Virtual reality system is capable of simulating events which are normal, abnormal, dangerous or unforeseen. They create scenes and situations in which human mind can participate, interact and exist. Virtual reality is a promising technology which is applicable in various domains like education, training, medicine, health care and entertainment industry. This paper focuses on virtual reality effect in education.

S.W.O.T analysis of virtual reality systems

Opportunities

- Tele-presence and Tele-conferencing
- Medicine and surgery science, education and training
- Entertainment and games
- Military
- Heritage and archaeology
- Fiction and fine arts
- Music
- Manufacturing and urban design

Threats

- Awareness is limited and these are unrealistic
- expectation
- Technical and cultural challenges
- Addiction to virtual reality
- False sense of security
- Cost issues

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