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3.2.2 Number of books and chapters in edited volumes/books published and papers published in national/ international conference proceedings per teacher during last five years (10)

Sl. No.	Name of the teacher	Title of the book/chapters published	Title of the paper	Title of the proceedings of the conference	Year of publication	ISBN/ISSN number of the proceeding	Whether at the time of publication Affiliating InstitutionWas same Yes/NO	Name of the publisher
1	T. Gangaiah	ICT and Education	ICT in teaching mathematics	International multidisciplinary Conference on Education for future: Issues and Challenges	2017	978-1-926488-51-6	No	Canadian Academic Publishing

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2	**Dr. Jai kishan ojha**	Materialstoday: proceedings	**Molecular geometry, NBO analysis, Hyperpolarizability and HOMO-LUMO energies of 2-azido-1-phenylethanone using Quantum chemical calculations**	International Conference on Materials Research and Applications ICMRA -2016 (11–13th March 2016), Department of Physics, CMR Technical Campus, Hyderabad, Telangana State, India	**2016**	ISSN: 2214-7853	**No**	Science Direct
3	**Dr. Jai kishan ojha**	**Journal of physics: conference series**	**Experimental and theoritical study of 3-methyl-4-Nitrobenzoic acid using DFT and IVP methods**	XXVII IUPAP Conference on Computational Physics (CCP2015) 2–5 December 2015, Guwahati, India	**2016**	ISSN:1742-6588 E-ISSN:1742-6596	**No**	IOPScience
4	**Dr. Jai kishan ojha**	International journal of Research and analytical reviews	E-Content development and OERS in Higher Education	National Conference on E-Content development and OERS in Higher Education	**2020**	E-ISSN 2348-1269, P-ISSN 2349-5138	**yes**	Atman publishing Academy

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5	**P.Savitha**	International journal of Research and analytical reviews	E-Content development and OERS in Higher Education	**National Conference on E-Content development and OERS in Higher Education**	**2020**	E-ISSN 2348-1269, P-ISSN 2349-5138	**yes**	Atman publishing Academy

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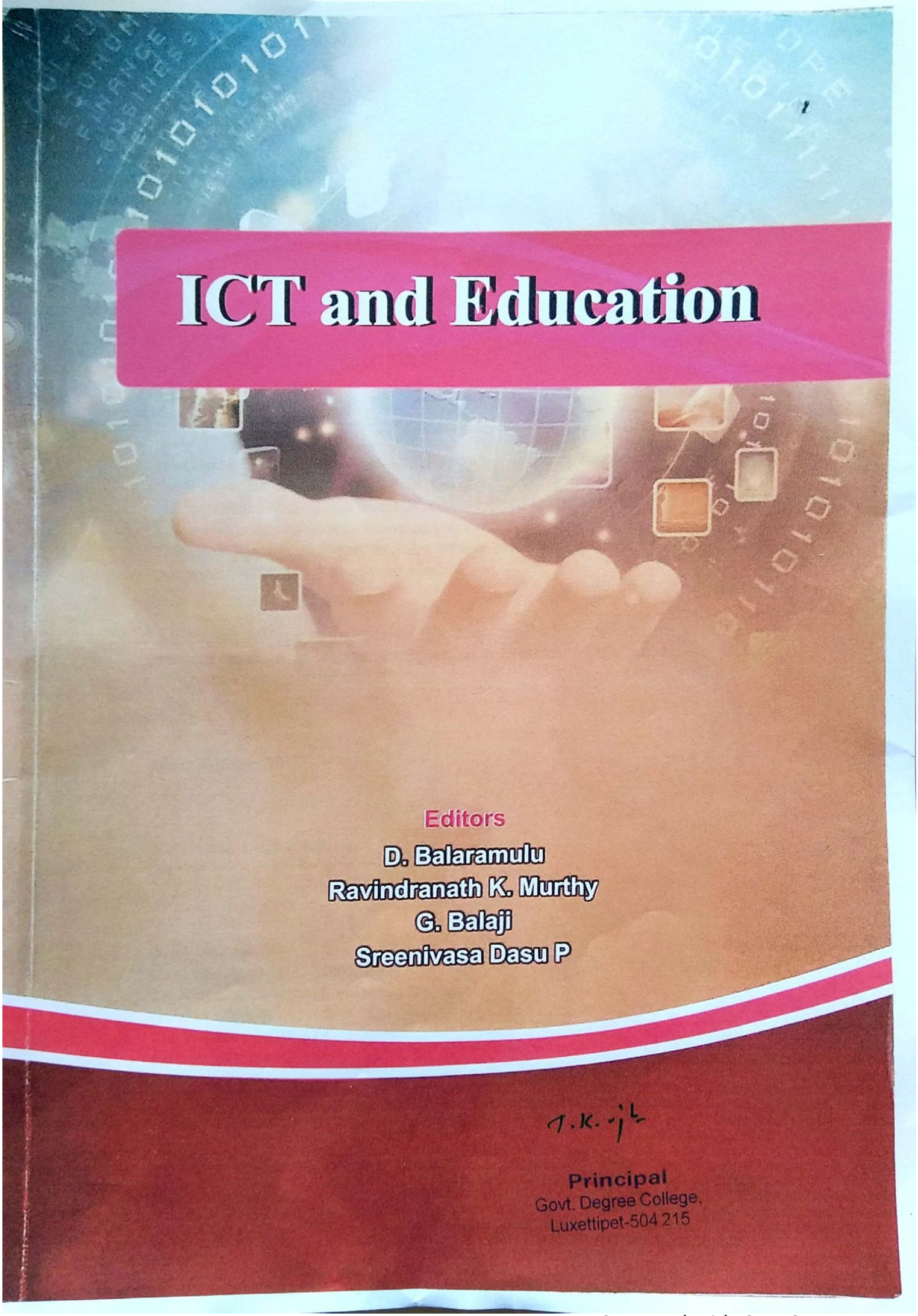

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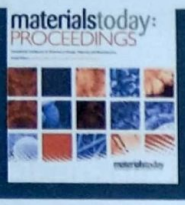

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Experimental and theoretical study of 3-methyl-4-nitrobenzoic acid using DFT and IVP methods

J Prashanth[1], Jai Kishan Ojha[2], B Venkatram Reddy[1] and G Ramana Rao[1]

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Abstract

The Fourier Transform Infrared (FTIR) and FT-Raman spectra of 3-methyl-4- nitrobenzoic acid have been recorded in the range 4000-400 cm^{-1} and 3500-50 cm^{-1}, respectively. The optimized geometry of the molecule, its vibrational frequencies have been computed using the Density Functional Theory (DFT) employing B3LYP/6-311++G basis set. The scaled values of harmonic vibrational frequencies so

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ICT IN TEACHING MATHEMATICS

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INTRODUCTION

From my experience as a student in mathematics and later as a teacher (for a short period) in this field, I believe that technology can be a supportive tool in teaching and learning mathematics. It was interesting to go through the steps of conducting this research, learning the pedagogical reasoning of using computer technology in education and particularly observing how students react to and interact with the program during the lessons.

I hope this study will be a good start for the implementation of computer programs in teaching practices and it will inspire mathematics teachers to think about using these tools in their teaching

Technology in education

Potential of technology in daily life

Over the last few decades technology has become a very important tool in everyday life. Computers have become a common tool for communication, text processing, and many other activities, including different forms of media, audio, graphics, videos, and virtual reality. The development of internet and the increase in accessibility have opened a whole new digital world. Children are not only exposed to new information and computer technology (ICT) at school, but also at home. Many children today have computers at home and have access to internet. They use computers and technology every day for entertainment, communication and education.

Computer literacy is also an essential skill in occupational activities, since technology is widely used in business, economics and many other professions.

The role of technology in education

Many educational institutions have taken into consideration the potential of technology, developing standards related to this new practice in education (Lawless & Pellegrino, 2007), and trying to integrate it into teaching and learning. We take a look at the role of technology in education, considering some pedagogical issues and how the technology integration can affect them.

Technology in mathematics education

One of the major goals in mathematics education is to ensure the success of all students in understanding the subject matter. Mathematics is considered as one of the most challenging and problematic subjects in the educational aspect. But at the same time it is one of the most important areas of science, given that mathematical skills and knowledge are important in everyday life, and there are also many mathematical applications in other subjects and sciences. Christy (1993) states that "mathematics is a basic tool in analysing concepts in every field of human endeavour"

For these reasons, mathematics is a subject which should be taken seriously. Teachers should focus on fostering the students' understanding of mathematical concepts and they should provide a quality education environment for them. Many students find it difficult to engage with mathematical concepts. For learning to take place, students need to be actively engaged with the explored concepts or objects – The cognitive operations are also a difficult part of mathematical activities for students, given that very often teachers attach more importance to the mathematical processes than to their applications to daily life situations or to physical problems. This leads students to solve problems mechanically, by following the algorithm steps without real awareness of their actual meaning (Milovanovic,Takaci&Milajic, 2010). Given these challenges in doing mathematics, it is teachers' and educators' responsibility to make the learning and the understanding of mathematics easier for students. A very important key for the understanding of mathematics is the use of visualization and representations in the learning and teaching

Experimental and theoretical study of 3-methyl-4- nitrobenzoic acid using DFT and IVP methods

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Experimental and theoretical study of 3-methyl-4-nitrobenzoic acid using DFT and IVP methods

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Abstract. The Fourier Transform Infrared (FTIR) and FT-Raman spectra of 3-methyl-4-nitrobenzoic acid have been recorded in the range 4000-400 cm^{-1} and 3500-50 cm^{-1}, respectively. The optimized geometry of the molecule, its vibrational frequencies have been computed using the Density Functional Theory (DFT) employing B3LYP/6-311++G basis set. The scaled values of harmonic vibrational frequencies so obtained have been compared with their experimental counter parts. The scaling factors have been refined to reproduce the frequencies with an RMS error of 9.26 cm^{-1} between the experimental and computed frequencies. The theoretically predicted FTIR and FT-Raman spectra agree satisfactorily with those of experimental spectra. A 89-parameter modified valence force field was evaluated by solving inverse vibrational problem (IVP) using Wilson's GF matrix method. The force constants were refined using 44 experimental frequencies of this molecule in overlay least-squares technique. The average error between observed and computed frequencies was found 11.61cm^{-1}. PED and eigen vectors computed in the process were used to make unambiguous vibrational assignments of all the fundamental vibrations of this molecule. The values of dipole moment and hyperpolarizability were determined to study the NLO behaviour of this molecule. The HOMO and LUMO energies were also evaluated for this molecule.

1. Introduction

Vibrational assignment for complex systems can be proposed based on frequency agreement between the computed and observed fundamental frequencies. The spectroscopists have been investigating to develop 'a priori' method of predicting vibrational frequencies of a given molecule for the past two and a half decades. In this process, two different and distinct methods, namely classical experimental approach [1] and theoretical quantum mechanics approach [2-13], have been evolved.

In experimental approach, Snyder and Schachtschneider [1] proposed the overlay least-square technique wherein a set of related molecules can be treated together to reduce the number of force constants. This method has been applied successfully to some representative molecular systems as reported in our earlier work on nitrotoluenes, dimethylanilines and some substituted methylbenzenes [14]; and on other molecules as mentioned therein.

Spectroscopic investigation has been carried out in theoretical approach in our earlier work on 3,6-dichloro-4-methylpyridazine and 3,6-dichloropyridazine-4-carboxylic acid by DFT method using B3LYP functional with 6-311++G(d,p) basis set [15]; and 4-methyl-3-nitrobenzoic acid employing DFT method employing B3LYP/6-311++G level of theory [16]. We have recently reported the results

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Outline

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Molecular geometry, NBO analysis, Hyperpolarizability and HOMO-LUMO energies of 2-azido-1-phenylethanone using Quantum chemical calculations

J. Prashanth [a], G. Ramesh [a], J. Laxman Naik [a], Jai Kishan Ojha [b], B. Venkatram Reddy [a]

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Abstract

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Molecular geometry, NBO analysis, Hyperpolarizability and HOMO-LUMO energies of 2-azido-1-phenylethanone using Quantum chemical calculations

J. Prashanth[a], G. Ramesh[a], J. Laxman Naik[a], Jai Kishan Ojha[b] and B. Venkatram Reddy[a*]

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Abstract

The Fourier Transform Infrared (FTIR) spectrum of 2-azido-1-phenylethanone (APE) has been recorded in the range 4000-400 cm^{-1} respectively. The optimized geometry of the molecule has been computed by evaluating the torsional potential energy as a function of angle of rotation about the interlinking bonds of APE using quantum chemical calculations. These calculations were carried out using density functional theory (DFT) employing B3LYP functional with 6-311++G(d,p) basis set. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. The values of dipole moment, polarizability and hyperpolarizability were computed to determine the NLO behaviour of the molecule under study. The HOMO and LUMO energies were also evaluated for this molecule to demonstrate the chemical stability.

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Keywords: 2-Azido-1-phenylethanone; FTIR spectrum; DFT; Molecular geometry; Hyperpolarizability; NBO analysis; HOMO-LUMO

1. Introduction

Azide is the anion with the formula N_3^- which is a conjugate base of hydrajoic acid (HN_3) and is isoelectronic with CO_2 and N_2O. It is also a functional group in organic chemistry, RN_3 [1]. Organic azides represent a unique substance class, which is able to undergo a multitude of reactions used for a variety of applications in industry [2]. They are versatile starting materials for the synthesis of a variety of nitrogen-containing compounds that attracts

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attention of both organic and inorganic chemists. The first organic azide (phenyl azide) was synthesized by P. Grieß in 1864 [3, 4]. It followed the discovery of hydrogen azide and the Curtius rearrangement of acyl azides to the corresponding isocyanates by T. Curtius from 1890 to 1894 [5]. The organic azides received considerable attention in the 1950s and 1960s with new applications in the chemistry of the acyl, aryl, and alkyl azides [6, 7]. Organic azides are used for the synthesis of heterocycles (triazoles, tetrazoles, aziridines), as blowing agents, and functional groups in pharmaceuticals e.g. azidonucleosides for the treatment of AIDS [8]. The chemistry of azides has been reviewed several times; some of these overviews focus only on some special subclasses of azides [9]. The organic azides were considered by inorganic chemists as readily accessible substrates for the preparation of nitrene (imido) complexes [10]. The dominant application of azides is as a propellant in air bags. Hence, experimental and theoretical investigation of organic azides gained importance in recent years. A variety of experimental methods and techniques have been used for their structural characterization. These include IR, NMR, microwave spectroscopy, electron diffraction, mass spectrometry and *ab initio* quantum chemical calculations [11-16]. Rocha et al carried out the kinetic resolutions of (±)-β-azidophenylethanols and synthesized by immobilized Candida Antarctica lipase [17].

From the above, it is clear that the study of molecular dynamics of 2-azido-1-phenylethanone (APE) is yet to appear in literature. Hence, a systematic investigation is carried out for this molecule using quantum chemical calculations by density functional theory (DFT) employing B3LYP functional with 6-311++G(d,p) basis set. The purpose of this investigation is:

1. To record FTIR spectrum of APE to get complete information on their vibrational frequencies.
2. To make DFT calculations of this molecule in order to
   (i) identify most stable rotational isomer in the ground state and optimize its geometry,
   (ii) make the NBO analysis to understand molecular structure by studying the interactions between the localized bonding and anti-bonding orbitals,
   (iii) obtain the values of polarizability and first order hyper polarizability to study the NLO behaviour,
   (iv) evaluate HOMO and LUMO energies to know the chemical stability of the molecule.

2. Spectral measurements

The molecule 2-azido-1-phenylethanone was obtained from TCI Chemical Company, Japan and used as such for the spectral measurements. The room temperature FTIR spectrum of the molecule was recorded using Thermo Nicolet Nexus 670 spectrometer employing KBr optics in 4000-400 cm^{-1} region with a resolution of 2.0 cm^{-1}.

3. Quantum chemical calculations

3.1. Molecular geometry

The quantum chemical calculations of APE were carried out with Becke's three parameter hybrid functional [18] combined with Lee-Yang-Parr correlation functional [19] employing 6-311++G(d,p) basis set. The starting point for the calculations in this type of study is to determine the most stable conformer for the molecule under investigation. Hence, the molecule was subjected to a rigorous conformational analysis, wherein torsional potential energy was computed as a function of angle of rotation around the bonds among phenyl, azide and ethanone of this molecule using Gaussian 09w software package [20] implemented on Pentium-V (3.2 GHz) Workstation. The optimized geometry was obtained by solving self-consistent field equation iteratively and the global minimum energy was found at -548.6182 Hartree for this molecule. Subsequent calculations were performed with this optimized structure shown in Fig. 1, which contains numbering of atoms also. As per the computations, the molecule APE possesses C_1 point group symmetry and optimized structure shown in Fig. 1. For plotting simulated IR spectrum, a pure Lorentzian band shape was used with a full width at half maximum (FWHM) 0f 10 cm^{-1}. The optimized structure parameters namely bond lengths, bond angles and torsional angles of APE in its most stable conformation were presented in Table 1. The experimental and simulated FTIR spectra are presented in Fig. 2.

3.2. Natural bond orbital (NBO) analysis

Natural Bond Orbitals (NBO) are localized few-centre orbitals that describe the Lewis-like molecular bonding pattern of electron pairs (or of individual electrons in the open-shell case) in optimally compact form. The NBO

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E-Content Development and OERs in Higher Education: Issues & Challenges

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Abstract

As goes the Sanskrit saying "Vidhwan Sarvatra Pujyate", a scholar is respected globally irrespective of his status, society, culture, and nation. Education is one that vital tool which makes mankind wise, peaceful and happy. The world is witnessing a high pace technological revolution in almost all aspects of human life and access to world-class knowledge through open learning resources like MOOCs, UDACITY, COURSERA, EDX, SHAKSHAT, NMEICT, NPTEL, SWAYAM, has become a cakewalk today. This development has more significance in the Indian context which is blessed with a demographic dividend. But these courses require self-regulated discipline and candidness.

The major challenge being poor connectivity, availability of infrastructure, potential teachers, quality students, genuine critiques and the linguistic constraint, the fruition of many piloted projects is not as expected. The efficacy of the micro-credentials granted by these virtual classrooms also needs to be peer-reviewed. The present paper shall try to enlighten on issues and challenges involved in e-learning.

Introduction

Mankind always exhibited a quest for superior quality knowledge that set him up on the path of innovation and technological growth and is making things happen that might have been felt impossible just a decade back. The access to renowned institutions that imparted domestic knowledge of high competence was always confined to a section of students with a high profile who can afford expensive learning

The credit for massive availability of Open Educational Resources goes to the most renowned and sought after institution, the Massachusetts Institute of Technology that launched the prestigious project MITOPENCOURSEWARE in 2002 which triggered the global open educational resources movement. The term Open Educational Resources was first adopted at UNESCO's 2002 forum on Impact of Open Course Ware in Higher Education for developing countries.

Open educational resources (OERs) are freely accessible, openly licensed text, media, and other assets – digital or otherwise – that are useful for teaching, learning, assessing and also research purpose. It permits users to use, remix, improve and redistribute with no or limited restrictions under some licenses.

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Indian Context

As quoted in EDUCATION IN INDIA BY STEFAN TRINES, RESEARCH EDITOR, WENR, during 2015-16 there were 260 million students of secondary grade produced by 1.5 million schools and as per the AISHE REPORT, 2015- 2016 about 35 million of Indians are graduating from 799 Universities that include around 40000 colleges as Government Degree Colleges and Private Degree Colleges which are catering to the educational needs of under-graduating students. There must be more than 50% dropouts at school levels which is an alarming situation in educational prospects. So India needs radical reforms.

A focus on enforcing higher standards of transparency, strengthening of the vocational and doctoral education pipeline, and professionalization of the sector through stronger institutional responsibility would help in reprioritizing efforts and working around the complexities. Establishment of OERs is a breakthrough for countries like India where diversified student community can find platforms of learning that satisfies their innate potentials. The enrollment into MOOCs is still limited to those students who are well versed with IT usage and English fluency.

Issues

1. Quality and Reliability of Material

Though the material and courseware get licensed, quality assurance has become a big concern. It is difficult to decide the quality and reliability of the material disseminated in the course process. MOOCs lack structure and rarely include the central role of an instructor or teacher. The most effective form of quality assurance and assessment comes from reflections and informal evaluations of enthusiasts who post comments using social media. In spite of that a person enrolled in a course if, at a particular point of the session, he /she find it meaningless in continuing the course not only discontinues but also doubts the quality of all online courses.

2. Significance of Credits

The credits earned by the students on the completion of a course are not channelized in becoming eligible for all sorts of government jobs or many private sectors where traditional qualifications are still in vogue. Hence, in many cases, students may enroll only to secure additional skills or to satisfy their repertoire.

3. Assessment and Award of Credits

In most cases, the assessments are through multiple choice questions with automated answers which give less scope for analyzing the domestic knowledge gained by the student. And even in case of essay submissions, it is difficult to review thousands of essays submitted, as also cross-checking the level of plagiarism. The mechanism does not identify the impersonation of participants in the submission of assignments either. Many courses do not require participants to take a formal examination and in cases where formal examinations are conducted, if the evaluator is the course instructor himself there is a chance of over evaluation. The credits gained also are less appreciated when compared to the ones awarded informal programs of certification.

4. Sustainability

Though there is a growing tendency towards e-learning most MOOCs start-ups do not have organized strategies for clinching the economic market and sustaining business growth. Some startups are trying to generate revenue by working in partnership with higher education educational institutions, Universities and charging a fee for examination, certification or even transcription. But this is against initial ideals of MOOCs which professes free access and availability. In these circumstances, the question of revenue generation becomes an issue of concern for sustainability.

Challenges

1. Connectivity

The courses many times require high-end internet connectivity which again plays a detrimental role in reaching the remote and rural areas more predominant in India. Though the cost of data is reduced significantly, a good section of the Indian population still finds it unaffordable.

2. Availability of Infrastructure

With the advent of smartphones, access to courseware has become surprisingly easy. But the level of comfortable learning is more through digital classrooms which again becomes unaffordable for the rural population.

3. Potential Teachers

The teachers with the utmost potential may not be able to participate in open courseware due to a lack of skill in digital communication. The courseware being one-sided; there is less scope for interaction thus landing the students in confusion.

4. Basic English and Basic Computer Knowledge

It also requires the students to have a certain level of digital literacy coupled with English fluency, which raises concern on inclusivity and equality of access.

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PAPER • OPEN ACCESS

Experimental and theoretical study of 3-methyl-4-nitrobenzoic acid using DFT and IVP methods

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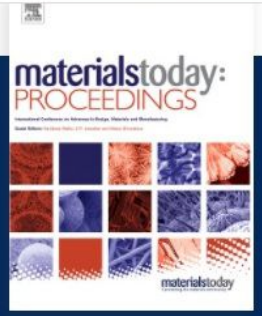
Abstract

The Fourier Transform Infrared (FTIR) and FT-Raman spectra of 3-methyl-4- nitrobenzoic acid have been recorded in the range 4000-400 cm^{-1} and 3500-50 cm^{-1}, respectively. The optimized geometry of the molecule, its vibrational frequencies have been computed using the Density Functional Theory (DFT) employing B3LYP/6-311++G basis set. The scaled values of harmonic vibrational frequencies so



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Molecular geometry, NBO analysis, Hyperpolarizability and HOMO-LUMO energies of 2-azido-1-phenylethanone using Quantum chemical calculations

J. Prashanth [a], G. Ramesh [a], J. Laxman Naik [a], Jai Kishan Ojha [b], B. Venkatram Reddy [a]

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