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About JUET

Jaypee University of Engineering & Technology (earlier Jaypee Institute of Engineering & Technology), Raghogarh, Guna is established under Madhya Pradesh Private University Adhiniyam 2010 vide Gazette (Extraordinary) Notification No. 273 of 29th April 2010. The JUET campus situated on the national highway linking Agra to Mumbai sprawls over 100 acre as a modern institution of higher learning in the field of engineering and technology education. It aims to produce professionals who can be leaders in innovation, entrepreneurship, creativity and management. The first academic activities started in the year 2003. Presently the institute offers 4 year (8 semester) B.Tech Programs, M.Tech. Programs and Doctoral Programs in Chemical Engineering, Civil Engineering, Computer Science and Engineering , Electronics and Communication Engineering and Mechanical Engineering. The Doctoral Programs are also available in Mathematics and Physics streams. Six Semester Diploma program in Building Materials and Cement Technology with strong practical gain is also offered.

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The Materials Research Society of India (MRSI) is an interdisciplinary society founded in 1989 by Prof. C N R Rao, F.R.S., dedicated to the field of materials science and engineering in India. The Society is committed to stimulate and integrate research in the field of materials for rapid industrial progress in the country. The society is currently functioning from IISC, Bangalore. Details are available at www.igcar.ernet.in/mrsi

National Conference on

Recent Advances in Materials Science & Engineering : A Multidisciplinary Approach

[RAMSE 2010]

October 23-24, 2010

Organized by

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in collaboration with

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About the conference

AIM & OBJECTIVES

From the very beginning of civilization, we are using materials in any form. With the advent of new technologies, the need of specific materials is growing very rapidly. Therefore, to fulfill these requirements, newer materials, advanced synthesis and characterization techniques need to be developed. This conference is being organized by JUET, Guna in collaboration with Lucknow Chapter of MRSI with the following objectives :

- To provide platform to exchange of information concerning fields and subjects of interest for national and international research groups both as concerns and scientific knowledge
- Development of research activities and drawing in young researchers to the field subject of the conference.
- Development of new research directions by establishing the opportunities in the field of materials and their applications.
- Identifying the demand for research, development and innovation.

Call for Papers

Technical papers, research findings and case studies on the conference theme are invited from academicians, researchers, and practitioners from the industry from India and abroad.

Detailed abstract (min. of one page max. of two pages in specified format) giving details of findings should be sent to ramse2010@gmail.com. The abstract will be reviewed and authors will be intimated accordingly. Papers presented in the conference will be published in the conference proceedings.

Contributions are solicited in all areas of Materials Science & Engineering namely, but not limited to:

- Synthesis and characterization
- Computational Chemistry
- Nanotechnology
- Electronic & Magnetic Materials
- Surface science (coating, thin films)
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Important Deadlines

Last date for detailed abstract submission	August 7, 2010
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DD should be drawn in favour of "Jaypee University of Engg. & Technology", payable at Guna.

The registration fee includes conference kit, high tea, lunch and dinner during conference days.

Travel/Accommodation

Participants will be provided travel assistance from Ruthiyai railway station to JUET on prior intimation of travel plan. Free hostel accommodation will be provided inside the campus on request. The accommodation may also be arranged in hotels in Guna, charges may vary from Rs. 1000 to Rs. 2000 per day. Advanced request is required for hotel booking.

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ABSTRACT FORMAT

DENSITY FUNCTIONAL THEORY STUDY OF STRUCTURE AND VIBRATIONAL SPECTRA OF 4-CHLORO-4'DIMETHYLAMINO-BENZYLIDENE ANILINE

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Keywords: *Nonlinear optical crystal; rotamers; Vibrational analysis; DFT*

Abstract: The nonlinear optical organic crystals may have potential applications in harmonic generation, amplitude and phase modulation, optical switching, optical communications, optoelectronics, optical computing, optical logic gates, laser radiati on protection, locked laser mode, laser fusion reactions, laser remote sensing, colour display, medical diagnostics etc.[1-3] 4-chloro-4'dimethylamino-benzylidine aniline (CDMABA) is a newly synthesized organic nonlinear optical crystal which shows a large third order nonlinear absorption.[4] Single crystal structure determinations showed that CDMABA belongs to a monoclinic system, space group $P2_1/c$ with unit parameters a = 9.852 (6) Å, b = 16.268 (9) Å, c = 9.512 (6) Å, and β = 119.904 (6)°.[5]

The structure of CDMABA crystal is of much interest, as these crystals do not contain any strong-hydrogen-bond-forming groups, such as -COOH, $-NH_2CO-$ or $-NO_2$; therefore various weak interactions, such as C-H...π[6], π-π[7], weak hydrogen-bonding interactions and the interplay between these interactions, must play an important role in determining conformation of molecule. In the present communication a conformational analysis of possible molecular structures of CDMABA crystal has been done. In order to investigate the possible stable rotamers, the potential energy surface (PES) was obtained by calculating the variation in the total energy of the molecule with change in dihedral angle ϕ1(C4-C5-C12-C13) and ϕ2(C12-C13-C15-C16) using HF/3-21G level of theory

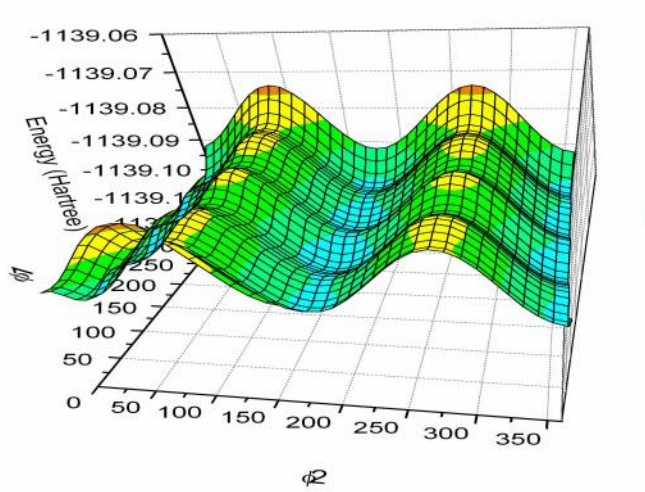

Figure 1. PES of ϕ1 and ϕ2 of CDMABA

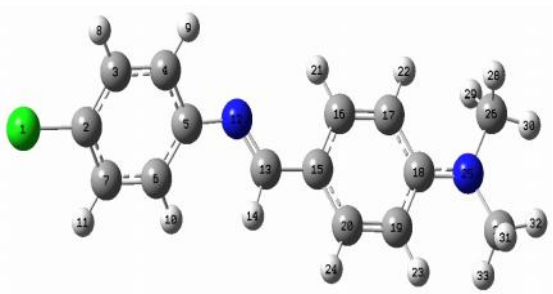

Figure 2. Optimized structure of CDMABA

Geometries of the obtained stable conformers were optimized and harmonic vibrational wavenumbers were calculated. Quantum mechanical calculations of geometry optimization, electrostatic potential surface and vibrational wavenumbers with Raman scattering activities and infrared absorption intensities have been carried out by density functional theory (DFT) method using 6-311++G (d,p) basis set and Becke's three-parameters hybrid functional (B3LYP). The optimized geometry of CDMABA(Figure 2) shows a good agreement with the geometry obtained by X-ray diffraction.[5] The values of the electrostatic potentials are obtained by generating cubes from the data of the checkpoint file. Calculated electrostatic potential surface for CDMABA crystal is shown in Figure 3. The total number of atoms in this molecule is 33; hence it gives 93(3n-6) normal modes. The calculated vibrational wavenumbers and IR/Raman intensities were found to agree well with the experimental FT-IR and Raman spectra (Figure 4).

Figure 3. Electrostatic potential surface of CDMABA

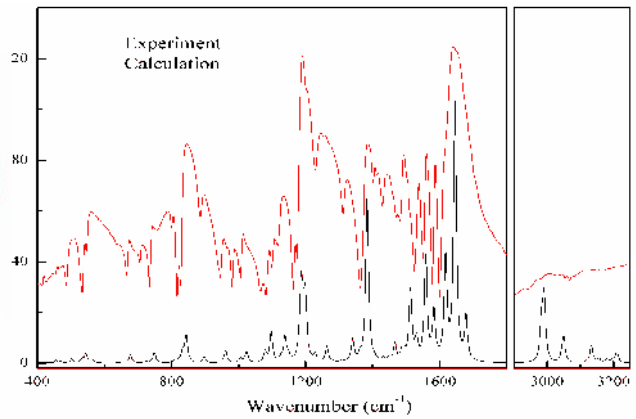

Figure 4. Experimental and calculated Infrared spectra of CDMABA

Isotropic ^{1}H- and ^{13}C-nuclear magnetic shielding tensors of CDMABA were calculated by employing the direct implementation of the single point Gauge-including-atomic-orbital (GIAO) method at the B3LYP density functional and HF levels of the theory using same basis set. ^{1}H-chemical shifts were also calculated with GIAO method, using corresponding TMS shielding calculated at the same theoretical levels as the reference. In addition to this, excited state TD-DFT calculations have also been done for the molecule and obtained cut off wavelength at 350 nm, this shows good agreement with the experimentally observed value at 367 nm.

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