PROJECT COMPLETION REPORT

PROJECT TITLE

Vibrational and Electronic Spectroscopic Studies of Some Organic Compounds

PROJECT CODE: SB/EMEQ - 396/2014, 10-03-2016

SERB INDIA

विज्ञान एवं प्रौद्योगिकी विभाग
DEPARTMENT OF
SCIENCE & TECHNOLOGY
भारत सरकार
GOVERNMENT OF INDIA

DST - SERB Sponsored

SUBMITTED BY

Dr. ADAMILLI VEERAIAH
Principal Investigator &Assistant Professor
Molecular Spectroscopy Laboratory
Department of Physics
D.N.R.College(A), Bhimavaram
Andhra Pradesh-534202

Annexure-IX

PROJECT COMPLETION REPORT

Notes: 1. The PCR should be in bound form.
2. Cover page should include the title of the project, file number, names and addresses of the investigation.

1. **Title of the project** : VIBRATIONAL AND ELECTRONIC SPECTROSCOPIC STUDIES OF SOME ORGANIC COMPOUNDS
Project Code: **SB/EMEQ-396/24**, Dated: **10/03/2016**

2. **Principal Investigator(s) and Co-Investigator(s)** : Dr. A. VEERAIAH
Principal Investigator &Assistant Professor
Molecular Spectroscopy Laboratory,
Department of Physics,
D.N.R.College(A), Bhimavaram, A.P.

3. **Implementing Institution(s) and Other collaborating Institution(s)** : D.N.R. College (A), Bhimavaram,
West Godavari (Dt.), Andhra Pradesh – 534 202

4. **Date of commencement** : 23-04-2016

5. **Planned date of completion** : 22-04-2018

6. **Actual date of completion** : 22-04-2018

7. **Objectives as stated in the project proposal:**

In this project, we studied the vibrational and electronic spectroscopic properties of some classes of heterocyclic organic compounds. We carried out, our research with the help of quantum computational simulation methods and experimental UV-Vis, FT-IT, FT-Raman, Fluorescence techniques. Further, we reported florescence, electro-chemical and commercial importance with broad applications. We presented the detailed vibrational frequencies analysis for further investigations. We have been working in this field for the last few years and published many research articles in high impact factor journals.

8. **Deviation made from original objectives if any, while implementing the project and reasons thereof:** NIL

9. Experimental work giving full details of experimental set up, methods adopted, data collected supported by necessary table, charts, diagrams &photographs: Publications attached below
Experimental Techniques used:
    1. FTIR Spectroscopy
    2. FT Raman Spectroscopy
    3. UV Vis Spectroscopy
    4. Fluorescence Spectroscopy
    5. XRD spectroscopy

Theoretical methods used

1. Ab initio methods
2. Density functional theory
3. Time dependent density functional theory
4. SAC CI method, etc.,..

Note: all the results have been published in Journals of high repute

10. **Detailed analysis of results indicating contributions made towards increasing the state of knowledge in the subject:**

We studied the vibrational and electronic spectra of different classes of organic and inorganic compounds. In this work, the geometrical, structural properties and vibrational frequencies of some commercially important molecules were investigated extensively using density functional theory (DFT) employing B3LYP exchange correlation by different basis sets. All the structural properties of the different compounds were determined by DFT with hyper exchange correlation functional using higher basis set. The fundamental vibrational modes are studied with use of theoretical and experimental simulations. The harmonic vibrational frequencies are theoretically calculated, presented and analyzed. The frontier molecular orbitals such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies are determined by using respective higher basis sets. The electron density distribution and site of chemical reactivity of molecules have been obtained by mapping electron

density iso-surface with molecular electrostatic potential (MEP). Stability of the molecules arising from hyper conjugative interactions, charge delocalizations, etc.,. have been analyzed by using natural bond orbital (NBO) analysis. Hyperpolarizability calculations of the investigated compounds show that the non-linear optical property of the some investigated compounds greater than the standard compound, Urea. Thus some of the compounds have been found to be useful in non-linear optical applications. Further, Electronic, structural and optical properties of the compounds have been studied extensively. Most of compounds were reported in various journals, conferences, etc., Furthermore, some of compounds were about to submit.

List of Organic Compounds studied:

S.NO	Name of Compound
1	6-(Y,Y-Dimethylallylamino)purine
2	2-coumaranone
3	2-Hydroxyquinoline-4-Carboxylic Acid
4	1,3-Diphenyl-2-propanone
5	4-nitrochalcone
6	2-(Trifluoromethyl)quinoline
7	7,9-Dimethylbenz[c]acridine
8	Indoline
9	Benzothiophenesulfone-2-methanol (BS2M)
10	1-(2-Aminophenyl) pyrrole
11	5-Bromo-2-(1-piperidinyl) pyrimidine
12	2-Amino-5-(4-methoxyphenyl)-1,3,4-oxadiazole
13	3-Amino-5-(4-fluorophenyl) isoxazole

14	4-Isoquinolineboronic acid
15	Tryptamine

11. Conclusions summarizing the achievements and indication of scope for future work:

First, we developed Modeling and Simulation Material Science Laboratory. In the present investigations of organic compounds, the structural, vibrational frequencies have been studied from which scientific community gets information regarding the structural behaviour of various class of compounds. The structural information obtained helps the drug designers to design/modify the drugs according to their diversified requirements. The complete vibrational and electronic spectra of different classes of compounds were studied by both theoretical and experimental observations. The complete analysis of NBO and HOMO, LUMO were reported. The geometries and normal modes of vibrations obtained from B3LYP calculations were compared with the experimental data and a good coherence is achieved during the process.

There are N number of methods to predict the chemical, electronic and vibrational frequencies of complex molecules with the theoretical simulations among which Density Functional Theory predictions are one of the most important and successful methods. The DFT calculations were very useful to support the experimental data.

Thus, the aim of the project is fulfilled to some level after which the study of different class of compounds may be continued so that new compounds can be designed / studied to help the scientific community to create a new path for synthesis and drug discoveries during the years to come.

12. S &T benefits accrued:

i. List of Research publications

S No	Authors	Title of paper	Name of the Journal	Volume	Pages	Year
[illegible]	[illegible]	[illegible]	[illegible]	4	40-45	2016
[illegible]	Ramachandra Rao, P.V. Chalapathi, M. Satyavani, **A. Veeraiah**	coumarancone by experimental and density functional theory calculations	structure	[illegible]	[illegible]	[illegible]
3	Katta Eswar Srikanth, K. Anand Solomon, **A. Veeraiah**	XRD, FT-IR, Electronic and Fluorescence Spectroscopic Studies, of Benzothiophenesulfone-2-methanol	International Journal of Pure and Applied Researches	Vol 1	05-25	2018
4	Katta Eswar Srikanth, **A.Veeraiah**	FT-IR, UV/Vis and Fluorescence spectra studies and Quantum Chemical Calculations on 3-Amino-5-(4-fluorophenyl)isoxazole	International Journal of Pure and Applied Researches	Vol 1 (1)	36-50	2018

5	Katta Eswar Srikanth, S Venkata Raju, M SatyaVani, D Vijay, P Paul Divakar, **A Veeraiah**	Characterization, NBO, NLO And Molecular Structural Analysis Of A Material -2-Hydroxyquinoline-4-Carboxylic Acid By Using DFT Method	International Journal of Engineering Science Invention	ISSN : 2319 – 6734	43-51	2018
6	Katta Eswar Srikanth, S Venkata Raju, **A Veeraiah,** D Vijay	A high energy material-1, 4-di nitro-1 H-imidazole its molecular structure and NLO analysis by using DFT method	AIP Conference Proceedings	1992 Issue1	040037 - 1 to 040037 - 8	2018
7	Yeddu Sushma Priya, Kokkiripati Ramachandra Rao, Pallavajhula Venkata Chalapathi, **Adamilli Veeraiah**	Vibrational and Electronic Spectra of 2-Phenyl-2-Imidazoline: A Combined Experimental and Theoretical Study	**Journal of Modern Physics**	8	753-774	2018
8	Sushma Priya Y, Ramachandra Rao K, Venkata Chalapathi P and **Veeraiah A**	Vibrational Spectral Studies and Electronics Properties of Non-Linear Optical Heterocyclic Compound 3-Amino Pyrazole - DFT Study	Journal of Clinical and Medical Images and Short Reports	1	1-9	2018

9	Katta Eswar Srikanth, D Jagadeeswara Rao, V Seetaramaiah, **A Veeraiah**	Molecular geometry and vibrational analysis of 1-(2, 5-dimethyl-furan-3-yl)-ethanone by using density functional theory calculations	Materials Today: Proceedings	18 Part 6	2019-2025	2019
10	K Eswar Srikanth, K Ramaiah, D Jagadeeswara Rao, K Prabhakara Rao, J Laxman Naik, **A Veeraiah,** J Prashanth	Experimental and theoretical analyses on structural (monomer and dimeric form), spectroscopic and electronic properties of an organic semiconductor 2, 6-dimethoxyanthracene	Indian Journal of Physics	https://doi.org/10.1007/s12648-019-01562-z	1-15	2019
11	Katta Eswar Srikanth, **A.Veeraiah**	4-Isoquinolineboronic Acid: Theoretical And Experimental Studies Using Ft-Ir, UV-Visible, Fluorescence Spectra With The Help Of DFT Method	Journal of Emerging Technologies and Innovative Research (JETIR)	6	184-195	2019

12	Y. Sushma Priya , K. Ramachandra Rao , P.V. Chalapathi , **A. Veeraiah,** Kattu Eswar Srikanth , Y. Sheena Mary , Renjith Thomas	Intricate spectroscopic profiling, light harvesting studies and other quantum mechanical properties of 3-phenyl-5-isooxazolone using experimental and computational strategies	Journal of Molecular structure	1203	127461	2020
	In addition to these, some more papers were presented at various International and National Conferences as Invited Talks, Oral Presentations, Posters, etc.,.. The respective details may be found at https://dnrcollege.org/en/department-of-physics/ 3 papers are under review and 3 more papers are supposed to be submitted to various journals of high repute					

ii. Manpower trained on the project

a) Research Associates : Katta Eswar Srikanth, M.Sc.,

b) No. of Ph.Ds produced : In progress (2)

c) Other Technical Personnel trained : 0

iii. Patents taken, if any :NIL

13. Financial Position:

No	Financial Position/ Budget Head	Funds Sanctioned	Expenditure	% of Total cost
I	Salaries/ Manpower costs	4,22,400.00	4,22,400.00	38.40
II	Equipment	3,11,962.00	3,14,489.00	28.59
III	Supplies & Materials	1,77,600.00	99,923.00	9.08
IV	Contingencies	75,000.00	74,901.00	6.81
V	Travel	75,000.00	67,481.00	6.13
VI	Overhead Expenses	1,00,000.00	1,00,000.00	9.09
VII	Others, if any	-	-	
	Total	11,00,000.00	10,79,194.00	98.11

14. Procurement/ Usage of Equipment:

a)

S No	Name of Equipment	Make/Model	Cost (FE/ Rs)	Date of Installation	Utilization Rate (%)	Remarks regarding maintenance
1	Desktop systems & UPS	DELL-V3800 APC110va UPS	1,07,900.00	17-05-2016	100%	NA

2	Gauss View Software	Gauss View 5.0.9	71,400.00	22-06-2016	100%	NA
3	Crystal software	Crystal-17	51,741.00	23-01-2018	In progress	NA
4	Wien2K Software	W2k-2964	33,882.00	22-02-2018	In progress	NA
5	Muffles Furnace	BTL-39	49,566.00	24-03-2018	In progress	NA

b) Plans for utilizing the equipment facilities in future:

Name and Signature with Date:

a. DR.A.Veeraiah
(Principal Investigator)

b. _____
(Co-Investigator)

PRINCIPAL,
D. N. R. COLLEGE
BHIMAVARAM-534 202.

D.N.R.COLLEGE(A)::BHIMAVARAM-534202

(A College with Potential for Excellence and Re-accredited at "B^{++}" level by NAAC)

Dr. A.VEERAIAH

M.Sc., M. Tech., Ph.D.

Principal Investigator (Project code - SB/EMEQ / 2014)

Assistant Professor in Physics and NCC Officer

PHONE: +91-8143395467, avru@rediffmail.com

To

The Under Secretary,
Science and Engineering Research Board,
Department of Science and Technology, Government of India,
5 & 5A, Vasant Square Mall, Sector B, Pocket 5,
Vasant Kunj, New Delhi - 110 070.

Sir,

Sub.: Expression of gratitude - reg.
Ref. : Project code - SB/EMEQ / 2014

This is to bring to your kind notice that I, Dr.A.Veeraiah have been sanctioned a research project by the SERB, DST, Government of India as per the project code cited in the reference above.

With the overall support from SERB, DST, Government of India and my Institute, I could complete my project in a befitting manner. In this process, few research scholars have been trained. Therefore, I express my deep sense of gratitude to the authorities of SERB, DST, Government of India in connection with the opportunity provided. Some of our students are being helped in various aspects.

Thanking you once again.

Dr.A.Veeraiah

DNR COLLEGE (A), BHIAMAVARAM, AP -534 202

DST PROJECT, Govt. Of India.

Publications List

1. Veeraiah, M.Satyavani, Katta Eswar Srikanth, Vibrational and UV/VIS Spectroscopic, NBO analysis of 6-(y,y-dimethylallylamino) purine by ab initio d calculations, International Journal of Engineering Research-Online Vol.4., S2., 2016 .48
2. Y. Sushma Priya, K. Ramachandra Rao, P.V. Chalapathi, M. Satyavani, A. Veeraiah , Vibrational and UV spectroscopic studies of 2-coumaranone by experimental and density functional theory calculations, Journal of Molecular Structure 1144 (2017) 535-544
3. Katta Eswar Srikanth, S Venkata Raju, M SatyaVani, D Vijay, P Paul Divakar & A Veeraiah, Characterization, NBO, NLO And Molecular Structural Analysis Of A Material -2-Hydroxyquinoline-4-Carboxylic Acid By Using DFT Method, International Journal of Engineering Science Invention, 2319 – 6734, 2018
4. Katta Eswar Srikanth, S. Venkata Raju, A. Veeraiah, and D. Vijay, A high energy material - 1, 4-di nitro-1 H-imidazole its molecular structure and NLO analysis by using DFT method, AIP Conference Proceedings 1992, 040037 (2018)
5. Yeddu Sushma Priya, Kokkiripati Ramachandra Rao, Pallavajhula Venkata Chalapathi, Adamilli Veeraiah, Vibrational and Electronic Spectra of 2-Phenyl-2-Imidazoline: A Combined Experimental and Theoretical Study, Journal of Modern Physics, 2018, 9, 753-774
6. Katta Eswar Srikanth, K. Anand Solomon, A. Veeraiah, XRD, FT-IR, Electronic and Fluorescence Spectroscopic Studies, of Benzothiophenesulfone-2-methanol, International Journal of Pure and Applied Researches, 2018, 1, 5-25
7. Katta Eswar Srikanth, A.Veeraiah, FT-IR, UV/Vis and Fluorescence spectra studies and Quantum Chemical Calculations on 3-Amino-5-(4-fluorophenyl)isoxazole, International Journal of Pure and Applied Researches, 2018, 1(1), 36-50
8. Katta Eswar Srikanth, A.Veeraiah, 4-isoquinolineboronic acid: Theoretical and experimental studies using FT-IR, UV-Visible, fluorescence spectra with the help of DFT method, JETIR, june 2019, volume 6, issue 6
9. Y. Sushma Priya, K. Ramachandra Rao, P.V. Chalapathi, A. Veeraiah, Katta Eswar Srikanth, Y. Sheena Mary, Renjith Thomas, Intricate spectroscopic profiling, light harvesting studies and other quantum mechanical properties of 3-phenyl-5-isooxazolone using experimental and computational strategies, Journal of Molecular Structure 1203 (2020) 127461
10. Katta Eswar Srikanth, D. Jagadeeswara Rao, V. Seetaramaiah, A. Veeraiah, Molecular geometry and vibrational analysis of 1-(2, 5-dimethyl-furan- 3-yl)-ethanone by using density functional theory calculations, Materials Today: Proceedings 18 (2019)
11. Katta Eswar Srikanth, A. Veeraiah, T. Pooventhiran b, Renjith Thomas, K. Anand Solomon, Ch.J. Soma Raju, J. Naveena Lavanya Latha, Detailed molecular structure (XRD), conformational search, spectroscopic characterization (IR, Raman, UV, fluorescence), quantum mechanical properties and bioactivity prediction of a pyrrole analogue, Heliyon 6 (2020) e04106

UGC-DAE (CRS) PROJECT
Publications List

12. D Vijay, Asim Kumar Das, B N Rajasekhar And A Veeraiah (2019), Quantum Chemical Calculations and FT-IR, UV Light Interactions on Benzofuran-2-Carbonyl Chloride, Journal Of Emerging Technologies And Innovative Research (JETIR), June 2019, Volume 6, Issue 6, Pages 169-179. Id JETIR1907J25
13. D Vijay, Y Sushma Priya, M Satyavani, Asim Kumar Das, B N Rajasekhar, A Veeraiah (2020) Structural, vibrational and electronic spectroscopic study of 6-hydroxycoumarin using experimental and theoretical methods, Spectrochimica Acta Part A: Molecular and Bio molecular Spectroscopy 229 (2020) 117930, 1-9. https://doi.org/10.1016/j.saa.2019.117930
14. Sushma Priya Yeddu, Pooventhiran Thangaiyan, Adamilli Veeraiah, Dharmarpu Vijay, Katta Eswar Srikanth, Ahmad Irfan, Renjith Thomas, Vibrational Spectral Studies, Quantum Mechanical Properties, and Biological Activity Prediction and Inclusion Molecular Self-Assembly Formation of N-N'-Dimethylethylene Urea, Volume 12, Issue 3, 2022, 3996 - 4017

PRINCIPAL,
D. N. R. COLLEGE
BHIMAVARAM-534 202.