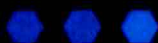


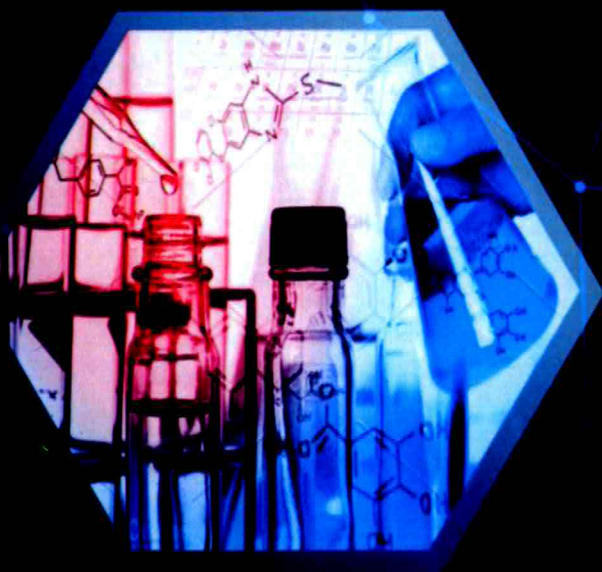
Proceedings of National Conference On

INNOVATIVE RESEARCH IN MEDICAL CHEMISTRY



Edited By

Dr.J.Jani Matilda



10th FEBRUARY 2023, FRIDAY



Organized By

DEPARTMENT OF CHEMISTRY

MUSLIM ARTS COLLEGE

THIRUVITHANCODE - 629167, KANYAKUAMRI DIST

TAMIL NADU - INDIA



Copyright © 2023 by Raj Pathippakam

All rights reserved.

Reproduction or translation of any part of this book by any means without prior permission from the publisher is unlawful. Requests for permission or further information should be addressed to the copyrighter.

The author of the book is fully responsible for the facts and figures presented in this book.

Further it is stated that the publisher is not responsible for the statements or opinions expressed by the author of the book.

ISBN : 978-93-84737-39-9



ISBN 978-93-84737-39-9

Published by

Raj Pathippakam,
3E, North Street,
Kurusady,
Nagercoil - 4

Preface.....

One Day National Conference On '**Innovative Research in Medicinal Chemistry**' (IRIMC-2023) organized by the Department of Chemistry, Muslim Arts College, Thiruvithancode on 10th February 2023. This seminar will be forum to specialize in the recent Innovation and to develop new therapeutic agents by involving synthetic organic and inorganic metal complexes in Medicinal Chemistry. We trust that this seminar would provide valuable insights to the participants to explore the deeper levels of chemistry towards the healthier life. We believe that the book of proceedings will be very useful and readable. It includes two invited talks and forty four contributed papers from research scholars, academicians and scientists. We thank all authors for their contributory papers. We look forward to a productive and successful seminar.

I take this opportunity to thank the Management, the Correspondent-Secretary and Principal of Muslim arts college, Thiruvithancode, for their unstinted cooperation, help and support. I must also thank all the conference office bearers, the organizers, members of the editorial board for their dedication, commitment and involvement in rendering the event unique and memorable. My thanks are also due to all the delegates and the scholar who really make a conference a conference with their paper presentation and sharing of notes, as it were, which is the very vital element in any intellectual activity for the benefit and betterment of humanity.

Dr. J. JANI MATILDA

About the conference

The Conference aims to provide a platform to the students, researchers and faculties of various nearby colleges and departments and also researchers from other institutes to come together and share their findings in various branches of chemistry. This conference will be one of the national meetings exclusively dedicated to medicinal chemistry. The national conference on innovative research in medicinal chemistry explores the deeper levels of chemistry towards a healthier life. The scientific session comprises research areas of Medicinal Chemistry, Bio Chemistry, Inorganic and Organic Materials, Coordination Chemistry, Polymer Chemistry, Nanoscience & Materials, Photo Chemistry, Environmental Chemistry etc. The very attractive speaker of the conference provides a unique opportunity to the participants to listen, interact and benefit from the invited talks and discussions.

CONTENTS

Sl.No	Topic	Page No
INVITED LECTURES		
I	GREEN CHEMICAL APPROACH IN MEDICINE <i>Dr.T.F Abbs Fen Reji</i>	1
II	ROLE OF TRANSITION METAL COMPLEXES IN MEDICINAL CHEMISTRY <i>Dr. Jijo Johnson</i>	2
CONTRIBUTED PAPERS		
1	SYNTHESIS AND CHARACTERIZATION OF DRUG LOADED EGG ALBUMIN- PECTIN NANOPARTICLES <i>A.Asha, G.S. Prabha Littis Malar</i>	3
2	SYNTHESIS OF SILVER NANOPARTICLE- NITROGEN-DOPED GRAPHENE OXIDE NANOCOMPOSITE <i>Asmitha Beegum S & Begila David</i>	6
3	SYNTHESIS AND CHARACTERIZATION OF SCHIFF BASE COMPLEX OF NICKEL(II) <i>M. Shyamala Devi Thankachi</i>	9
4	EVALUATION OF SURFACE WATER QUALITY IN SOUTHERN PARTS OF KANYAKUMARI COASTAL AREAS <i>K.Vinila Mary , G.V.Shyly Sree</i>	13
5	PRELIMINARY PHYTOCHEMICAL SCREENING OF <i>CYNODON DACTYLON (L.) PERS.</i> FROM TWO DIFFERENT SITES. <i>Bashidha Banu. S And Iren Amutha.A</i>	17
6	A STUDY ON HEAVY METALS (CD AND PB) CONCENTRATION IN THE MOST POLLUTED SOIL OF KALKULAM TALUK AND ITS REMOVAL BY PHYTOREMEDIATION PROCESS USING ANANAS COMOSUS <i>Dr.D. Helen And A C Cini Roach</i>	20
7	GEOMETRICAL AND ELECTRONIC PARAMETERS OF 2-[2-ETHYLAMINO-4-(4-CHLOROPHENYLAMINO)THIAZOL-5-OYL]NAPHTHALENE <i>J. Jebaleneta, & T. F. Abbs Fen Rejia</i>	24
8	QUANTUM CHEMICAL CALCULATIONS AND VIBRATIONAL SPECTRA OF 3-[5-(2-PHENYLETHENYL)-1H-PYRAZOL-3-YL]-1-METHYLINDOLE <i>J. Jani Matilda, T. F. Abbs Fen Reji</i>	27

QUANTUM CHEMICAL CALCULATIONS AND VIBRATIONAL SPECTRA OF 3-[5-(2-PHENYLETHENYL)-1H-PYRAZOL-3-YL]-1-METHYLINDOLE

J. JANI MATILDA^{*A}, T. F. ABBS FEN REJI^B^aDepartment of Chemistry, Muslim Arts College, Thiruvithancode-629174.^bDepartment of Chemistry and Research Centre, Nesamony Memorial Christian College, Marthandam-629165, Kanyakumari Dist (TN), India. *Corresponding Author E-mail: jani.matilda91@gmail.com**Abstract**

The compound of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole was synthesized and characterized by elemental analysis and IR spectral studies. The optimized structural parameters of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole was done using Gaussian '09 program package using B3LYP method with the 6-31G basis set, which has been successfully applied in order to derive the optimized geometry, bonding features, harmonic vibrational wave numbers and Mulliken population analysis. Theoretical calculation of the title compounds were carried out using density functional theory method (DFT) and the observed wave numbers were compared with calculated results. The calculated HOMO and LUMO energy gaps also confirm that charge transfer occur within the molecule.

Keywords: DFT, Gaussian, Mulliken charges, HOMO-LUMO.

Introduction

Indole is one of the important heterocyclic compounds and is found in natural products as well as synthetic materials. Many of the clinically approved drugs are naturally or synthetic occurring substituted Indoyl compounds, some of which are fused with other heterocyclic moieties. In addition, Indole and other heterocyclic derivatives have been reported to possess a wide variety of pharmacological properties and biological activities including anticancer, antiinflammatory, antihypotensive, antidepressant, anticonvulsant, antimicrobial, and antitubercular activities [11–12]. The vibrational spectroscopic techniques are powerful molecular structural techniques for the investigation of biological systems.

The present work describes the quantum calculations and vibrational spectral studies of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole, supported by density functional theory (DFT) calculations. DFT calculations have been carried out to elucidate the correlation between the optimized structure, biological activity, bonding features, and electron delocalization. The bond lengths, bond angles, atomic coordinates, equivalent isotropic displacement parameters were measured.

The DFT computations for the 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole was carried out in the Gaussian '09 program package. The calculations were performed at the B3LYP with the standard 6-31G basis set to derive the optimized geometry and vibrational wave numbers.

Results and Discussion**Optimized Geometry**

The molecular structure along with atom numbering of the title compound is shown in **Figure 1**. The optimized bond lengths and bond angles of the 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole molecule at B3LYP level with 6-31G as basis set is collected and is given in **Table 1**. From the experimental values of literature C – C bond length is 1.4 Å, C – O length is 1.26 Å, C – N length is 1.37 Å, C – H length is 1.07 Å. In phenyl ring the C – C length is 1.4 Å. Taking account of the effect of conjugation the theoretically computed values in reasonable agreement with the above mentioned literature data. The B3LYP/6-31G bond length are closed to the literature data due to slightly exaggerated electron correlation effect. The optimized structure is shown in **figure 1**.

**Experimental Details
Computational Details**

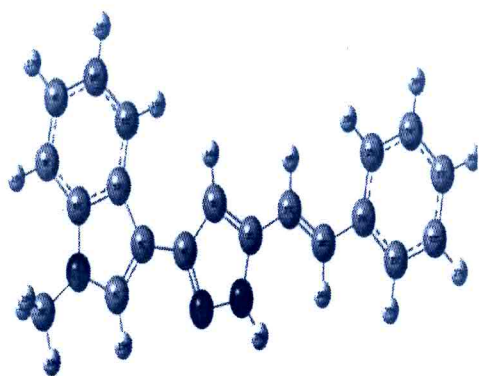


Figure 1: Optimized molecular structure of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole

Atom	Bond length (Å)	Atom	Bond angle (°)
N ₁ -C ₄	1.3596	N ₁ -C ₄ -C ₃	110.36
C ₄ -C ₃	1.4218	C ₄ -C ₃ -H ₁₄	127.57
C ₃ -H ₁₄	1.0769	C ₄ -C ₃ -C ₂	106.62
C ₃ -C ₂	1.3965	N ₁ -C ₄ -C ₅	120.17
C ₂ -N ₃₄	1.3764	C ₃ -C ₄ -C ₅	129.44
N ₃₄ -H ₃₅	1.0045	C ₄ -C ₅ -C ₆	124.65
C ₄ -C ₅	1.4535	C ₅ -C ₆ -H ₁₅	128.53
C ₅ -C ₆	1.3818	C ₅ -C ₆ -N ₇	110.34
C ₆ -H ₁₅	1.0782	N ₇ -C ₁₂ -C ₈	129.76
C ₆ -N ₇	1.3884	C ₁₂ -C ₈ -H ₁₆	121.47
N ₇ -C ₁₂	1.3920	H ₁₆ -C ₈ -C ₉	120.90
C ₁₂ -C ₁₃	1.4288	C ₈ -C ₉ -C ₁₀	120.95
C ₁₂ -C ₈	1.4004	C ₉ -H ₁₇ -C ₁₀	119.50
C ₈ -H ₁₆	1.0852	C ₉ -C ₁₀ -H ₁₈	119.88
C ₈ -C ₉	1.3943	C ₁₀ -C ₁₁ -H ₁₉	119.53
C ₉ -H ₁₇	1.0853	C ₁₀ -C ₁₁ -C ₁₃	119.29
C ₉ -C ₁₀	1.4120	H ₁₉ -C ₁₁ -C ₁₃	120.81
C ₁₀ -H ₁₈	1.0854	C ₁₁ -C ₁₃ -C ₅	134.73
C ₁₁ -H ₁₉	1.0840	C ₂₀ -C ₂₁ -C ₂₂	121.26
C ₁₁ -C ₁₃	1.4075	H ₂₇ -C ₂₂ -C ₂₃	120.13
C ₂₀ -C ₂₁	1.4118	C ₂₂ -C ₂₃ -C ₂₄	119.43
C ₂₁ -H ₂₆	1.0867	C ₂₃ -C ₂₄ -C ₂₅	120.48
C ₂₁ -C ₂₂	1.3966	H ₂₉ -C ₂₄ -C ₂₅	119.12
C ₂₂ -H ₂₇	1.0855	C ₂₄ -C ₂₅ -C ₂₀	120.87
C ₂₂ -C ₂₃	1.3991	C ₂ -N ₃₄ -H ₃₅	128.41
C ₂₃ -C ₂₄	1.4020	N ₇ -C ₃₀ -H ₃₁	111.02
C ₂₄ -C ₂₅	1.3947	C ₃₀ -H ₃₁ -H ₃₂	35.689

Table 1: Optimized geometrical parameters of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole

Mulliken Atomic Charges

The net atomic charges can be obtained from the molecular orbital calculations based on the Mulliken Population analysis. It also plays an important role in the application of quantum chemical calculations to molecular systems. In the title compound the magnitude of the carbon atomic charges was found to be positive and negative. The oxygen atom exhibit negative charge which are donor atom. Hydrogen atoms exhibit positive

Parameter (a.u)	3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole
E _{HOMO}	-0.2262
E _{LUMO}	0.0104
ΔE	-0.2366
Ionization Potential (I)	0.2262
Electron affinity (A)	-0.0104
Electronegativity (χ)	0.1078
Hardness (η)	0.1183
Softness (S)	4.2261

charge, which are the acceptor atoms. The magnitude of the Nitrogen atomic charge was found to be negative. C₁₃ has large positive charge (0.471) due to its attachment with electronegative oxygen. N₈ has large negative charge (- 0.783). **Figure 2** show the Mulliken charge distribution of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole

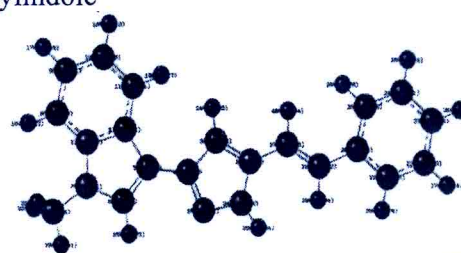
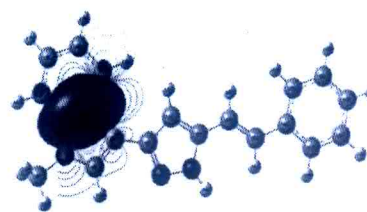


Figure 2: Mulliken Charge distribution of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole

HOMO – LUMO Energy Gap

The HOMO – LUMO (Highest Occupied Molecular Orbital – Lowest Unoccupied Molecular Orbital) analysis has been carried out to explain the charge transfer within the molecule. Energy difference between HOMO and LUMO orbital is called as energy gap which is prove that bioactivity of the molecules, ie. intramolecular charge transfer from electron donating part to the electron acceptor part. The energy difference between the HOMO and LUMO is about - 0.2366eV. The atomic orbital component of the molecular orbital is shown in **figure 3**.



HOMO



Figure 3:

HOMO – LUMO Vibrational Assignment

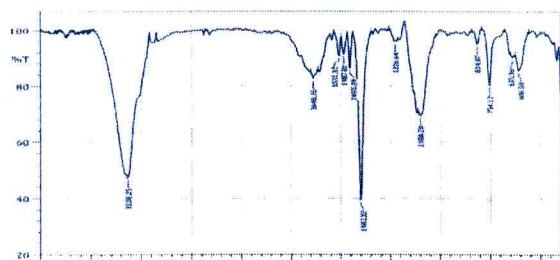


Figure 4: Theoretical FT-IR spectrum of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole

The vibrational assignments in the present work are based on B3LYP/6-31G frequencies. In 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole, the experimental IR spectral values was recorded in the range of 4000-400 cm^{-1} . Aromatic compounds exhibit C-H stretching vibrations in the region 3100-3000 cm^{-1} . Calculated band at 3120 cm^{-1} is due to asymmetric stretching of Phenyl group. Calculated band at 1511 cm^{-1} is due to C = C stretching vibration. Calculated band at 1108 cm^{-1} is due to C = O stretching vibration. Calculated band at 1640 cm^{-1} is due to C = N stretching vibration. Calculated band at 1226 cm^{-1} is due to C – N in-plane bending vibration. Calculated band at 1255 cm^{-1} is due to C – O – C asymmetric stretching vibration. The ring C – C stretching vibrations appears in the region 1640 – 1400 cm^{-1} . Skeletal vibration takes place because of C – C vibrations. In the present work the frequencies are observed at 1455 cm^{-1} , 1487 cm^{-1} as skeletal vibration. The C – H out of plane bending vibrational frequencies observed at 814 cm^{-1} and 754 cm^{-1} . The vibrational assignments computed by B3LYP/6-31G method is in good agreement with literature observation

Conclusion

The structure of 3-[5-(2-phenylethenyl)-1H-pyrazol-3-yl]-1-methylindole was optimized

by quantum chemical calculations using the basis set 6-31G, DFT method. The optimized geometry, vibrational frequencies have been found to agree well with the literature reported values. From the Mulliken charge analysis the atomic charge values of the atom were obtained. The HOMO – LUMO energy gap shows that charge transfer occur within the molecule.

References

- [1] Chiyanzu, C Clarkson, P J Smith, J Lehman, J Gut, P J Rosenthal, K Chibale, *Bioorg. Med. Chem.*, Vol. 13, pp. 3249-3261, 2005.
- [2] T R Bal, B Anand, P Yogeewari, D Sriram, *Bioorg Med Chem Lett.*, Vol. 15, pp. 4451-4455, 2005.
- [3] K A Rama Krishna Reddy, P B Suneetha, C S C Kariga, N H D Manjunath and K N Mahendra, *J. Chil. Chem. Soc.*, Vol. 53, pp. 1653-1657, 2008.
- [4] K Manna, Y K Agrawal, "benzofuran and their antimicrobial activity", Vol. 19, pp. 2688-2692, 2009.
- [5] B Bhrigua, D Pathaka, N Siddiquib, M S Alamb, Waquar, "Search for biological active Isatins: A short review", Vol. 2, pp. 229-235, 2010.
- [6] M O Shibinskya, S A Lyakhov, A V Mazepa, S A Andronati, *Euro. J. Med. Chem.*, Vol. 45, pp. 1237-1243, 2010.
- [7] D Sriram, P Yogeewari, G Gopal, *Euro. J. Med. Chem*, Vol. 40, pp. 1373-1376, 2005.
- [8] S N Pandeya, D Sriram, G Nath, "Euro. J. Med. Chem.", Vol. 35, pp. 249-255, 2000.
- [9] C R Prakash, S Raja, G Saravanan, P Dinesh Kumar and T Panneer Selvam, *Asian J. Res. Pharm. Sci.*, Vol. 1, pp. 140-143, 2011.
- [10] S Ramachandran, V Uma Maheshwari, *Int. J. Pharm. Bio Sci.*, Vol. 2, pp. 251-260, 2011.
- [11] G Kiran, M Sarangapani, T Gouthami, A R Narsimha Reddy, novel bis-isatin carbohydrazone derivatives", Vol. 95, pp. 367-378, 2013.
- [12] K. Maquelin, L.-P. Choo-Smith, C. Kirschner, T.N.A. Ngo, D. Naumann, G.J. Puppels, *Handbook of Vibrational Spectroscopy*, John Wiley, Chichester, 2002.
- [13] R. Petry, M. Schmitt, J. Popp, J. Raman Spectrosc. 4 (2003) 14–30.
- [14] E. Urlaub, J. Popp, W. Kiefer, G. Bringmann, D. Koppler, H. Schneider, U. Zimmermann, B. Schrader, *Biospectroscopy* 4 (1998) 113–120



MUSLIM ARTS COLLEGE



ISO 9001:2000
Reg. No.: R0913488

(Affiliated to Manonmaniam Sundaranar University, Tirunelveli)
Azhagi Mandapam, Thiruvithancode – 629174, Kanyakumari District, Tamil Nadu.
Ph: 04651-24842, 24881, 248803, E-mail : muslimartscollege@gmail.com

DEPARTMENT OF CHEMISTRY

National Conference On

INNOVATIVE RESEARCH IN MEDICINAL CHEMISTRY [IRIMC-2023]

Certificate

This is to certify that Mr/Ms/Mrs/Dr. *J. JANI.MATILDA., Asst... Professor...,... Mujahim... Arts... College...,... Thiruvithancode*.....has participated in the National Conference on Innovative Research in Medicinal Chemistry (IRIMC-2023) organized by the Department of Chemistry, Muslim Arts College, Thiruvithancode, Kanyakumari District on 10th February 2023.

He/She has presented a paper *Oral/Poster* entitled *Quantum... Chemical... Calculations... And... Vibrational... Spectra... Of... 3... 5... (2... phenylethynyl)... 1H... Pyrazol... 3... 4... 5... Methylinole*

[Signature]
Lion. Dr. H. Mohammed Ali
Secretary

[Signature]
Dr. G. Edwin Sheela
Principal

[Signature]
Principal