Journal of Advances in Science and Technology
Vol. 16, Issue No. 1, March-2019, ISSN 2230-9659

Vibrational Spectra of 1,3-bis-acto-5-substituted methyl Benzimidazoline-2-thiones: An Antiviral and Antifungal Drug

D. B. Singh[1]* Kiran Pandey[2] Deepika Nishad[3]

[1,2,3] Micromolecular and Biophysics Laboratory, Department of Physics, Dr. Shakuntala Mishra National and Rehabilitation University, Mohan Road, Lucknow

Abstract – A chemically active compound 1,3-bis-acto-5-substituted benzimidazoline-2-thionesshows the property of Antiviral and Antifungal Drug. The vibrational spectroscopy of1, 3-bis-acto-5-substituted benzimidazoline-2-thionesiscompletely deals in this assignment. The fundamental vibrational frequencies and intensity of vibrational bands of 1,3-bis-acto-5-substituted benzimidazoline-2-thiones compound were evaluated by density functional theory (DFT) using standard B3LYP/6-31G methods and basis set combinations. The vibrational spectra were interpreted, with the aid of normal coordinate analysis based on a scaled quantum mechanical force field. The infrared and Raman spectra were also predicted from the calculated intensities. The comparison of experimental spectra with the simulated spectra provides us the important information about the ability of the computational method to describe the vibrational modes. The optimized geometric structure of 1, 3-bis-acto-5-substituted benzimidazoline-2-thiones has been studied by using Density Functional Theory (DFT). On the basis of ground and excited state geometries, the absorption spectra have been calculated using the DFT method. To understand the Non-Linear Optical properties of1,3-bis-acto-5-substituted benzimidazoline-2-thiones, we computed HOMO-LUMO, dipole moment (μ) and mid and far FTIR and FT-Raman spectra were measured in the stateusing B3LYP density functional theory method in conjunction with 6-31G basis set. The detailed study shows that the given compound exhibits the antifungal and antiviral properties.

Keywords: DFT, FTIR, Vibrational Spectra, HOMO, LUMO, Antifungal, Antiviral.

----------X----------

INTRODUCTION

1,3-bis-acto-5-substituted benzimidazoline-2-thionesis a chemically active compound that shows the property of Antiviral and Antifungal Drugs. Benzimidazole derivatives are being explored in pharmaceutical industries and substituted benzimidazole derivatives have also been found in the diverse therapeutic applications such as in anti-ulcers, antihypertensive, anti-viral, anti-fungal, anti-cancers and anti-histaminics. On the other hand, such benzimidazole derivatives are condensed with other heterocycles like pyrazole, thiadiazole, triazole, thiazole, coumarin and 2- azetidinone moieties which have shown diverse pharmacological activities. compound.Benzimidazoles have different activities as they can act as bacteriostats or bactericides, anticarcinogens, etc. They are often bioactive.Bezimidazole fungicides are commercialized. They act by binding to the fungal microtubules and stopping hyphal growth. They are applied to cereals, fruits, vegetables and vines, and are also used in post-harvest handling of crops. The solubility of Bezimidazole fungicides is low at physiological pH and becomes high at low ph. Since 1952 the antiviral activity of benzimidazole has been studied extensively. A major stimulus during this work has been the central finding that virus-inhibiting activity and cell toxicity of chemical derivatives of benzimidazole may vary independently. The introduction of 1,3-bis-acto-5-substituted benzimidazoline-2-thiones as an antiviral and antifungal agent marked a most important step of the investigations on selective inhibition of viral and fungal replication. Benzimidazoles are also known as benziminazoles and 1,3-benzodiazoles.1,2 They possess both acidic and basic characteristics. The NH group present in benzimidazoles is relatively strongly acidic and also weakly basic. Another characteristic of benzimidazoles is that they have the capacity to form salts. Benzimidazoles with unsubstituted–NH-groups exhibit fast prototropic tautomerism, which leads to equilibrium mixtures of asymmetrically substituted compounds.

The molecular geometry optimization, energy and Vibrational frequency calculations have been performed for 1,3-bis-acto-5-substituted benzimidazoline-2-thiones using Gauss view

program packages at the Becke3-Lee-Yang-Parr (B3LYP) level with standard 6-31G basis set.DFT computational codes are used in practise to investigate the structural, magnetic and electronic properties of molecules, materials and defects DFT calculations allow the prediction and calculation of material behaviour on the basis of quantum mechanical considerations, without requiring higher order parameters such as fundamental material properties. DFT computational methods are applied for the study of systems to synthesis and processing parameters. In such systems, experimental studies are often encumbered by inconsistent results and non-equilibrium conditions.

METHOD, MATERIAL AND THEORY:

The optimized geometry, frequency and intensity of the vibrational bands of 1, 3-bis-acto-5-substituted benzimidazoline-2-thiones were obtained by the Restricted Hartree-Fock (RHF) density functional theory (DFT) with complete relaxation in the potential energy surface using 6-31G basis set. The harmonic vibrational frequencies for 1,3-bis-acto-5-substituted benzimidazoline-2-thiones were calculated and the scaled values have been compared with experimental values of FTIR and FT-Raman spectra. The observed and the calculated frequencies are found to be in good agreement. The harmonic vibrational wave numbers and intensities of vibrational bands of 1,3-bis-acto-5-substituted benzimidazoline-2-thiones with its cation and anion were calculated and compared with the neutral 1,3-bis-acto-5-substituted benzimidazoline-2-thiones. The DFT calculated HOMO and LUMO energies shows that charge transfer occurs within the molecule. DFT calculations allow the prediction and calculation of material behavior on the basis of quantum mechanical considerations, without requiring higher order parameters such as fundamental material properties. Optimized geometrical structure of 1,3-bis-acto-5-substituted benzimidazoline-2-thiones;

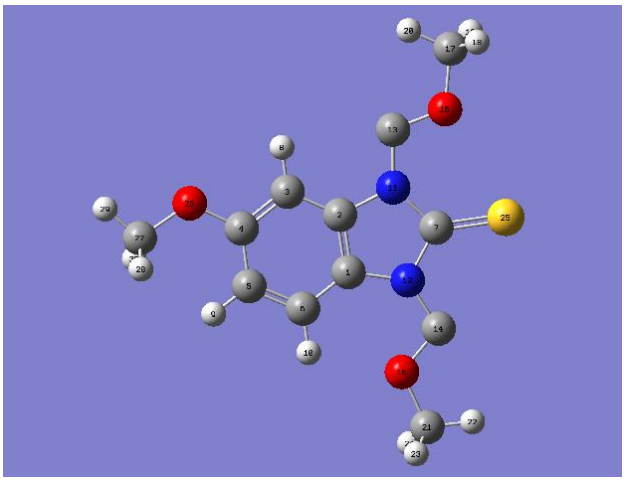

FIG.1

IR and Raman Frequencies

In Vibrational spectroscopy the infrared and Raman spectra of optimized geometrical structure of chemical compound1,3-bis-acto-5-substituted benzimidazoline-2-thioneswere also evaluate from the calculation of intensities. Then the followingfigures show the calculated IR and Raman spectra of Optimized geometrical structure1,3-bis-acto-5-substituted benzimidazoline-2-thiones .These calculations were done by using B3LYP/6-31G methods.

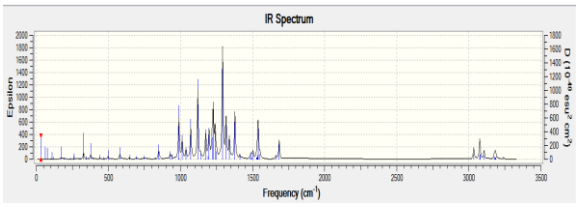

FIG.2

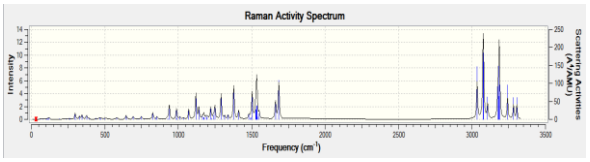

FIG.3

Energy and Dipole Moment

Bond dipole moment of Optimized geometrical structural compound is the measurement of polarity of a chemical bond and also known as the mathematical product of the separation of the ends of a dipole and the magnitude of the charges. The dipole moment creates by unequal sharing of electron in optimized geometrical molecules by their atoms.

Dipole moment and energy of the medically active compound 1,3-bis-acto-5-substituted benzimidazoline-2-thionesis shown in following table:-

Dipole Moment	4.6535 Debye
Total Energy	-1197.43047333 a.u.

(1 Debye = $3.34*10^{-30}$ cm.)

(1 *a.u.* of *energy* = 1hartree = 4.360×10^{-18} J. = 27.211*eV* = 2625kJ/mol = 627.5kcal/mol.)

Molecular Orbital Energies

The most important orbitals in a molecule are the frontier molecular orbitals, called highest occupied molecular orbital (HOMO) and lowest unoccupied

molecular orbital (LUMO).These orbitals determine the way the molecule interacts with other species. The frontier orbital gap helps characterize the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule.

HOMO and LUMO are types of molecular orbitals. The acronyms stand for "highest occupied molecular orbital" and "lowest unoccupied molecular orbital", respectively. The energy difference between the HOMO and LUMO is termed the HOMO**–**LUMOgap. HOMO and LUMO are sometimes called frontier orbitalsin frontier molecular orbital theory. The difference in energy between these two frontier orbitals can be used to predict the strength and stability of transition metal complexes, as well as the colors they produce in solution.

Energy levels of the frontier molecular orbital's especially HOMO, LUMO as well as their spatial distributions are important parameters for determining the optoelectronic properties. The density plot of the HOMO and LUMO of 1,3-bis-acto-5-substituted benzimidazoline-2-thionesis calculated at B3LYP/6-31G level of theory and are shown in Figure;

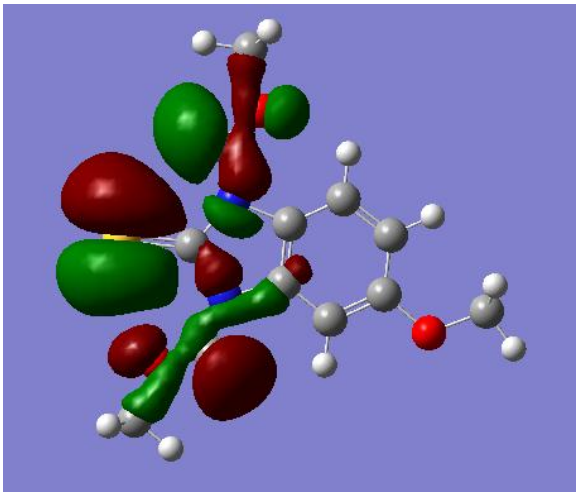

FIG.4HOMO

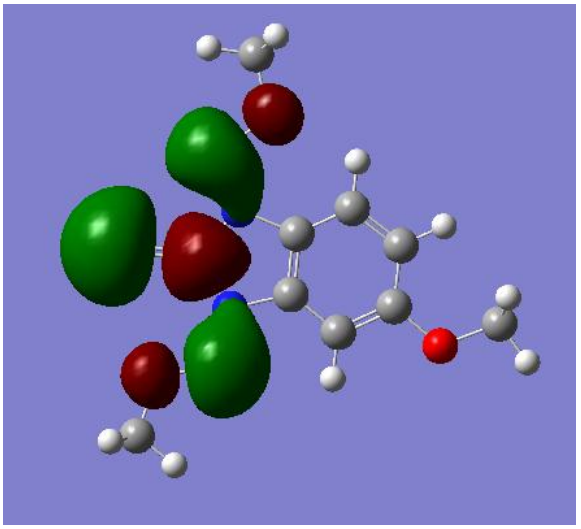

FIG.5LUMO

The energy gap between HOMO and LUMO has been used to prove the bioactivity from intermolecular charge transfer. The energy gap measures the kinetic stability of the molecules. The HOMO and LUMO energy gap show the charge transfer interaction taking place within the molecule.

The HOMO and LUMO energy calculated by B3LYP /6-31G method as shown below in table:-

HOMO Energy	-0.19197 a.u.
LUMO Energy	-0.07268 a.u.
ENERGY GAP (LUMO-HOMO)	0.1929 a.u.

Bond Length and Bond Angle

In molecular geometry, bond length or bond distance is the average distance between nuclei of two bonded atoms in a molecule. It is a transferable property of a bond between atoms of fixed types, relatively independent of the rest of the molecule. Molecular geometries can be specified in terms of bondlengths, bond angles and torsional angles. The bond length is defined to be the average distance between the nuclei of two atoms bonded together in any given molecule. A bond angleis the angle formed between three atoms across at least two bonds. The such as bond lengths, bond angle are the optimized structural parameters , so these parameters were determined at B3LYP level theory with 6-31G basis set and they are presented in a table, which is given below –

ATOMS	BOND LENGTH
H22-C21	1.09124
O16-C14	1.36054
N12-C7	1.43565

S25-C7	1.67970
C2-C1	1.39846
N11-C13	1.46862
O15-C17	1.46862
C17-H20	1.09178
C3-H8	1.07994
C1-C6	1.39283
H9-C5	1.08227
C5-C4	1.40513
C4-O26	1.38954
O26-C27	1.45165
C27-H29	1.08921
H30-C27	1.09641

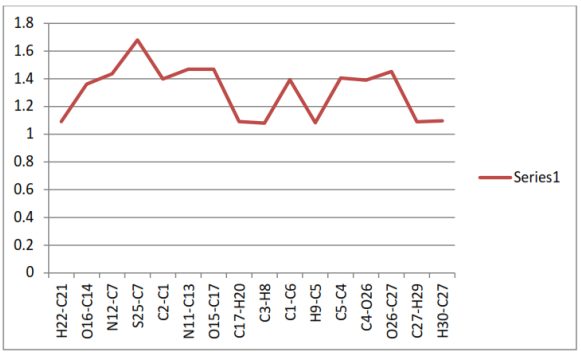

Fig.6 Graph of Bond Length

ATOMS	BOND ANGLE
H22-C12-H24	111.268
H23-C21-O16	107.593
O16-C14-N12	107.413
N12-C7-S25	126.203
C7-N11-C2	109.547
C7-N11-C13	133.889
O15-C13-C17	33.630
H18-C17-H20	111.506
H19-C17-O15	107.120
C2-C1-N12	107.020
C1-C6-C5	118.131
H9-C5-C4	120.628
H8-C3-C4	121.360
C27-O26-C4	118.990
H30-C27-O26	111.294
H28-C27-H29	109.725

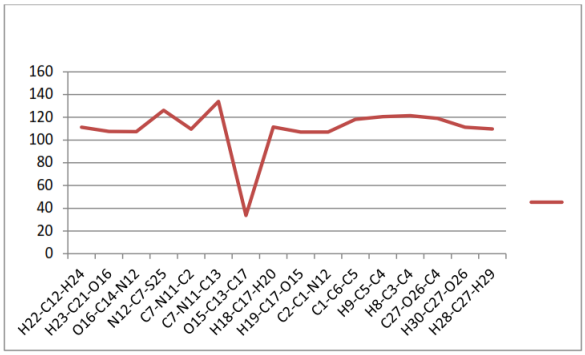

Fig. 7 Graph of Bond Angle

CONCLUSION:

Thus, the Simulation report of1,3-bis-acto-5-substituted benzimidazoline-2-thionesis on progress. It will be reported very soon.

ACKNOWLEDGMENT:

I would like to thank my parents, who push me towards good education.I wish to thank my teachers, They made me enjoy learning new things and take new heights in life. We are very grateful to the DSMNR University Lucknow for the facility provided.

REFERENCES:

1. A. Hegedus, Z. Hell and A. Potor (2006). Synth. Commun., 36, pp. 3625.

2. S.Y. Lin, Y. Isome, E. Stewart, J.F. Liu, D Yohannes and L. Yu (2006). Tetrahedron Lett., 47, pp. 2883.

3. Mumtaz, A.; Saeed, A.; Malik, I. Synthesis, Characterization and Antimicrobial Activities of Mercaptoxadiazoles, Mercaptotriazoles and their Derivatives. J. Chem. Soc. Pak. 2014, 36, pp. 852–857.

4. Liu, X.H.; Zhai, Z.W.; Xu, X.Y.; Yang, M.Y.; Sun, Z.H.; Weng, J.Q.; Tan, C.X.; Chen, J. (2015). Facile and efficient synthesis and herbicidal activity determination of novel 1,2,4-triazolo[4,3-a]pyridin-3(2H)-one derivatives via microwave irradiation. Bioorg. Med. Chem. Lett. 25, pp. 5524–5528.

5. Tan, C.X.; Weng, J.Q.; Liu, Z.X.; Liu, X.H.; Zhao, W.G. (2012). Synthesis, crystal structure and fungicidal activity of a novel 1,2,3-thiadiazole compound. Phosphorus Sulfur Silicon Relat. Elem., 187, pp. 990–996.

6. Liu, X.H.; Weng, J.Q.; Wang, B.L.; Li, Y.H.; Tan, C.X.; Li, Z.M (2014). Microwave-assisted synthesis of novelfluorinated 1,2,4-triazole derivatives, and study of their biological activity. Res. Chem. Intermed., 40, pp. 2605–2612.

7. Liu, X.H.; Xu, X.Y.; Tan, C.X.;Weng, J.Q.; Xin, J.H.; Chen, J. (2015). Synthesis, crystal structure, herbicidal activities and 3D-QSAR study of some novel 1,2,4-triazolo[4,3-a]pyridine derivatives. Pest Manag. Sci., 71, pp. 292–301.

8. Liu, X.H.; Tan, C.X.; Weng, J.Q. (2011). Synthesis, dimeric crystal, and fungicidal activity of 1-(4-methylphenyl)-2- (5-((3, 5-

dimethyl-1H-pyrazol-1-yl) methyl)-4-phenyl-4H-1, 2, 4-triazol-3-ylthio) ethanone. Phosphorus Sulfur Silicon Relat. Elem., 186, pp. 558–564

9. Blaine T. Smith (2014). Brian Luke Seaward. Pharmacology for Nurses. Jones & Bartlett Publishers=year=2014.

10. Murillo A, Vera-Estrella R, Barkla BJ, Méndez E, Arias CF (2015).

11. Tuthill, Tobias J.; Groppelli, Elisabetta; Hogle, James M.; Rowlands, David J. (2010).

12. B.G. Mohamed, A.M. Abdel-Alim and M.A. Hussein, Acta. Pharm., 2006, 56, pp. 31.

13. Rossignol JF (2014). "Nitazoxanide: a first-in-class broad-spectrum antiviral agent". Antiviral Res. 110: pp. 94–103. doi:10.1016/j.antiviral.2014.07.014.

14. Rick Daniels; Leslie H. Nicoll. "Pharmacology - Nursing Management". Contemporary Medical-Surgical Nursing. Cengage Learning, 2011. p. 397.

15. Kisung Ko, Yoram Tekoah, Pauline M. Rudd, David J. Harvey, Raymond A. Dwek, Sergei Spitsin, Cathleen A. Hanlon, Charles Rupprecht, Bernhard Dietzschold, Maxim Golovkin, and Hilary Koprowski (2003). "Function and glycosylation of plant-derived antiviral monoclonal antibody". PNAS. 100: 8013–8018. doi:10.1073/pnas.0832472100. PMC 164704 .

16. X. Jing, Q. Zhu, F. Xu, X. Ren, D. Li and C. Yan, Synth. Commun., 2006, 36, pp. 2597.

17. V.K. Tandon and M. Kumar, Tetrahedron Lett., 2004, 45, pp. 4185.

18. K. Bougrin, A. Loupy, A. Petit, B. Daou and M. Soufiaoui, Tetrahedron., 2001, 57, pp. 163.

19. D.S. VanVliet, P. Gillespie and J.J. Scicinski (2005). Tetrahedron Lett., 46, pp. 6741.

20. Stapleford, Kenneth A.; Miller, David J. (2010)

21. Cook, S.; Moureau, G.; Harbach, R. E.; Mukwaya, L.; Goodger, K.; Ssenfuka, F.; Gould, E.; Holmes, E. C.; de Lamballerie, X. (2009).

22. Schnitzler, P; Schön, K; Reichling, J (2001). "Antiviral activity of Australian tea tree oil and eucalyptus oil against herpes simplex virus in cell culture". Die Pharmazie. 56 (4): 343–7. PMID 11338678.

23. Kunin, Marina; Engelhard, Dan; Thomas, Shane; Ashworth, Mark; Piterman, Leon (15 October 2015). "Challenges of the Pandemic Response in Primary Care during Pre-Vaccination Period: A Qualitative Study". Israel Journal of Health Policy Research. 4 (1).

24. Lindegren, Mary Louise; Griffin, Marie R.; Williams, John V.; Edwards, Kathryn M.; Zhu, Yuwei; Mitchel, Ed; Fry, Alicia M.; Schaffner, William; Talbot, H. Keipp; Pyrc, Krzysztof (25 March 2015).

25. NACCHO (December 2010)

26. Marc A. Fritz; Leon Speroff (28 March 2012)

27. N.A. Hamdy, H.A. Abdel-Aziz, A.M. Farag and Issa M.I. Fakhr (2007). Monatsh. Chem., 138, pp. 1001.

28. Ukrit Jitropas and Chung-Hao Hsu (2017). "Study of the first-principles correlation functional in the calculation of silicon phonon dispersion curves".

29. Richard J. Fitzgerald "A simpler ingredient for a complex calculation"(2016).

30. Michelini, M. C.; Pis Diez, R.; Jubert, A. H. (2016). "A Density Functional Study of Small Nickel Clusters.

31. Somayeh F. Rastegar, Hamed Soleymanabadi (2013). "DFT studies of acrolein molecule adsorption on pristine and Al- doped graphenes".

32. Hanaor, D.A.H.; Assadi, M.H.N; Li, S; Yu, A; Sorrell, C.C. (2012). "Ab initio study of phase stability in doped TiO2".

Corresponding Author

D. B. Singh*

Micromolecular and Biophysics Laboratory, Department of Physics, Dr. Shakuntala Mishra National and Rehabilitation University, Mohan Road, Lucknow