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VIBRATIONAL STUDIES OF 2-PHENYL-4,5-DIHYDRO-1H-IMIDAZOLE

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Abstract: *The ground state vibrations of 2-Phenyl-4,5-dihydro-1H-imidazole were accounted for through investigational and theoretical techniques. The computed optimized properties and vibrational frequencies were correlated with the investigational values with good agreement, indicating good harmony.*

Introduction

In present days, the derivatives of the Imidazole compound found to have NLO properties. Because of the high molar extinction coefficient imidazole is used in metal-free organic dyes. 2-imidazoline is the isomer derivative from imidazole. Imidazole's show the most important biological and pharmacological activities such as anesthetic [1], antidiabetic [2], antihypercholesterolemic [3], antiphlogistic [4], and blood pressure lowering agent [5,6].

The main object of this investigation is to study the geometry, vibrational wavenumbers, UV-Vis absorption spectrum, etc., of 2-Phenyl-4,5-dihydro-1H-imidazole. In this chapter, we characterize and describe the structural parameters and vibrational parameters, of 2-Phenyl-4,5-dihydro-1H-imidazole, both theoretically and experimentally.

Investigational Details

The compound 2-phenyl-2-imidazoline (2PI) was obtained from Sigma Aldrich chemical company and was used as such in the following subsequent spectroscopic

Investigations without any further purification about 302^0 K. The FT-IR spectra are recorded by the KBr pellet method.

Computational details

All the computational details used to perform all the calculations viz., the methods, calculation procedure, software/programs, scaling procedure, obtaining P.E.D.

Results and discussion

The optimized geometrical parameters with a high-level basis set are summarized in Table 5.1 according to Fig 1. A potential energy surface (PES) scan for C3-C4-C5-H15 dihedral angle is performed. The form of the potential energy curve as a The global minimum

energy for the title molecule is computed to be 454.9756695 Hartrees.

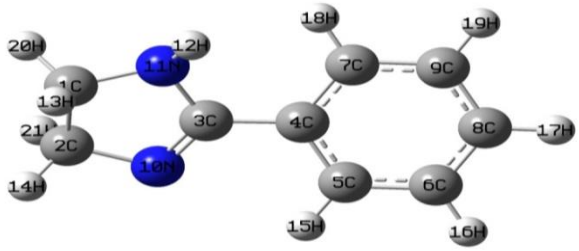

Fig 1: Optimized Molecular structure of 2-Phenyl-4,5-dihydro-1H-imidazole along with numbering of atom

While Experimental crystal data of 2PI is not presented, Experimental data of the reference molecule 2-[2-(2-Hydroxyethoxy) phenyl]-4, 4, 5, 5-tetramethyl-2-imidazoline-1-oxyl 3-oxide [9] was taken for comparison. These deviations may be caused because the theoretical calculations of the compound were executed in the gas phase while investigational calculations were done in the solid state

Vibrational analysis

The title compound is a nonlinear molecule having 21 atoms with Cs symmetry with 57 normal modes of internal vibrations. Total vibrations were active in Raman and IR. The task of assigning vibrational frequencies was done by NCA-normal coordinate analysis. The internal coordinates were identified. We constructed non-redundant local symmetry coordinates as listed in table 5.3 from the guidelines of author Fogarasi [10, 11]. Later computed force fields from the DFT method were transformed to the vibrational coordinates.

Complete analysis with FT–IR experimental frequencies and IR intensities are reported i. All vibrations are active in both IR and Raman. The investigational FT–IR spectra along with the corresponding simulated spectra of 2PI are illustrated in Fig 2.

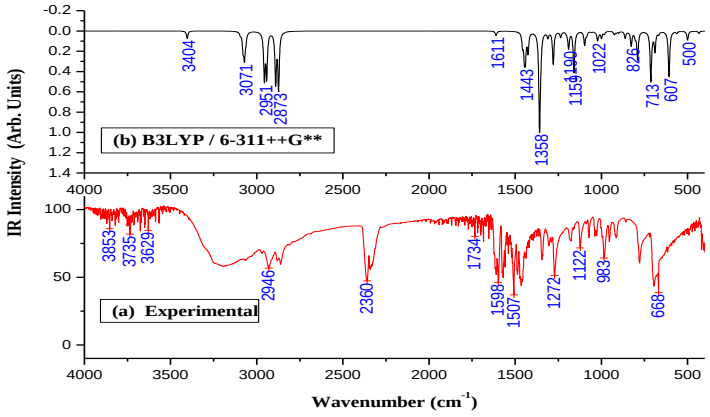

Fig 2: (a) Investigational, (b) Theoretical FT-IR spectra of 2-Phenyl-4,5-dihydro-1H-imidazole

Carbon–Hydrogen Vibrations

Ring structures have acute or average spikes between 3100 – 3000 cm^{-1} [12]. FT Raman band noticed at 3065 cm^{-1} belongs to C-H stretching vibrations of PED percentage 99. The benzene in-plane C-H bending vibrations and their derivatives are observed in the range 1300-1000 cm^{-1} [13]. The computed and experimental frequency 1122 cm^{-1} is distributed to in-plane C-H bending vibration.

Methylene Group Vibrations

The final result is that the IR peak appears broadened, as it is an average of all these slightly different absorptions. For CH_2 group frequencies, the asymmetric vibrations examined 3000 - 2900 cm^{-1} region.The stretching asymmetric vibrations observed at 2842 and 2855 cm^{-1} were compared to a week dip at 2946 cm^{-1} in mid IR spectrograph.

Conclusions

2-Phenyl-4,5-dihydro-1H-imidazole is characterized by vibrational spectroscopic techniques election of enough exchange-correlation functional and basis set.

References

[I] Vizi, E. S. Med. Res. Rev. 1986, 6,431-449.

[2] Le Bihan, G.; Rondu, F.; Pele-Tounian, A.; Wang, X.; Lidy, S.; Touboul, E.; Lamouri, A.; Dive, G.; Huet, J.; Pfeiffer, B.; Renard, P.; Guardiola-Lemaitre, B.; Manechez, D.; Penicaud, L.; Ktorza, A.; Godfroid, J.-J. J. Med. Chem. 1999,42, 1587-1603.

[3] Li, H. Y.; Drummond, S.; De Lucca, I.; Boswell, G. A. Tetrahedron 1996, 52, 11153-11162.

[4] Ueno, M.; Imaizumi, K.; Sugita, T.; Takata, I.; Takeshita, M. Int. J. Immunopharmacol. 1995, 17,597-603.

[5] Schorderet, M. In Pharmacologie: Des Concepts Fondamentaux aux Applications The'rapeutiques; Frison-Roche:Paris, 1992; pp 130-153.

[6] L.M. Rodriguez-Valdez, W. Villamisar, M. Casales, J.G. Gonzalez-Rodriguez, A.Martinez-Villafane, L. Martinez, D. Glossman-mitnik, Computational simulations of the molecular structure and corrosion properties of amidoethyl, aminoethyl and hydroxyethyl imidazolines inhibitors, Corros.Sci. 48 (2006) 4053-4064.

[7] C.A. Gonzalez-Rodriguez, F.J. Rodriguez-Gomez, J. Genesca-Llongueras, The influence of Desulfovibrio vulgaris on the efficiency of imidazoline as a corrosion inhibitor on low-carbon steel in seawater, Electrochim. Acta 54(2008) 86-90.

[8] Contreras, C.D., Montejo, M., Lopez Gonzalez, J.J., Zinczuk, J. and Brandan, S.A. (2011) Journal of Raman Spectroscopy, 42, 108-116.

[9] Jing, L.-L., Ma, H.-P., He, L., Fan, P.-C. and Jia, Z.-P. (2011) Acta Crystallographica Section E, 67, 03503.

[10] P. Pulay, G. Fogarasi, F. Pang, and J. E. Boggs, J. Am. Chem. Soc. IOI (1979) 2550.

[11] G. Fogarasi, X. Zhou, P.W. Taylor, P. Pulay, J. Am. Chem. Soc. 114 (1992) 819I.

[12] Lambert, J.B., Shurvell, H.F., Verbit, L., Cooks, R.G. and Stout, G.H. (1976) Organic Structural Analysis. Macmillan Publ. Co. Inc., New York.

[13] Silverstein, R.M., Basseler, G.C. and Morill, C. (1981) Spectrometric Identification of Organic Compounds. John Wiley and Sons, New York.