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DENSITY FUNCTIONALIZED L-ARGININE: A THEORETICAL STUDY TO SPECULATE THE BIOLOGICAL RELEVANCE OF THE MOLECULE

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ABSTRACT L-Arginine is among the most fascinating compounds being studied in amiono acid chemistry. Because of the involvement in multifacet industrial and medicinal applications, herein we report a schematica optimized frame-work under 63-11G,dp basis set and B3LYP as functional for the respective computation process. The resultant geometries was evaluated to explain the related computational approach of the respective bio-relevant processes. From the study, a well-defined agreement has been found between theoretical and experimental outcomes. Molecular electrostatic potential surfaces were discussed in linking the appropriate hydrophobic and hydrophilic site of the compound.

KEYWORDS : Arginine; DFT; Geometry

Introduction

Amino acids represent important life supporting molecules[1-3]. L-arginine is one of the essential amino acids found in humans. By its involvement in the regulation of nitric oxide synthesis, exhibits responsible role for the vasodilator tone in the regulation of blood pressure and in neurotransmission for the formation of memory. Due to the fact of its biological importance arginine supplements are used at dietary level considerably[4]. In medical field the compound is significant in serving it under physiological stress, for example during recovery from burns, injury, and sepsis, or when the respective biosynthesis is deffective[5-7].

Density functional theory is the most advanced theoretical tool to predict biophysical and chemical properties of known or unknown compounds[8]. Since the compound under study possesses potential role in biological world, hence it seems worthy to present a study on its theoretical speculation of biochemical parameters like stability, reaction tendency and electron density localization[9]. The present work is an effort to report the optimized structural status of the molecule in combination with various biological relevant chemical descriptors.

Methodology applied in the study

First of all the geometric optimization was carried out followed by frequency and energy calculations using Gaussian 09 programme[10,11]. B3LYP functional and 631g(d,p) were the formulae applied. The bands procured from frequency computation were established on normal coordinate analysis. Each frequency value was compared with the real one to confirm that the corresponding geometry is a minimum in terms of potential energy surface analysis. Gauss View 5.0, a graphical visualizer was also intervened to present the shape of the vibrational modes.[12] The molecular orbital approach under computational study helped to explore energies of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels. The molecular electrostatic potential (MESP) energy surface of the molecule under investigation was used for bordering the intermolecular and intramolecular reactive behaviour.[13] In addition to above time-dependant density functional theory (TD-DFT) and atomic charge analysis have been the useful additives to explain the motive of the work.

Results and discussion

Geometry and stability

From the geometrical optimization it can be seen that the observed stereochemistry is the energy minimal state of the compound. The 3-D structure with the respective numerical and color labeling is given in Fig. 1. This is generally confirmed while looking at the frequency results showing the absence of imaginary frequency i.e., no negative value of any band is obtained. By referring to Fig. 2, it is clear that all the vibrational bands lie between 0 and 4000 cm^{-1} without any instability indicating value. Hence explains the stability in the given structural framework[8-11].

Fig. 1: Optimized structure of L-Arginine

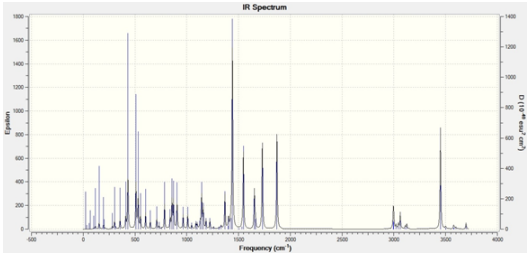


Fig. 2: Theoretical IR spectrum of the compound

Theoretical speculation of biological relevance

For a biomolecule it has always been a subject of great interest to explain the structural and physio-chemical parameters in relation to biological requirement. A compound is always inspected for its lipophilicity, lipophobicity, size, quantity and reactive beahiour. From the optimized figure it can be seen that the terminal Nitrogen (Amine) is 9.7 Å away from hydroxyl type oxygen of carboxylic side (C-OH). From the molecular electrostatic analysis (Fig. 3) it seems that three color regions that are used to present the overall appearance of a molecule in comparison to the rest of universe/biological environment. Red zone is meant for highly electron dense region and blue represents reduction centre, and greenish as intermediate of the two. From the respective analysis it seems that the terminal sites have equal opposite behaviour of this sort and hence could be the reason of its tendency to easily get converted to ammonium ion and carboxylate ion a natural tendency. This can further be explained on the basis of Mulliken charge analysis. The carbon located in COO region is positive along with hydrogen atoms, while rest atoms are negatively charged9,10.

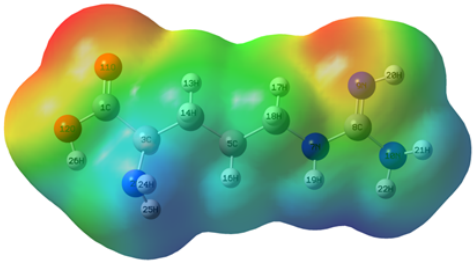
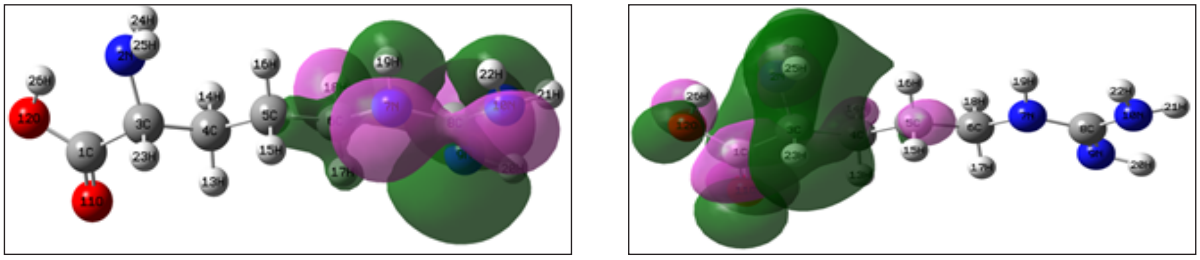


Fig. 3: Electrostatic potential surface of Arginine

The reactive behavior can also be established on MO treatment and respective TD-DFT data. From the MO-diagram HOMO lies at -0.22 and LUMO at -0.01 a.u. The respective TD-DFT data gives 5 to 6 eV excitation probability. Which helps to speculate the coulombic interaction among terminal functional groups. From the HOMO and LUMO appearances of their electron density plots in Fig 4 it again addresses the same to spots for the respective feasibility to get converted to carboxylate ion and ammonium ion.



HOMO LUMO

Fig. 4: MO structure of the compound

Conclusion

From the overall theoretical analysis it is clear that the biophysical parameters can be easily understood by such study for the amino acid under study and all other related class of compound. The study can be though as a useful platform for featuring various physico-chemical parametrization. The further study in relation to its assimilation and protein synthesis can be thought as a future tool for such type of study.

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