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Effect of Na, K, Ca, Mg, Fe and Zn on the Structure and Physical Parameters of Protein

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ABSTRACT

The amino acid alanine is choosen as a model molecule for protein structure. To study the effect of metals upon protein Na, K, Ca, Mg, Fe and Zn were respectively coordinated to alanine through the H-bonding of Carboxyl group. Both Na and K are coordinated with one alanine unit while Ca, Mg, Fe and Zn are coordinated with two alanine units. Calculations are conducted with density functional theory at B3LYP/6-31g(d,p) level of theory. The geometrical parameters are calculated including bond lengths and bond angle of COOH group. The total dipole moment, HOMO/LUMO band gap energy and C=O vibration of COOH group are also calculated. Results indicate that, the bond length L_{C-O} is decreased while $L_{C=O}$ and L_{O-H} are increased, a shift in the characteristic band of carboxyl group (C=O) toward lower wavenumbers is recorded. The total dipole moment and band gap energy are changed. It could be concluded that the studied elements are changing both the structural, Physical and vibrational characteristics of protein.

Keywords: Protein, Alanine, COOH, B3LYP/6-31g(d,p)

INTRODUCTION

Although semiempirical methods are fast there are other approximate quantum mechanical methods which were developed to study organic molecules. The parameters of this model are calculated from density functional theory and known as Self-Consistent Charge and Density-Functional Tight-Binding (SCCDFTB) method [1-3]. Amino acids are special class of organic molecules. There are 20 different standard L-α-amino acids used by cells for protein construction. Amino acids, contain both a basic amino group and an acidic COOH group [4]. Alanine is one of the simplest α-amino acids, it is classified as an aliphatic amino acid. It is worth to mention that, the methyl group of alanine never directly interfered in protein function [5-8]. Both experimental and DFT calculations were conducted to study molecular structure and vibrational spectra of nonlinear optical crystal L-alanine cadmium chloride [9].

Carboxyl group are one of the most important functional group which dedicate it for many studies [10,11]. Many structures containing carboxyl group were subjected to both theoretical and experimental study [12].

Molecular modeling was supporting FTIR to study the molecular structure of protein [13]. The effect of heavy metals on protein structure was elucidated with molecular modeling calculations and FTIR spectroscopy [14]. Interaction between metal and amino acids continue to be a topic of research work worldwide according to its wide range of applications [15-17].

In the present work B3LYP/6-31g(d,p) was utilized to optimize alanine then alanine interacted with Na, K, Ca, Mg, Fe and Zn respectively. The total dipole moment, HOMO/LUMO band gap energy and vibrational characteristics were calculated at the same level of theory.

COMPUTATIONAL DETAILS

The geometries of alanine; alanine-Na; Alanine-Ca-Alanine; Alanine-Mg-Alanine; Alanine-Fe-Alanine and Alanine-Zn-Alanine were built as indicated in Figure 1. The studied model molecules were optimized with Gaussian 09 soft code at Spectroscopy Department, National Research Centre [18]. The calculations were conducted with density functional theory at B3LYP/6-31g(d,p) quantum mechanical level [19-21]. Vibrational spectra were calculated at the same level of theory.

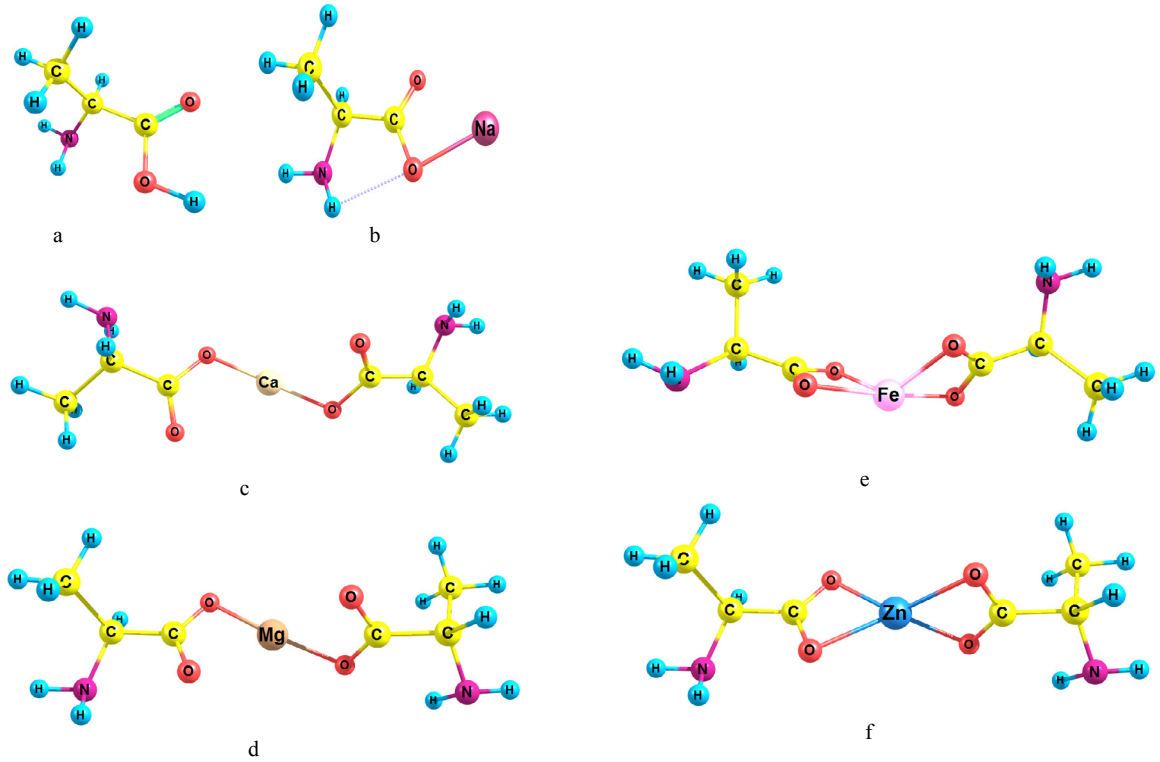

Figure 1: B3LYP/6-31g(d,p) calculated optimized structures for a-alanine; b-alanine-Na; c-Alanine-Ca-Alanine; d-Alanine-Mg-Alanine; e-Alanine-Fe-Alanine; f-Alanine-Zn-Alanine

RESULTS AND DISCUSSION

Amino acid which is used as a model molecule in the present study is alanine which is an α-amino acid that is used in the biosynthesis of proteins. The interaction between metals and alanine is supposed to happen through the hydrogen bonding of COOH group. Figure 1 presents the calculations of B3LYP/6-31g(d,p) optimized structures for alanine whereas it interacts with Na while it requires two hydrogen bondings for interaction with Ca; Mg; Fe and Zn as indicated in the figure.

The change in the geometry of COOH as a result of interaction is recorded in terms the bond lengths L_{C-O}; $L_{C=O}$; L_{O-H} and bond angle C-O=C as shown in Table 1. COOH of alanine shows L_{C-O}; $L_{C=O}$; L_{O-H} and C-O=C parameters as respective values 1.3575, 1.2095, 0.9720, 122.6. As far as Na is interacted with alanine through the H-bonding of COOH L_{C-O} is decreased while $L_{C=O}$ is increased.

As divalent alkalies like Ca and Mg interact with two alanine units the same behaviour took place a decrease in the L_{C-O} bond length with an increased in the $L_{C=O}$ bond length. Regarding heavy metals Fe and Zn one can observe the same behaviour such as other studied metals.

The bond length L_{O-H} is increased corresponding to the interaction between metals and alanine. The bond angle C-O=C is increased as Na, K interacted with alanine then remain unchanged corresponding to Ca and Mg then decreased corresponding to Fe and Zn.

Table 2 presents the B3LYP/6-31g(d,p) calculated physical parameters for the studied structures including total dipole moment (TDM) HOMO/LUMO band gap energy (ΔE) and the C=O vibration of carboxyl group. The calculated values in case of alanine were 2.5578, 6.8200 and 1855.4 respectively.

TDM is increased as a result of Na and K interaction then decreased corresponding to the other divalent metals. ΔE is decreased as a result of interaction with Na, K, Fe and Fe respectively. The decrease is slightly in case of Ca (5.3664 eV) and were very small for Mg and Zn 6.3765 eV; 6.3311 eV. It is stated earlier that both total dipole moment and band gap energy are reflecting the reactivity of a given structure [22,23]. For reactive compound its total dipole moment is high while its band gap energy is low. These two physical quantities measure the reactivity of a given compounds when it interacts with their surrounding molecules.

Regarding the vibrational characteristics which recorded in terms the C=O characteristic band of carboxyl group.

Table 1: B3LYP/6-31g(d,p) calculated optimized parameters for the studied structures including the bond lengths L_{C-O}; $L_{C=O}$; L_{O-H} and bond angle C-O=C

Structure	L_{C-O}	$L_{C=O}$	L_{O-H}	C-O=C
Alanine	1.3575	1.2095	0.972	122.6
Alanine-Na	1.2736	1.2695	2.1857	124.2
Alanine-K	1.2713	1.2666	2.5249	125.2
Alanine-Ca-Alanine	1.2745	1.2778	2.3401	122.3
	1.2778	1.2745	2.3414	122.3
Alanine-Mg-Alanine	1.27755	1.27985	2.0211	119.6
	1.2799	1.2775	2.022	119.6
Alanine-Fe-Alanine	1.2896	1.2686	1.915	116.5
	1.2871	1.2708	1.9116	116.5
Alanine-Zn-Alanine	1.2777	1.2761	2.0088	118.9
	1.2761	1.2776	2.0043	118.9

Table 2: B3LYP/6-31g(d,p) calculated physical parameters for the studied structures including total dipole moment (TDM) HOMO/LUMO band gap energy (ΔE) and the C=O vibration of carboxyl group

Structure	TDM	ΔE	$C=O_1$	$C=O_2$
Alanine	2.5578	6.82	1855.4	-
Alanine-Na	5.7571	4.0677	1606.1	-
Alanine-K	7.8511	3.9177	1614	-
Alanine-Ca-Alanine	1.2458	5.3664	1593.8	1593.6
Alanine-Mg-Alanine	1.4741	6.3765	1579.6	1579.4
Alanine-Fe-Alanine	1.9081	3.8967	1585	1561.1
Alanine-Zn-Alanine	1.5316	6.3311	1581.6	1581.4

The characteristic band was shifted toward lower wavenumber as a result of interaction this was noticable for all the studied metals.

CONCLUSION

Monovalent and divalent elements are supposed to interact with alanine through the hydrogen bonding of COOH. Although Ca, Mg, Fe and Zn are divalent but their cooridation with the two alanine units are different. Both Ca and Mg show bidentate coordination while Fe and Zn shoe bidentate cooridation. The geometry of the studied amino acid is changed as one bond length is decreased (L_{C-O}) while other bond lenthgs are increased ($L_{C=O}$ and L_{O-H}) with a change in the bond angle C-O=C. The change in the geometrical parameters are followed with a shift in the characteristic band of carboxyl group which shift the C=O toward lower wavenumbers. Both the total dipole moment and HOMO/LUMO band gap energy are changed as a result of interaction between the studied metals and the studied amino acid.

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