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KASTAMONU UNIVERSITY
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GLYCINE-CARBON NANO RING INTERACTIONS: A DFT STUDY

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MASTER OF SCIENCE
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APPROVAL

The thesis study entitled "**Glycine-Carbon Nano Ring Interactions: A DFT Study**" submitted by **Abeer I. Soulman ABDULRAHIM**, has been argued in front of the following examining committee members and accepted as **THE DEGREE OF MASTER OF SCIENCE in Physics Department,** The Graduate School of Natural and Applied Sciences in Kastamonu University by unanimity/majority of votes.

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COMMITMENT

All information in this thesis have written according to the ethical behaviour and academic regulations of Kastamonu University, in addition what does not belong to me in this study was prepared in accordance with the rules of thesis in Kastamonu University, all kinds of statements and reports writing that fully referenced to the source of knowledge and commitment.

Signature
Abeer I. Souliman Abdulrahim

ÖZET

Yüksek Lisans Tezi

GLİSİN-KARBON NANO HALKA ETKİLEŞİMLERİ: BİR DFT ÇALIŞMASI

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Bu tez çalışmasında Glisin molekülünün Karbon nano halka (C_{12}) ve halkalarıyla olan etkileşimi teorik olarak incelenmiştir. Glisin molekülünün temel durum optimize geometrisi Yoğunluk Fonksiyonel Teorisi (DFT) ile B3LYP metodu ve 6-311G baz seti kullanılarak hesaplanmıştır. Sınır molekül orbitalleri (Frontier molecular orbitals-FMOs), bant aralığı enerjileri, uyarılma enerjileri, dalga boyları, salınım frekansları, dipol moment, kimyasal sertlik, kimyasal yumuşaklık ve elektronegativite gibi kimyasal reaktivite parametreleri aynı yöntem ve baz seti kullanılarak elde edilmiştir. UV ve IR hesaplamalarının yanı sıra HOMO-LUMO ve Elektrostatik potansiyel (ESP) yüzeyleri çizilmiş ve reaksiyonun yapısı aydınlatılmaya çalışılmıştır. Elde edilen tüm veriler detaylı bir şeklide incelenerek yorumlanmıştır.

Anahtar Kelimeler: Glisin, Yoğunluk Fonksiyonel Teorisi (DFT), Karbon Nano Halka.

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ABSTRACT

MSc. Thesis

GLYCINE-CARBON NANO RING INTERACTIONS: A DFT STUDY

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Abstract: In this thesis, the interaction of Glycine molecule with Carbon nano ring (C_{12}) and rings was theoretically investigated. The ground state optimized geometries of the glycine molecule was calculated using the B3LYP method and the 6-311G base set with Density Functional Theory (DFT). Chemical reactivity parameters such as frontier molecular orbitals (FMOs), band gap energies, excitation energies, wave lengths, oscillation frequencies, dipole moment, chemical hardness, chemical softness and electronegativity were obtained using the same method and base set. In addition to UV and IR calculations, HOMO-LUMO and Electrostatic potential (ESP) surfaces were drawn and the structure of the reaction was elucidated. The all obtained data are analyzed and interpreted in detail.

Key Words: Glycine, Density Functional Theory (DFT), Carbon Nano Ring.

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Abeer I. Souliman ABDULRAHIM

Kastamonu, 01.2017

CONTENTS

SYMBOLS and ABBREVIATIONS INDEX

a.u : Atomic Unit
DFT : Density Functional Theory
EV : Electron Volt
$E(_{HOMO)}$: HOMO Energy
$E(_{LUMO)}$: LUMO Energy
ESP : Electrostatic Potential
HOMO : High Occupied Molecular Orbital
LUMO : Low Unoccupied Molecular Orbital
χ : Electronegativity
η : Chemical Hardness
σ : Chemical Softness
$\mathcal{E}$: Epsilon

FIGURE INDEX

TABLE INDEX

GRAPHICS INDEX

1.INTRODUCTION

Amino acids are highly biologically important organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups. In the nature, approximately 500 kinds of amino acids are known. Amino acids are formed by the combination of peptide or polypeptide chains.

Proteins contain only 20 kinds of amino acids. However, 10 of these 20 amino acids can be produced in the human body, while others can be obtained from the foods. Amino acids in the protein form are the second largest component of human muscles, cells and other tissues [1]. All the chemical reactions that occur in the human body depend on the amino acids and proteins. Proteins are generally shown in three-letter abbreviations, for convenience, as in the following table (Table 1.1).

Table.1.1. *Names of natural 20 amino acids, and chemical definitions of their side chains.*

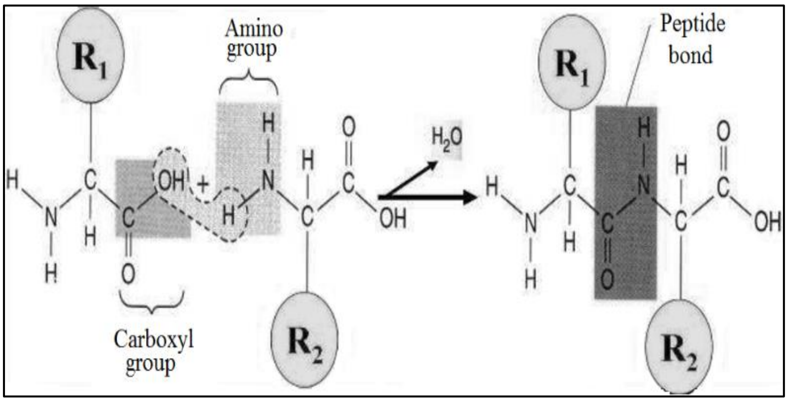
Group	Full Name	Three-letter Name	One-letter Name	Side-Chain Group
Nonpolar	Glycine	Gly	G	–
	Alanine	Ala	A	Methane
	Valine	Val	V	Propane
	Leucine	Leu	L	2-Methyl-propane
	Isoleucine	Ile	I	Butane
	Proline	Pro	P	Pyrrolidine
	Methionine	Met	M	(methyl-sulfanyl)ethane
Polar-Neutral	Serine	Ser	S	Methanol
	Threonine	Thr	T	Ethanol
	Cysteine	Cys	C	Methanethiol
	Asparagine	Asn	N	Acetamide
	Glutamine	Gln	Q	Propanamide
Electrically Charged	Glutamate	Glu	E	Propanoate
	Sspartate	Asp	D	Acetate
	Lysine	Lys	K	Butan-1-amine
	Arginine	Arg	R	1-propyl-guanidine
	Histidine	His	H	4-methyl-1H-imidazole
Aromatic	Phenylalanine	Phe	F	Methyl-benzene
	Tyrosine	Tyr	Y	4-methyl-phenol
	Tryptophan	Trp	W	3-methyl-1H-indole

Protein is derived from the Greek word "proteios" and means "in the forefront". Proteins are highly complex molecules that are actively involved in the most fundamental and most important aspects of life. For this reason, the science of protein is at the center of biological research, and has even been applied to medicine, agriculture, biotechnology and even battlefields [2].

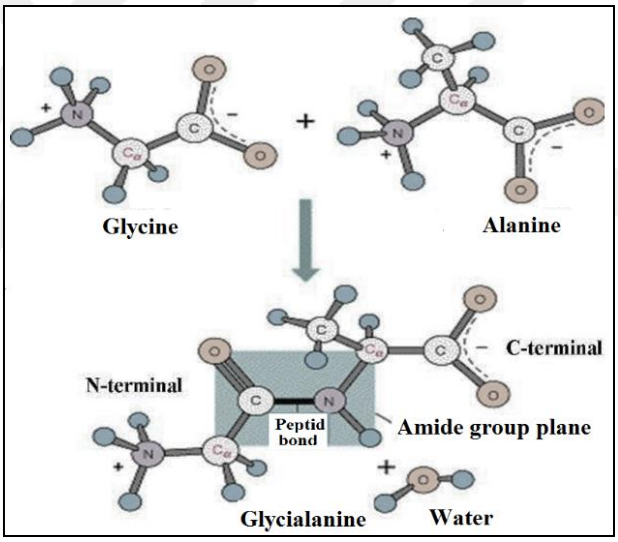
Proteins are molecules that are necessary for the smooth functioning of all the cells in our bodies. A Protein, in the human body, is the most common compound after water, and it is an organic molecule that constitutes about 20% of the body and about 50% of the dry weight of the cell. Approximately 78-80% of the dry weight of liver, muscle and kidney tissue is protein. Proteins play a crucial role in almost all of our cells' functions.

Every protein in the body has its own unique functions. Proteins have many functions such as food storage, biological catalysis, body structure and movement, growth, self-repair, defense system and communication etc. Proteins also act as chemical information carriers (neurotransmitters) throughout the nervous system and contribute to the transport of oxygen in the body. Proteins contain carbon (50%), oxygen (23%), nitrogen (16%) and hydrogen (7%) as well as small amounts of sulfur (0-3%), phosphorus (0-3%), iron, zinc and copper. Proteins can usually be isolated as pure crystals [2].

Amino acids combined with peptide bonds to form proteins. Proteins can also occur from a single polypeptide chain or in multiple polypeptide chains. According to the number of amino acids, they are expressed as dipeptide, tripeptide, hexapeptide, oligopeptide, polypeptide. The peptide bond occurs between the carboxyl group of the first amino acid and the amino group of the adjacent amino acid. Carbonyl oxygen and the hydrogen of the amino group is in the transposition: the one above the peptide plane and the other below. The peptide bond is partially double-bonded, and the carbonyl oxygen is negatively charged when the amino nitrogen is positively charged.



The number of amino acids in each protein is constant. Proteins can be built up from a polypeptide chain or from a large number of polypeptide chains. The amino acids in the proteins are monomeric and therefore proteins are polymers [3].



If the proteins are classified according to their functions [3]:

- Catalytic Proteins
- Carrier and Storage Proteins
- Proteins responsible for Coordinated Motion
- Mechanically supportive proteins
- Immune protective proteins
- Proteins responsible for nerve impulse generation and transmission
- Growth-Responsible Proteins (regulator proteins)

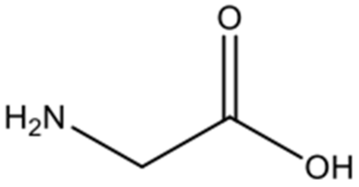
The proteins are structurally separated into four different classes:

(i) Primary structure,
(ii) Secondary structure,
(iii) Tertiary structure,
(iv) Quaternary structure.

Glycine: Glycine is the simplest molecule and the only amino acid that has no asymmetric carbon atom. And was first isolated from gelatin in 1820. It is also found in silk fibrils. Also the glycine does not show a hydrophobic or hydrophilic property. Glycine does not participate in hydrophobic interactions because it has a very short (almost absent) side chain [4].

Except for the glycine amino acid, the carbon atoms of all other amino acids are asymmetric. While the other amino acids exhibit optical activity, the glycine is not an optically active molecule because of this property. In addition, glycine can give flexibility in the region it is in, so they are more common in the rotation regions of the proteins [5].

Glycine can be synthesized by the organism. *Serin* (another amino acid) and glycine can be converted into each other. Another important feature of the glycine is that it combines with benzoic acid and some other acids and thus plays a role in detoxification mechanism. Besides, the glycine, cysteine and flutamin are combined with foreign substances, and make them harmless for the organism. Such substances are called conjugation agents [2].



2-aminoacetic acid

Chemical Formula : $C_2H_5NO_2$
Molecular weight : 75,07 g/mol
Elemental analysis : C, %32,00; H, %6,71; N, %18,66; O,%42,63

Figure 1.1. Glycine molecule.

Glycine is required for protein and nucleic acid synthesis. In addition, Glycine amino acid must be present in the body for absorption of the calcium. Glycine also helps to delay muscle degeneration. It is found in high amounts in the prostate fluid and is important for prostate health. Glycine amino acid is used in the treatment of hyperactivity, in manic depression and in the prevention of epileptic seizures. It also shows a function as a neurotransmitter inhibitor in the nervous system.

Glycine has many applications. Some of these can be ordered as follows:

- It can be used for organic synthesis and biochemical analysis.
- It can be used as a buffer to prepare tissue culture media and to test copper, gold and silver.
- It is used in the treatment of myasthenia gravis and progressive muscle atrophy, hyperacidity, chronic enteritis and hyperprolineemia in children.
- It can reduce irritation when used with aspirin; It can be used in the treatment of hyperprolineemia in children.
- Glycine is used especially as a nutritional additive ingredient in chicken feed.
- It is used together with Alanine for alcoholic beverages; the addition amount: 0.4% for grape wine, 0.2% for whiskey, 1.0% for champagne.
- It has inhibitory effects on Bacillus subtilis and E. coli.
- Glycine has amphiprotic ions containing amino and carboxyl groups, so it has a strong buffering property for salt and vinegar.

- The storage time is increased by 3 to 4 times by adding butter, cheese and margarine.
- Glycine can also be used as a raw material for synthesis such as threonine amino acids.
- Glycine, also known as amino acetic acid, is also used in a variety of industries such as fertilizers, pharmaceuticals, food additives and spices.
- It can be used as pH adjuster in other industries, added to coating solution or used as raw material for other amino acids.
- It can also be used as biochemical reagents and solvents in organic synthesis and biochemistry.
- It can be used as a solvent for carbon dioxide removal in the fertilizer industry. In addition, it can be used as a pH adjusting agent and can be used to prepare the coating solution.
- Glycine can be used as biochemical reagents for drug, food and feed additives; it can also be used as a non-toxic carbon-removing agent in the fertilizer industry [6].

2. THEORETICAL SECTION

2.1. Atom Clusters And Ring Structures

Works on the clusters started in 1950 and accelerated in the 1970s. With the development of computer technology, and therefore the efficient use of theoretical calculations, it has become easier to examine clusters containing large numbers of atoms. The geometry, electronics and vibration properties of the clusters consisting of hundreds of atoms can be calculated by computers. So, experimental methods such as photoelectron spectroscopy (PES), trapped ion electron diffraction (TIED) and infrared spectroscopy can be compared with the theoretical data [7-11].

Evaporation of graphite by the laser causes the formation of carbon clusters. Depending on the size of the cluster, the structures such as linear chains, rings, bowls, plates, and cages can be formed. Very small clusters such as C2 and C3 are linear chains, and the rings are formed in larger sizes. The carbon rings are stable in the in the range of C_6-C_{30}, but slight changes can be seen according to the experimental conditions. In higher dimensions, high-energy ESP hybridized clusters begin to turn into sp2 hybridized forms such as the plates and cages. Thus, the fullerens, which are highly interested in the scientific world, occurs. The ring structures are relatively stable, but monocyclic rings are more stable than other ring configurations [12].

Also, small size carbon structures are highly reactive in the gas phase, and for this reason, their preparation and analysis is difficult. Difficulties in making experiments on highly reactive clusters and conflicting experimental results challenge theory. Numerous theoretical calculations have been made on atomic clusters up to 10", focusing on the relative energies of the ring and chain isomers. However, the calculations on the larger clusters have presented great difficulties. For this reason only a small number of C isomers containing only 10-30 atoms have been studied [13].

The questions about the structure of small carbon clusters have a historical origin dating back to the first days of molecular quantum mechanics and spectroscopy. The basic assumption in these studies was that neutral clusters smaller than C10 are linear conjugate chains having an electronic structure and stability with sharp double/single transition. While it was estimated that the even numbered pellets were open shelled and had a high electron affinity, single-numbered pellets were closed shells, and their electron affinity was expected to be quite low. Researches have shown that that single or even atomic arrangement of linear carbon chains have caused differences in their electronic structures. Odd-numbered atom clusters exhibits lower electron affinity than even numbers [14].

The discovery of carbon fullerenes and carbon nanotubes has opened up material research for practical applications. Unfortunately, the studies for understanding the structural and electronic properties of the carbon nanostructures is not at a satisfactory level. The experiments have shown that semi-dimensional structures such as chains and rings are among the major preliminary elements in the formation of fullerenes and nanotubes. However, because of their complex nature, there are great difficulties in understanding their characteristics and behavior [15].

2.2. Density Functional Theory (DFT)

Density functional theory is a very powerful theory and has come to the forefront in recent years as a method that yield fairly accurate results at low cost. For example, in calculations of bonding energy of molecules and the band structure of solids have been used frequently. Besides, there are applications, even in areas that are thought to be farther away from quantum mechanics, such as biology and mineralogy. The DFT calculations have taken an important place in many branches of science such as superconductivity, classical fluids and magnetic properties of alloys. However, some approaches are necessary to apply the theory, and results can be obtained with fairly variable accuracy. For this reason, in a certain system class, calibration studies are required to determine truth [16].

In the quantum mechanics, all information of system is contained in the wave function Ψ. This wave function is calculated by the Schrödinger equation. For an electron moving at potential $V(\boldsymbol{r})$, Schrödinger equation is given by

$$\left[-\frac{\hbar^2\nabla^2}{2m}+V(\boldsymbol{r})\right]\Psi(\boldsymbol{r})=\varepsilon\Psi(\boldsymbol{r}) \tag{2.1}$$

This expression, for many-body systems, is given below

$$\left[\sum_i^N\left(-\frac{\hbar^2\nabla_i^2}{2m}+V(\boldsymbol{r_i})\right)+\sum_{i<j}U(\boldsymbol{r_i},\boldsymbol{r_j})\right]\Psi(\boldsymbol{r_1},\boldsymbol{r_2},\dots,\boldsymbol{r_N})=E\Psi(\boldsymbol{r_1},\boldsymbol{r_2},\dots,\boldsymbol{r_N}) \tag{2.2}$$

Where N is the number of electrons and $U(\boldsymbol{r_i},\boldsymbol{r_j})$ is the electron-electron interaction. The Schröodinger equation determines the wave function Ψ y and then finds the expected values of the operators with this wave function and calculates their observability. One of the observable calculated in this way is the particle density given as:

$$n(\boldsymbol{r})=N\int d^3r_2\int d^3r_3\dots\int d^3r_N\,\Psi^*(\boldsymbol{r},\boldsymbol{r_2},\dots,\boldsymbol{r_N})\Psi(\boldsymbol{r},\boldsymbol{r_2},\dots,\boldsymbol{r_N}) \tag{2.3}$$

Many powerful methods have been developed to solve the Schrödinger equation. For example, in chemistry, while the configuration interaction (CI) methods based on the systematic expansion of Slater determinants are often used, the diagrammatic perturbation theory is used in the physics. There are also other special techniques. The problem of these methods is that it is difficult to effectively apply them to large and complex systems. For example, for calculations of a system with 10 electrons, it is necessary to use an account set that is 1034 times more than an electronically system set [16].

3. MATERIALS AND METHODS

In this study, the interaction of the 12-atom carbon nano-rings with the glycine molecule was calculated using the Density Functional Theory (DFT). Becke three-parameter hybrid functional combined with Lee-Yang-Parr correlation functional (B3LYP) method with 6-311G base set were used for the calculations. All the calculations in the study were made by using the Gaussian 09 [17] software. The UV and IR spectral analyzes of each system were performed by using stable structures obtained from optimization of the molecules.

In addition, the highest occupied molecular orbital-HOMO and lowest unoccupied molecular orbital-LUMO surfaces of the systems were obtained. These orbitals are also called Frontier Molecular Orbitals (FMOs) and are used to describe reactivity, in a simple way. When a molecule gives an electron, this electron is separated from the HOMO, and on the contrary, when the molecule takes an electron, this electron gets into LUMO. So, we can say that the electrons in the highest energy molecular orbital HOMO are the first electrons to break during ionization. If there is no relaxation process, we can reach the conclusion that the ionization energy is $-E_{\mathrm{HOMO}}$ and the electric charge is $-E_{\mathrm{LUMO}}$.

As a part of this thesis, the molecular electric potential surfaces (or electrostatic potential-ESP) energy maps of the Glycine-carbon nano-ring interaction were also obtained. ESP maps are a three-dimensional representation of the charge distributions of molecules in general terms. Electrostatic potential maps are very useful for three-dimensional diagrams of molecules. It allows us to visualize the charge distributions of molecules and to understand the properties of molecules in terms of the charge distribution. It also contributes to visualizing the size and shape of the molecules. Electrostatic potential maps have a very important role in predicting the behavior of complex molecules in the organic chemistry. The first step in creating an electrostatic potential map is to calculate the electrostatic potential energy.

Advanced computer programs calculate the electrostatic potential energy at a certain distance from the nuclei of the molecule. Electrostatic potential energy can be defined as a measure of the power of the charge, the nuclei and the electrons in a certain location. To analyze the charge distribution of a molecule correctly, the electrostatic potential energy must be calculated in very large quantities. One of the best ways to analyze this data is to visually represent it, as the electrostatic potential map. In order to facilitate the interpretation of electrostatic potential energy data, the red (for the lowest electrostatic potential energy value) and the blue (for the highest electrostatic potential energy value) color spectra are used to demonstrate the varying intensities of the electrostatic potential energy values.

In the later stages of the study, the values of the energy gaps, chemical hardness (η), chemical softness (σ) and electronegativity (χ) were also calculated by using the HOMO-LUMO energies. The chemical hardness mentioned above is one of the most useful concepts, allowing scientists (especially chemists) to understand the reaction data without supercomputers and databases. Although it was originally developed as an intuitive and qualitative concept, it is now a quantity accepted by quantum chemistry. In many experimental and theoretical studies, chemical hardness is considered as a useful theoretical descriptor and there are many important applications of this concept.

Besides, chemical hardness, after chemical potential, is seen as the most important concept in describing chemical reaction rates of atoms and molecules. Chemical stiffness is defined as the resistance to changing the electron cloud density of a chemical system. Chemical softness is defined as the opposite of chemical hardness, which means that the chemical hardness tends to be maximum when the chemical hardness approaches zero. Electronegativity is a chemical property that defines the tendency of an atom or a functional group to attract electrons towards it. Within the scope of this study, these properties were calculated and interpreted for the structures being investigated. In this study, these properties are calculated and interpreted for constructions. In this study, these quantities are calculated and interpreted.

3.1. Quantum Chemical Calculations

In this thesis study, the DFT approach was used to investigate the interaction of the Glycine molecule with the carbon nano rings. The UV-Vis and IR spectral analyzes were performed, HOMO-LUMO and ESP maps were created and some chemical parameters were obtained by using DFT. All calculations were performed by the Gaussian09 program. Details of the calculations are given in the next section.

3.2. Calculation Method

In this study, ground state geometries, IR and UV-Vis spectra of the structures were investigated by DFT and TD-DFT methods. Firstly, a quick preliminary calculation using G3LYP/3-21G and B3LYP/6-31G was made for the geometry optimization of the glycine molecule. Then ground state geometry with the lowest energy value was obtained by using B3LYP method and 6-311G basis set.

Similar calculations for the charge of -1 and +1 were also made using the same method and base set. The UV-Vis and IR spectra of the glycine molecule were obtained using the same functional and basis set. UV-Vis and IR calculations were also performed in gas phase and $nstate = 60$ was used. As a result of UV and IR calculations, absorption wave length (λ) and oscillation strength were obtained.

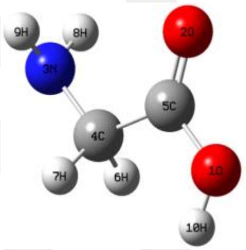
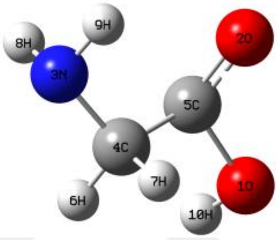
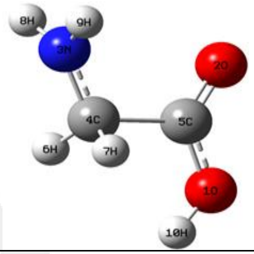
Moreover, a carbon nano ring with 12 atoms was optimized directly using the B3LYP method and 6-311G basis set without any geometry constraint, and as a result of the optimization, it was observed that the ring structure was observed in the planar ring geometry. It should be noted that carbon nano rings designed using 10 and 11 carbon atoms are not able to maintain symmetrical ring properties after optimization. The interaction of the glycine molecule with the 12-atom carbon nano-ring was investigated in two parts. In the first step, a single ring was used to study the interaction of the glycine molecule with the carbon ring.

The geometric optimization of the interaction was also performed by the same method and basis set. In order to analyze the properties of the interaction, the geometry obtained from the optimization is used for UV and IR calculations. The UV and IR calculations were performed to analyze the interaction glycine with carbon ring, and it was used the optimized geometry in the calculation. Two carbon nano rings were used in the second step of the carbon ring-glycine interaction study, where the glycine molecule was placed between two carbon nano rings parallel to each other. Geometry optimization, UV and IR spectrum calculations were also made in a similar way for this structure.

4. RESULTS AND DISCUSSION

The geometry optimization with lowest energy of the glycine molecule was carried out in the gas phase using the B3LYP method with 6-311G basis set. The energy values, the dipole moments, the bond lengths and bond angles between the atoms of the geometric structure of the optimized Glycine molecule are given in detail in Table 4.1. In the table, three different structures are given according to the charge values of the glycine molecule (charge: neutral, -1 and +1).

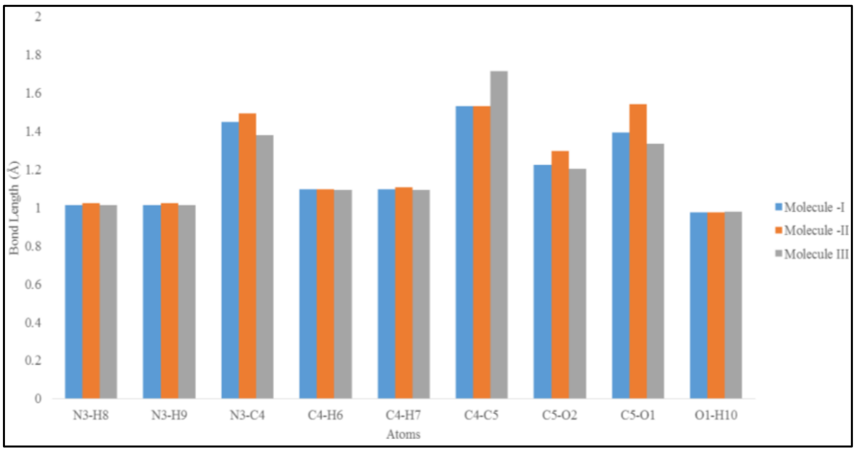
Table 4.1. *Energy, dipole moment and geometric parameter values of the optimized Glycine: charge 0, -1 and 1, respectively.*

	Molecule -I	**Molecule -II**	**Molecule -III**
Optimized structures			
Energy (au)	-284.40064810	-284.36456517	-284.06856996
Dipole moment (Debye)	3.4532	3.5127	6.4253
Atoms	**Bond lenght (Å)**		
N3-H8	1.0109	1.02371	1.0136
N3-H9	1.0109	1.0225	1.0136
N3-C4	1.4481	1.4914	1.3785
C4-H6	1.0946	1.0939	1.0899
C4-H7	1.0946	1.1061	1.0899
C4-C5	1.5299	1.5312	1.7144
C5-O2	1.2211	1.2952	1.2003
C5-O1	1.3909	1.5413	1.3329
O1-H10	0.9750	0.9753	0.9772
Atoms	**Bond angle (°)**		
H8-N3-C4	113.830	107.528	121.60
H9-N3-C4	113.830	105.330	121.60
N3-C4-H6	109.296	108.986	112.07
N3-C4-C5	115.488	112.094	114.91
N3-C4-H7	109.293	112.094	112.07
H6-C4-H7	105.973	107.327	113.33
H6-C4-C5	108.182	111.800	101.85
O2-C5-O1	119.653	114.824	127.00
O2-C5-C4	125.011	117.085	121.03
C5-O1-H10	113.474	105.374	121.60

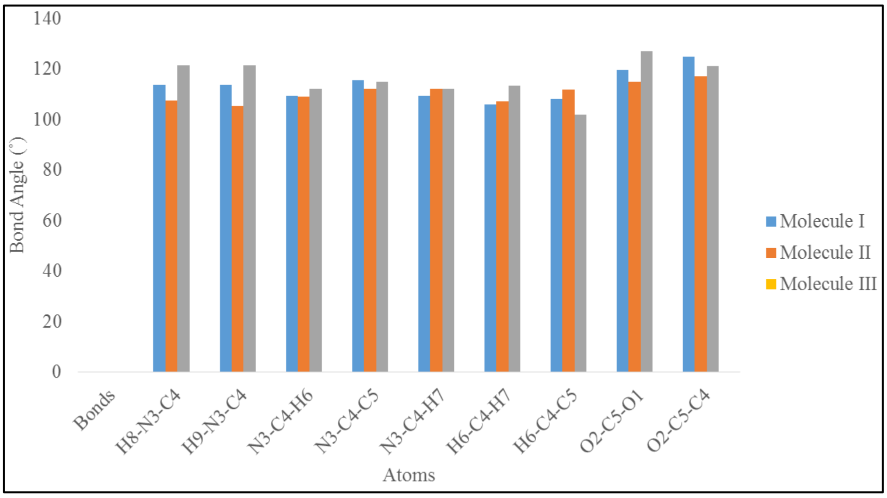
As a result of calculations, some differences were emerged due to the change in charge values. The lowest energy value was observed in Molecule I (-284.4006 au) where the charge was zero (neutral). The highest energy value was observed in Molecule III (-284.06856996 au) where the charge was +1. The increase or decrease in the number of electrons in the system naturally also caused a change in the dipole moment values. There is a great difference (about twice) between the dipole moments of molecule I and molecule III. The Energy and Dipole moment values of the calculations of Molecule II with charge of -1 were generally close to the results obtained by Molecule I.

The bond length between the C4 atom, which we can call the central carbon atom, and the nitrogen (N3) atom showed changes for different values of the charge. The bond length between N3 and C4 was calculated as 1.4481, 1.4914 and 1.3785 A^o, respectively (Table 4.1). When the bond lengths between C4-N3, C4-C5, C5-O2 and C5-O1 atoms were examined, the maximum bond lengths were observed in Molecule II compared to other molecules. When the bond angles of the molecules are examined, it is seen that the bond angles between the N3-C4-C5 atoms are the largest for Molecule I and the smallest for Molecule III.

For bond angles containing oxygen atoms (O2-C5-O1), the oxygen atom has a high electron affinity, while the Molecule III has the greatest angle, and Molecule II has the smallest angle. Molecule III has the largest, and Molecule II has the smallest angle for O2-C5-C4. In (Graphs 4.1 and 4.2), bond lengths and bond angles of selected atoms of the Glycine molecule are given.



Graphic 4.1. Calculated bond lengths of structures MI, MII and MIII.



Graphic 4.2. Calculated bond angle of structures MI, MII and MIII.

When bond lengths and bond angles between the atoms of the molecules are compared, it was generally observed that the atoms of Molecule II were optimized further away from each other while smaller bond angles were observed in Molecule II. In this study, a carbon nano ring with 12 atoms was used. As a result of optimization without any geometric constraints, it was observed that the ring maintained construction.

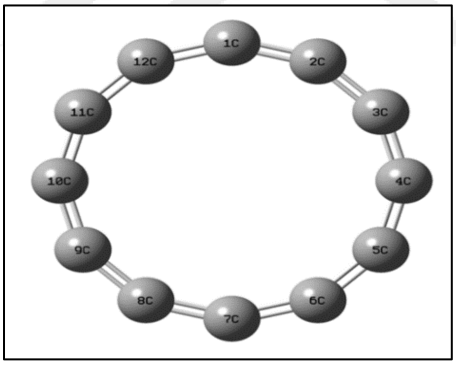


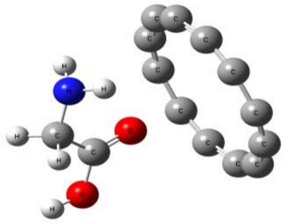
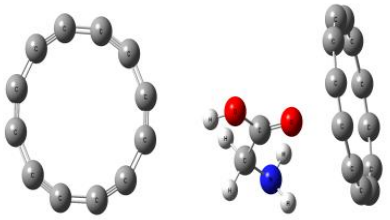
Figure 4.1. Carbon ring with 12 atoms.

As a result of the optimization, the bond lengths and bond angles between the atoms of the carbon ring were found as 1.292 Å and 150.0 °, respectively.

In the next stage of the study, the interaction of Molecule I with carbon nano ring was firstly investigated. In the first step, the glycine molecule was placed on the perpendicular axis to the center of the carbon ring, and performed the geometry optimization.

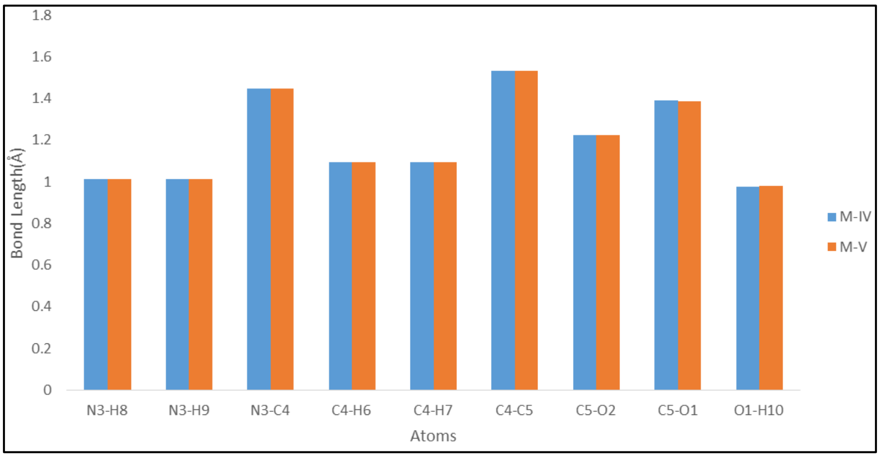
After that, the glycine molecule is placed on a perpendicular axis to the center of two carbon rings, parallel to each other, and the structure was optimized by the same method. The calculated energy, dipole moment and geometry parameters of the structures are given in Table 4.2. When the dipole moments of the structures resulting from the interaction of the glycine molecule with the carbon nano ring were examined, it was observed that the dipole moment did not change much, especially in the interaction with the single ring. While the dipole moment for Molecule I was 3.4532 Debye, the values were calculated as (3.7189) and (5.3347) Debye for structures IV and V, respectively. As a result of the calculations, it has been observed that the glycine molecule retains its molecular structure as a result of the interaction with the carbon rings. Similarly, the carbon rings also retained its geometric structure. As a result of the interactions, no significant change in the bond lengths and bond angle of the glycine molecule was observed. The calculated values are given in Table 4.2.

Table.4.2. *Energy, dipole moment and geometric parameters of the glycine molecule interacting with the carbon ring.*

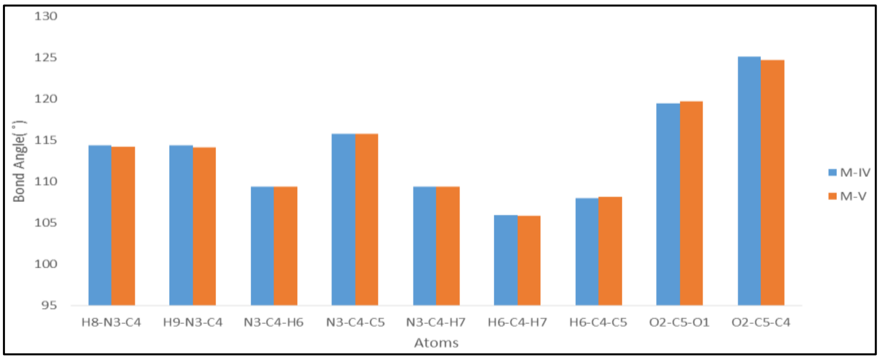
	Structure-IV	**Structure-V**
Optimized structures		
Energy (au)	-741.19296195	-1197.98584774
Dipole moment(Debye)	3.7189	5.3347
Atoms	**Bond lenght (Å)**	
N3-H8	1.0102	1.01051
N3-H9	1.0103	1.01052
N3-C4	1.4458	1.44732
C4-H6	1.0948	1.09402
C4-H7	1.0948	1.09448
C4-C5	1.5304	1.53061
C5-O2	1.2226	1.22442
C5-O1	1.3885	1.38377
O1-H10	0.9751	0.97789
Atoms	**Bond angle (°)**	
H8-N3-C4	114.38	114.18
H9-N3-C4	114.35	114.15
N3-C4-H6	109.37	109.36
N3-C4-C5	115.78	115.75
N3-C4-H7	109.34	109.35
H6-C4-H7	105.92	105.82
H6-C4-C5	107.99	108.17
O2-C5-O1	119.46	119.65
O2-C5-C4	125.10	124.70

As a result of the interaction of the Glycine molecule with the carbon ring, it was observed that the bond lengths between the central atoms (C4-N3, C4-C5, C5-O2) and (C5-O1) are small. After the reaction, it was seen that the bond length between the O2 oxygen atom, which is closest to the interaction with the carbon ring, and the C5 atom increased. However, the bond lengths between the N3-C4 and C5-O1 atoms are reduced. A similar phenomenon was observed between the (N3-C4, C4-C5, C5-O2) and (C5-O1) atoms in the interaction of the glycine molecule with the two carbon rings. There is also no significant change in the bond angles between the N3-C4-C5, O2-C5-O1 and O2-C5-C4.

It has been derived from calculations that the glycine molecule did not undergo a visible change as a molecular structure, neither in single ring nor double ring interactions. The geometrical parameters of the Structures IV and V are given in (Graphic4.3 and 4.4). As can be seen from these graphs, it can be said that the second carbon ring did not affect the geometrical structure of the Glycine. However, a significant increase in the dipole moment of this structure was observed. In addition, as can be seen in Table 4.2, the second carbon ring has significantly changed the parallel state with the first carbon ring. The first ring, however, continued to protect the position. For this reason, it can be said that the glycine molecule can form more stable structural units with single carbon rings.



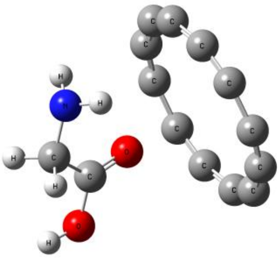
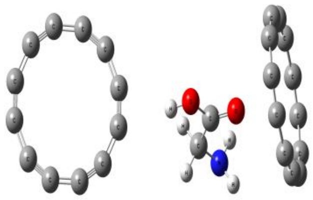
Graphic 4.3. Bond lengths of Structures IV and V.



Graphic 4.4. Bond angles of Structures IV and V.

When the carbon rings interacting with the glycine molecule were examined, it was observed that The bond length between the consecutive carbon atoms before the interaction was found 1.292 A$^{\mathrm{o}}$, but after the interaction it was observed, with very little change, as 1.225 and 1.37, consecutively. The bond angles were calculated as 150^{o} . Before the interaction, but after the interaction it was observed as 1.225 EV 1.37 A$^{\mathrm{o}}$ .With a slight change. The calculated values are given in Table 4.3.

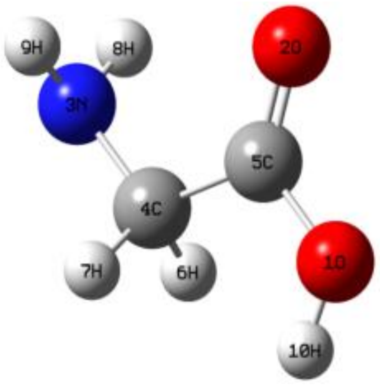
Table 4.3. *Geometrical parameters of only carbon rings.*

	Structure-IV	Structure-V
Optimized structures		
Atoms	**Bond lenght(A)**	
C1-C2	1.22526	1.37417
C2-C3	1.37524	1.22518
C3-C4	1.22544	1.37375
C4-C5	1.37604	1.22507
C5-C6	1.22555	1.37440
C6-C7	1.37542	1.22530
C7-C8	1.22532	1.37538
C8-C9	1.37446	1.22556
C9-C10	1.22503	1.37576
C10-C11	1.37384	1.22562
C11-C12	1.22500	1.37498
Atoms	**Bond angle(°)**	
C1-C2-C3	149.535	148.323
C2-C3-C4	150.404	151.333
C3-C4-C5	149.757	148.916
C4-C5-C6	149.709	150.839
C5-C6-C7	150.455	149.385
C6-C7-C8	149.431	150.790
C7-C8-C9	150.756	149.012
C8-C9-C10	149.439	151.125
C9-C10-C11	150.245	148.405
C10-C11-C12	150.010	151.754

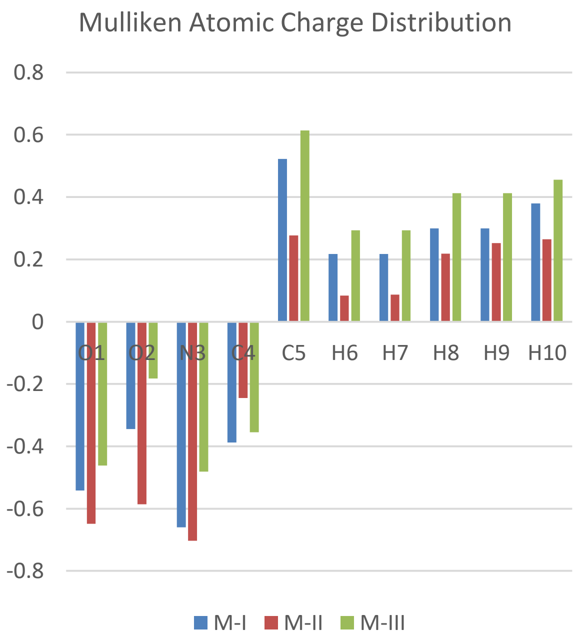
In this study, an analysis of Mulliken charge distributions was made before and after the interaction of the glycine with the carbon nano rings. As seen in Table 4.4, in case of the charge -1, it was calculated that the Mulliken charge of oxygen and nitrogen atoms, which have higher electronegativity, are larger than others.

The situation is the opposite for other Carbon and Hydrogen atoms. In general, the highest Mulliken atomic charge density is calculated on the Nitrogen atom. The least charge density was calculated for the 6H atom. Due to it was attached the Oxygen atoms, the charge density of the C5 carbon atom was greater than the other 4C carbon atom. A similar phenomenon was observed for the hydrogen atom (10H) due to the bond made by the oxygen atom. The positive value of the charge naturally caused to have larger charge densities of the Carbon and Hydrogen atoms than the others. The values for the Mulliken charge distributions of the atoms and the comparative graphic are given in Table 4.4.

Table 4.4. *Mulliken charge distribution of glycine structures.*

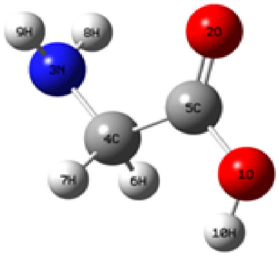
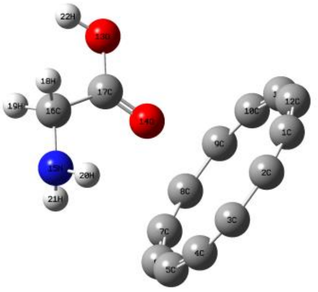
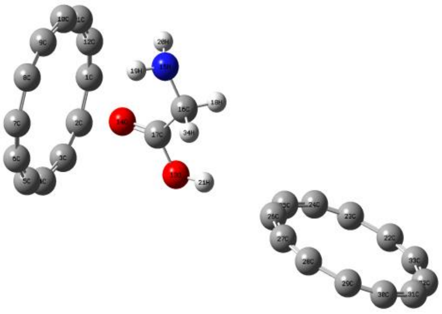


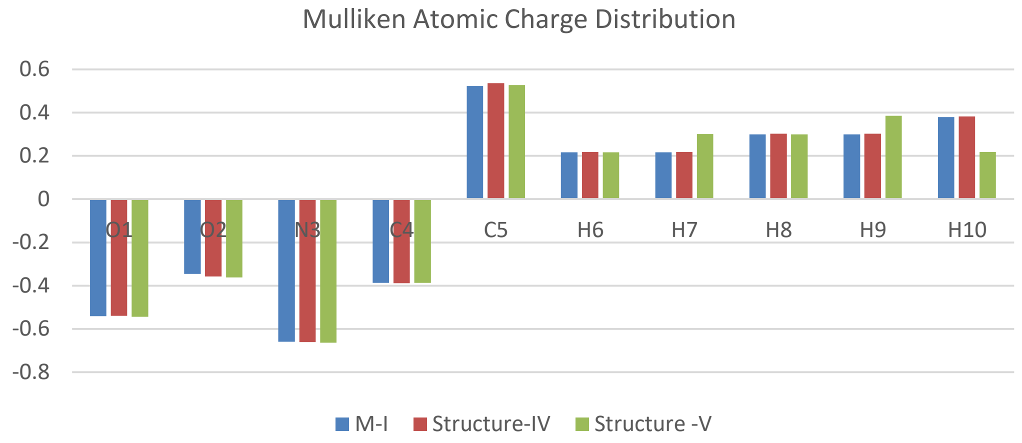
Atoms	M-I	M-II	M-III
O1	-0.541	-0.649	-0.4618
O2	-0.345	-0.586	-0.1826
N3	-0.660	-0.703	-0.4816
C4	-0.387	-0.245	-0.3550
C5	0.522	0.277	0.6142
H6	0.217	0.084	0.2936
H7	0.217	0.086	0.2934
H8	0.299	0.219	0.4123
H9	0.299	0.252	0.4123
H10	0.379	0.264	0.4552



In the study of how the atomic Mulliken charge distributions change, the following results were obtained: As a result of the interaction of the glycine molecule with the carbon nano-rings, no significant change in the charge density of atoms of the glycine was observed. In the interaction with the double ring, the charge densities of the hydrogen atoms (7 and 9) increased, but decreased the charge density of the hydrogen atom (10). If we talk about the small charge density changes of the interaction, it is seen that the Mulliken charge density of oxygen atoms of both Structure IV and V increased. While the charge density of the O1 atom for the molecule I was -0.5414, the values were calculated as -0.53996 and -0.5435 for "Structure IV and V". Mulliken charge density values were calculated as -0.3450, -0.35680 and -0.3618 for the oxygen atom (2O), respectively. A similar situation has also been observed for Nitrogen having high electron affinity. The charge densities for nitrogen were calculated as -0.6598, -0.66085 and -0.6632, respectively. It has also been observed that carbon atoms are not much affected by Interactions. The calculated values are given in Table 4.5.

Table 4.5. *Mulliken charge distribution of Glycine, Structure IV and V.*

	M-I	**Structure-IV**	**Structure-V**
			
O1	-0.5414	-0.53996	-0.5435
O2	-0.3450	-0.35680	-0.3618
N3	-0.6598	-0.66085	-0.6632
C4	-0.3874	-0.38797	-0.3864
C5	0.5218	0.53507	0.5272
H6	0.2170	0.21818	0.2160
H7	0.2170	0.21838	0.3004
H8	0.2991	0.30142	0.2994
H9	0.2991	0.30214	0.3856
H10	0.3796	0.38244	0.2171



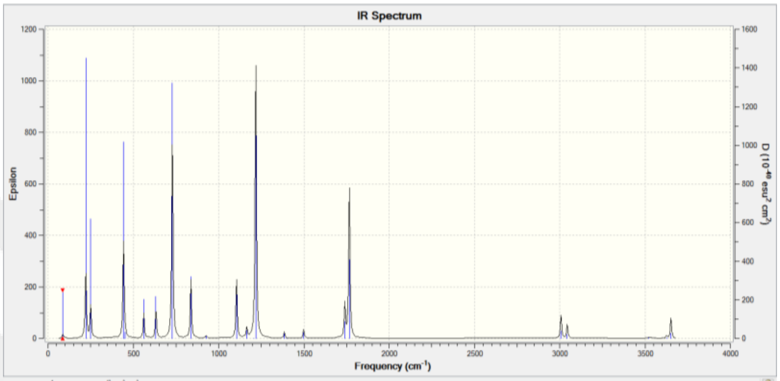
At this stage of the study UV and IR spectral analysis of the interaction of the glycine molecule with the carbon nano rings was theoretically performed. The oscillation frequencies and intensities of the IR calculations of the all structures are given in Table 4.6.

Table 4.6. *Calculated IR values of the molecular structure.*

Molecule-I		**Molecule-II**		**Molecule-III**		**Structure-IV**		**Structure-V**	
F	**I**	**F**	**I**	**F**	**I**	**F**	**I**	**F**	**I**
87	5.47	133	1.74	9.96	2.6942	-2.32	0.8784	3.06	0.0031
221	80.52	204	84.07	250.61	8.0803	15.75	0.9751	6.06	0.0172
250	38.70	237	31.50	308.969	51.1846	28.79	1.6307	6.64	0.0534
443	112.88	296	59.12	344.75	38.3801	40.80	0.0549	10.81	0.1268
453	3.70	406	5.26	407.88	131.2035	46.27	0.0515	14.42	0.2991
562	28.37	471	33.51	472.69	30.4399	53.82	0.5641	16.62	0.1664
633	34.19	511	43.87	596.55	13.1784	65.49	0.4425	25.37	0.3506
729	241.40	755	43.56	612.80	46.4399	86.90	3.9962	32.97	0.5730
838	67.20	885	124.47	795.00	249.5218	134.15	0.0137	39.63	0.2913
927	3.37	929	136.02	901.97	19.4443	135.17	0.0077	45.10	0.1066
1105	68.96	978	53.21	1054.60	656.5408	163.11	0.0064	50.17	0.0727
1165	12.04	1078	164.85	1123.39	55.6952	165.43	0.1235	67.16	0.1088
1205	0.00	1117	80.11	1134.21	1.3069	223.98	73.8123	74.74	0.3816
1218	328.04	1451	24.99	1202.03	17.5126	252.29	30.6744	82.67	1.2885
1386	8.04	1329	9.32	1291.39	15.0869	303.25	0.0041	130.88	0.0649
1399	0.16	1734	17.75	1390.56	1.9858	315.02	0.0054	135.04	0.0052
1499	10.66	2854	300.92	1508.21	24.7330	326.18	0.0022	135.22	0.0095
1740	38.58	3008	76.11	1709.25	70.8605	367.35	0.0267	137.31	0.8278
1766	180.48	3351	74.94	1794.92	135.4585	382.88	0.4482	161.99	0.0017
3008	27.96	3446	14.81	3045.87	3.1176	445.35	80.6310	163.56	0.0336
3044	16.73	3617	13.67	3132.60	6.1705	453.20	2.1797	164.30	0.0068
3522	1.46	-	-	3500.18	281.4194	457.46	0.4634	165.80	0.0442
3627	3.02	-	-	3623.87	110.2561	476.58	0.2941	191.93	0.2543
3652	24.61	-	-	3639.58	167.3615	479.47	0.5584	216.26	51.5599
-	-	-	-	-	-	480.07	0.4822	-	-

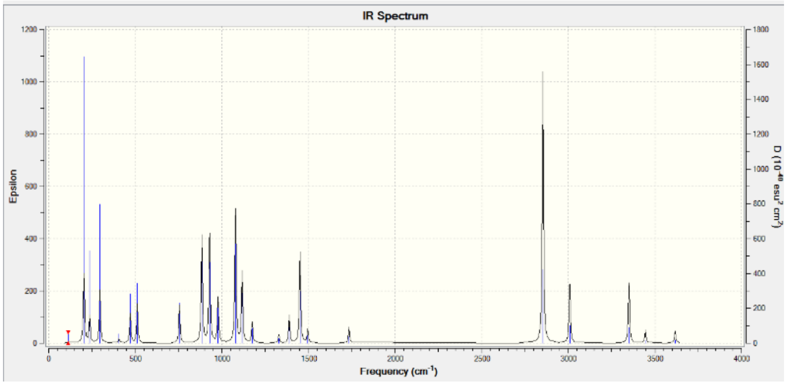
F: frequency (cm^{-1}), **I**: intensity

As a result of the IR calculations, some important modes of vibration of the glycine molecule (Moleceule-I) were observed: O-H stretching at 3652 cm^{-1}, (N-H) antisymmetric stretching at 3627 cm^{-1}, N-H symmetric stretching at 3522 cm^{-1}, (C-H) antisymmetric stretching for C4 at 3044 cm^{-1}, C-H symmetric stretching for C4 at 3007 cm^{-1}, C=O stretching at 1766 cm^{-1}, C-N stretching at 1165 cm^{-1}, C-O is stretching at 1105 cm^{-1} and (N-H) is wagging at 728 cm^{-1}.

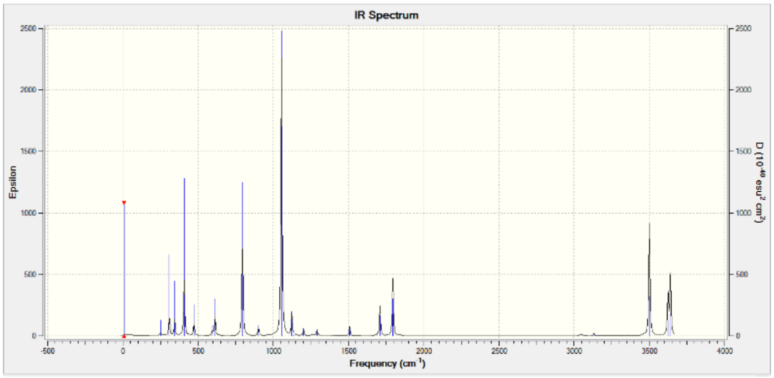


Graphic 4.5. The calculated IR values of M-I.

Vibration frequencies for Molecule II and Molecule III are given in Table 4.6. In addition, vibration frequency graphics of Molecules I, II and III are given in (Graphs 4.5-4.7).

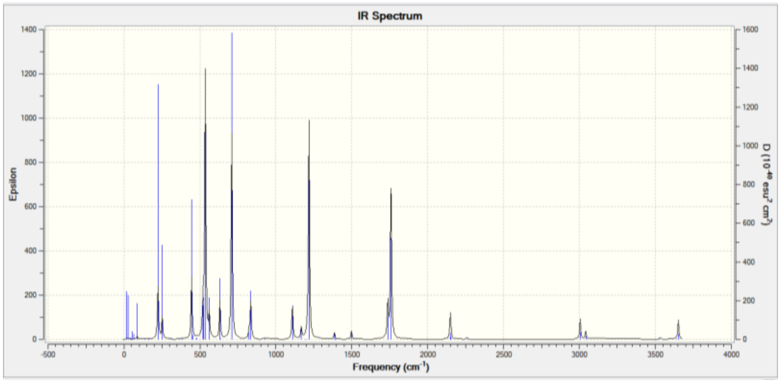


Graphic 4.6. The calculated IR values of M-II.



Graphic 4.7. The calculated IR values of M-III.

As a result of interaction of the carbon rings with the glycine molecule, it appears that there is no significant change in the vibration frequencies of the glycine. Some important vibration frequencies for Structure IV: O-H stretching at 3651 cm^{-1}, N-H antisymmetric stretching at 3636 cm^{-1}, N-H symmetric stretching at 3530 cm^{-1}, C-H antisymmetric stretching for C4 at 3041 cm^{-1}, C-H symmetric stretching for C4 at 3005 cm^{-1}, Various C=C vibrations of the carbon ring between 2260-2074 cm^{-1}, C=O stretching at 1759 cm^{-1}, C-N stretching at 1167 cm^{-1}, C-O stretching at 1109 cm^{-1} and N-H is wagging at 710 cm^{-1}. Calculated vibrational frequency of the interaction Glycine-Carbon ring is given in Graphic 4.8.

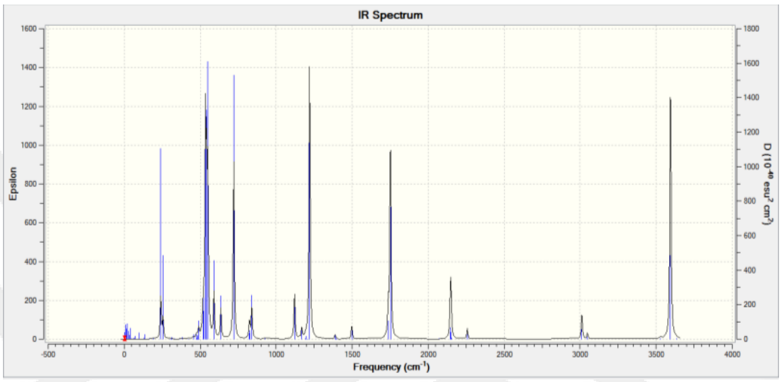


Graphic 4.8. Calculated IR values for Structure IV.

Some significant IR frequencies for the interaction of the double carbon ring with the glycine molecule: N-H antisymmetric stretching at 3632 cm^{-1}, O-H stretching at 3594 cm^{-1}, N-H symmetric stretching at 3527 cm^{-1}, C-H antisymmetric stretching for C4 at 3048 cm^{-1}, CH symmetric stretching for C4 at 3011 cm^{-1}, various C=C vibrations of carbon rings between 2257-2071 cm^{-1}, C=O stretching at 1751 cm^{-1}, N-

H scissoring at 1737 cm^{-1}, C-H scissoring at 1579 cm^{-1}, C-N stretching at 1168 cm^{-1}, C-O stretching at 1120 cm^{-1} and NH wagging at 721 cm^{-1}.

It has been observed that the frequencies in the high frequency region shifted more than in the low region. In addition, it was observed that there is no significant frequency shifting in the molecular structure as the result of the interaction of the glycine-double ring.



Graphic 4.9. Calculated IR values for Structure V.

The spectral analysis part of the study was continued with the theoretical calculations in the UV-Vis region. Theoretical data for UV calculations were obtained by the same method using the previously obtained optimization geometry. The theoretical UV data on the interaction of the glycine molecule with the carbon rings are given in Table 4.7.

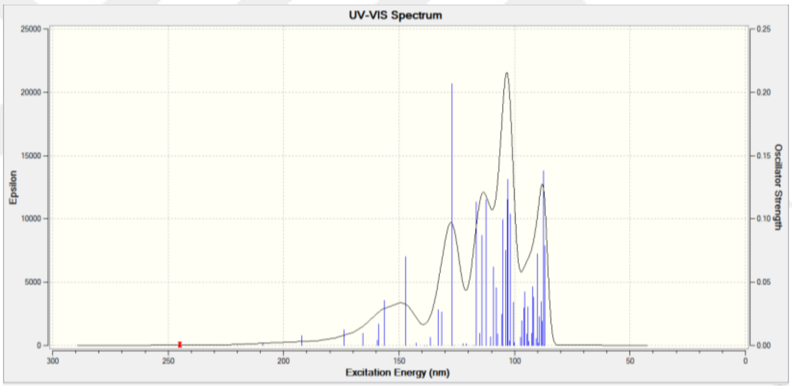
Table 4.7. *Calculated UV values of molecular structures.*

Molecule-I		**Molecule-II**		**Molecule-III**		**Structure-IV**		**Structure-V**	
E	**ε**	**E**	**ε**	**E**	**ε**	**E**	**ε**	**E**	**ε**
244.93	0.0012	551.34	0.0121	556.05	0.0726	787.15	0	822.47	0
219.93	0.0001	461.01	0.0336	298.7	0.0809	303.43	0.0137	327.93	0
191.94	0.0076	339.4	0.0588	175.58	0.0113	251.78	0.0193	303.68	0.0026
156.54	0.0354	322.88	0.0118	150.51	0.0075	250.73	0.0172	303.1	0.176
-	-	320.22	0.0204	-	-	191.05	0.0227	302.34	0.0001
-	-	249.41	0.0147	-	-	177.82	0.0145	302.49	0.0001
-	-	233.4	0.0083	-	-	175.25	0.0039	301.85	0
-	-	202.8	0.0062	-	-	174.55	0.0073	286.51	0.0021
-	-	188.15	0.0184	-	-	173.33	0.002	279.09	0.0058
-	-	173.72	0.0063	-	-	172.89	0.2058	-	-
-	-	179.63	0.0727	-	-	171.54	0.0676	-	-
-	-	165.99	0.012	-	-	-	-	-	-
-	-			-	-	-	-	-	-

E: Excitation (nm), ε: Epsilon.

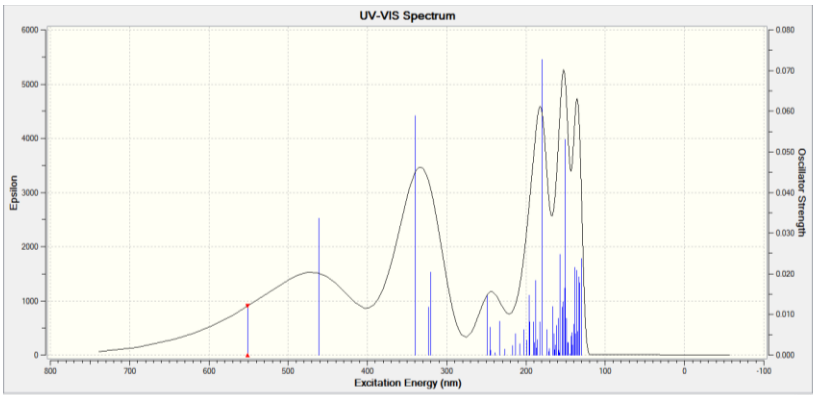
UV-Vis analyzes were performed using the geometrical data of the optimized structures. Firstly, the Glycine molecule was examined separately, then the interaction between Glycine with single and double carbon rings was considered. The relevant spectra are given in (Graphs 4.10-4.14).

According to the results obtained by UV calculations, the maximum absorption points are below 200 nm since there is no chromogenic group in the structure of Glycine. There is a maximum absorption point due to $n \rightarrow \pi^*$ electronic transitions due to $\pi \rightarrow \pi^*$ electron transitions originating from the π bonds and unpaired electron pairs on the Nitrogen and Oxygen. Since the $n \rightarrow \pi^*$ electronic transition of absorption at wavelengths close to 200 nm requires less energy, it has been shown that wave lengths exhibit more bathochromic shift than wave lengths due to $\pi \rightarrow \pi^*$ electronic transmission (Graphic 4.10).

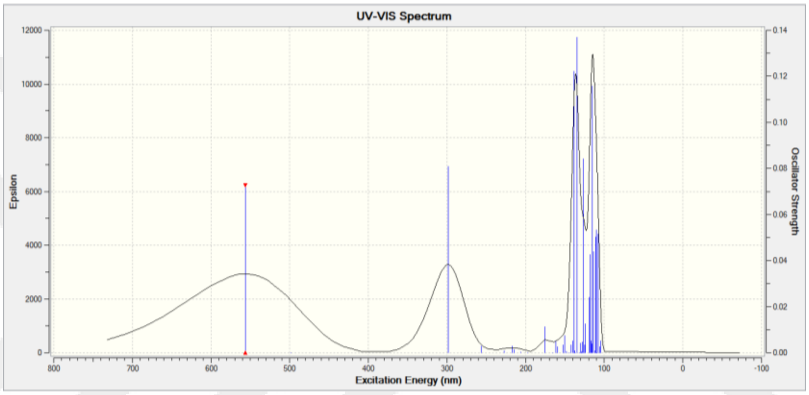


Graphic 4.10. The calculated UV values of M-I.

In the case of the charge was -1, it was observed that the peaks showed bathochromic shift. In the case of the charge was +1, it was observed that the second absorbtion showed hyperchromic shift while there was not much shift for λ_{max} (Graphic 4.11, 4.12).

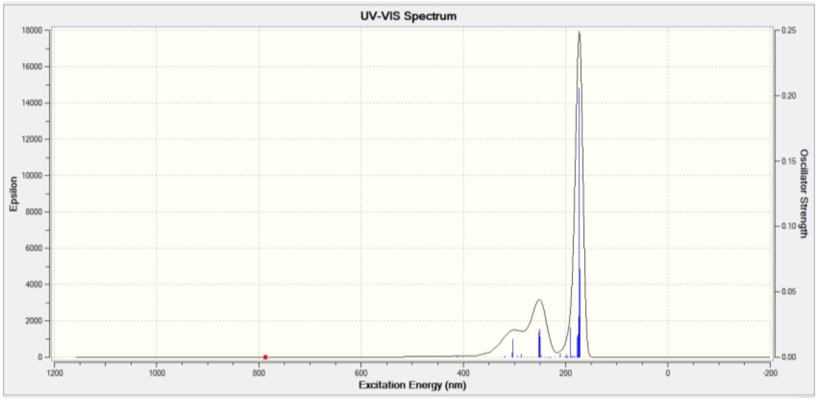


Graphic 4.11. The calculated UV values of M-II.

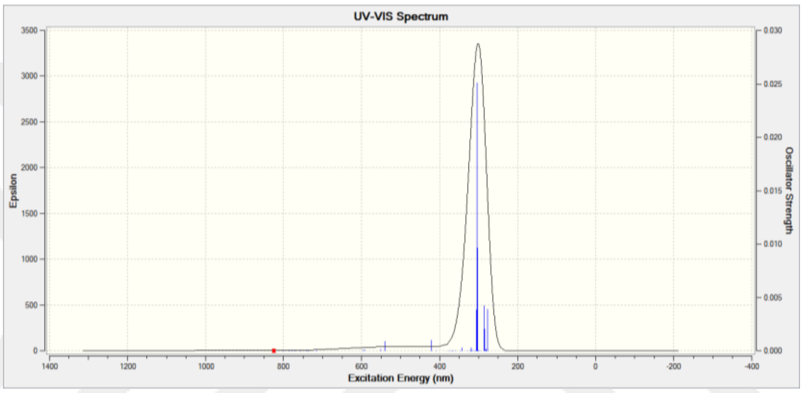


Graphic 4.12. The calculated UV values of M-III.

As a result of the interaction of the glycine molecule with the carbon ring, the first and second absorbers second absorbtions were superimposed, and so a bathochromic shift occurred. Furthermore, when the UV data is examined, it was concluded that the effect of the intramolecular hydrogen bond was increased, therefore the band resulting from this transition was the hipsochromic shift since the energy required for $n \rightarrow \pi^*$ electronic transitions was increase, the band originating from the $\pi \rightarrow \pi^*$ transition showed a bathochromic shift. İt was observed that since the intensity of the band due to the $\pi \rightarrow \pi^*$ transition is greater, it suppresses the other band and causes a single absorption band at the wavelength of 304 nm (Graphic 4.13, 4.14).

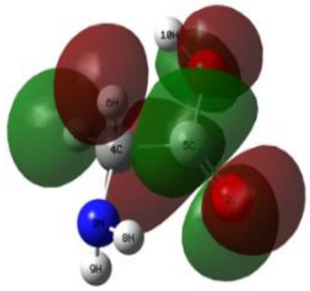
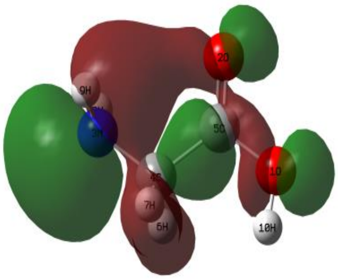
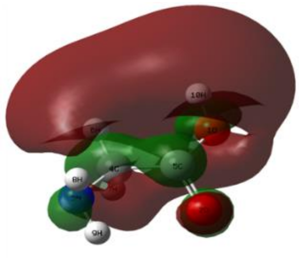
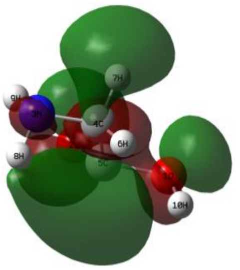
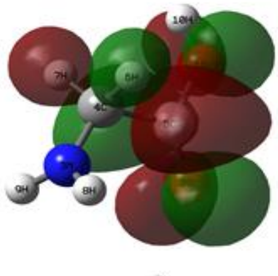
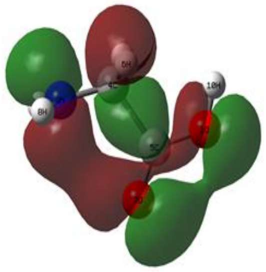
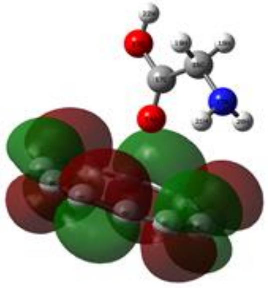
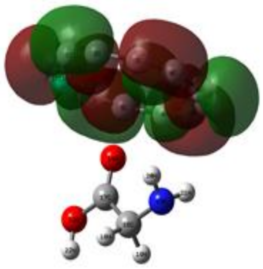


Graphic 4.13. Calculated UV values of Structure S-IV.



Graphic 4.14. Calculated UV values of Structure S-V.

The HOMO-LUMO surfaces of the glycine molecule and its interaction with the carbon nano-ring are given in Figure 4.2. When these surfaces are examined, it is seen that LUMO and HOMO are on carbon rings.

	LUMO	HOMO
M-I		
M-II		
M-III		
M-IV		

M-V

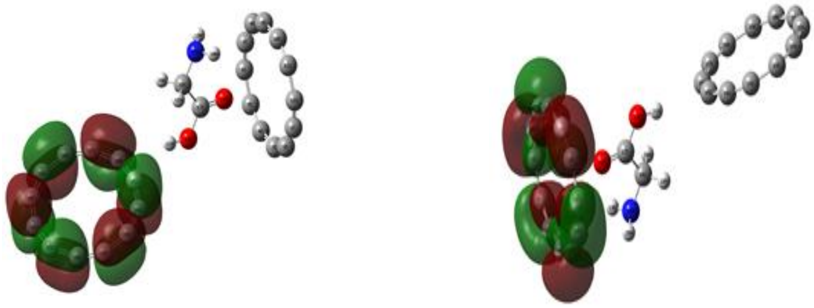
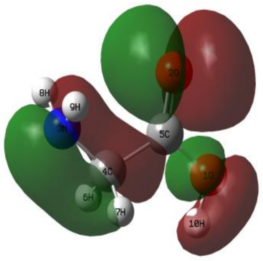
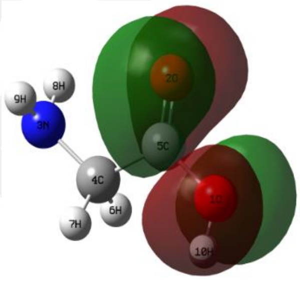
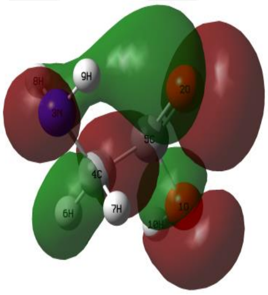
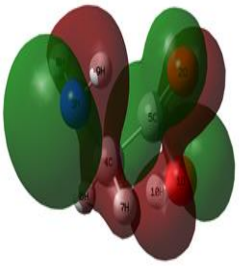
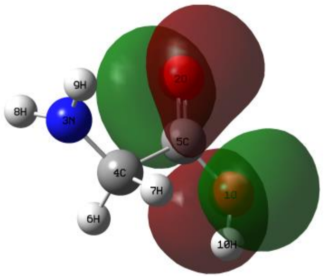
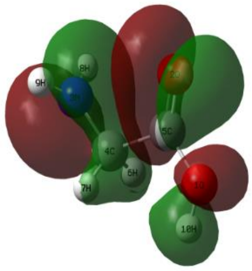
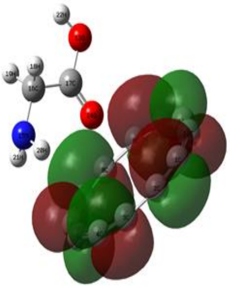
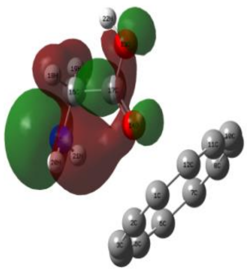


Figure 4.2. HOMO-LUMO distributions of molecular structures.

	HOMO-1	HOMO-2
M-I		
M-II		
M-III		
M-IV		

M-V

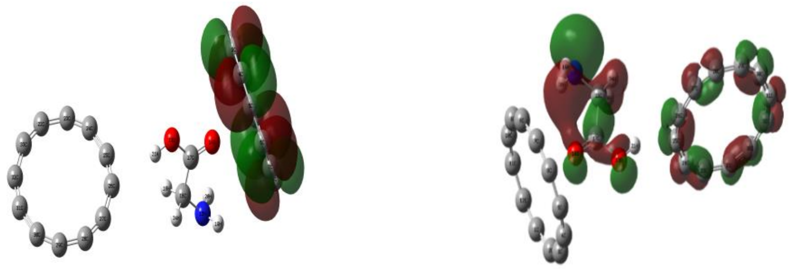
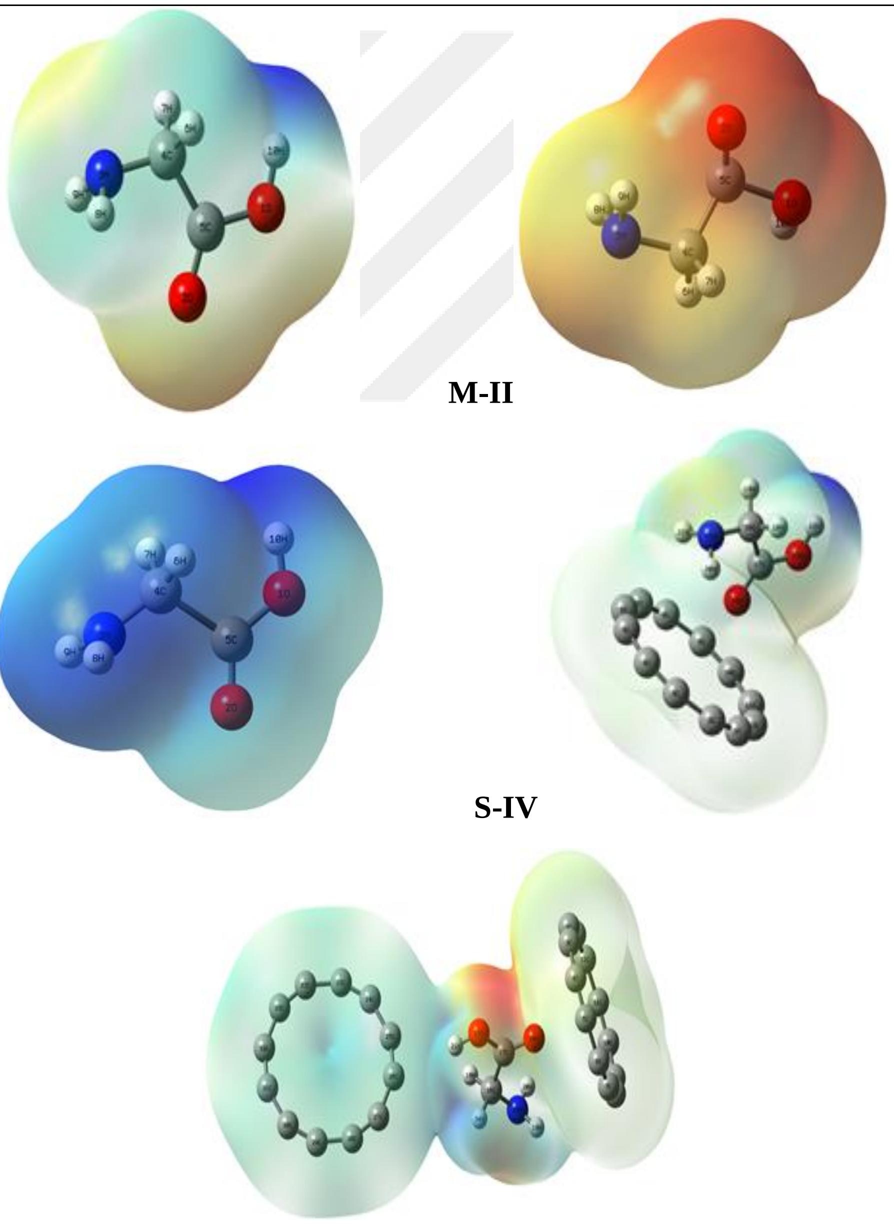


Figure 4.2. Continued

The ESP surfaces of the studied structure are given in (Figure 4.3).



M-I

M-II

M-III

S-IV

S-V

Figure 4.3. The ESP surfaces of the structures.

Electronegativity (χ), Chemical Hardness (η) and Chemical Softness (σ) values were calculated and interpreted at this stage of the thesis. Electronegativity is a very useful concept for explaining and understanding a chemical reaction. It is defined as a measure of how strong the electrons are drawn from an atom (or atom groups), and it is given as:

$$\chi = -\frac{1}{2}(E_{HOMO} + E_{LUMO}) \tag{4.1}$$

where E_{homo} is the energy of highest occupied molecular orbital, and E_{lumo} is the energy of lowest occupied molecular orbital. Chemical hardness is a measure of the resistance of an atom to charge transfer and is given by the following equation:

$$\eta = -\frac{1}{2}(E_{HOMO} - E_{LUMO}) \tag{4.2}$$

Chemical softness is defined as the capacity of an atom (or group of atoms) to receive electrons and is calculated by the following equation:

$$\sigma = \frac{1}{\eta} \tag{4.3}$$

Here η is the value of chemical hardness. The calculated values of the structures are given in Table 4.8.

Table 4.8. *The calculated chemical parameters of the systems.*

Mol	**Energy (a.u)**	**E_{HOMO} (eV)**	**E_{LUMO} (eV)**	**ΔE (eV)**	**η (eV)**	**σ (eV)**	**χ (eV)**	**Dipole moment (Debye)**
M-I	-284.40	-6.76	-0.53	6.23	3.12	0.32	3.64	3.45
M-II	-284.36	2.18	5.49	3.31	1.65	0.60	-3.83	3.51
M-III	-284.07	-13.77	-6.33	7.44	3.72	0.27	10.05	6.43
S-IV	-741.19	-5.86	-3.20	2.66	1.33	0.75	4.53	3.72
S-V	-1197.99	-5.78	-4.00	1.78	0.89	1.12	4.89	5.33

As a result of the calculations, the charge values of glycine molecule (-1 or +1) cause to change of the chemical parameters very much. Naturally, in the case of the charge was +1, it was found that the electron affinity of molecular is very large. However, a slightly different situation has emerged as a result of the interaction of glycine with carbon nano rings. When the interaction of glycine with single and the double ring were compared, the electronegativity value did not change significantly.

In addition, the second carbon ring in the double ring interaction with glycine increased the electron affinity of the system (4.528 for S-IV, 4.8907 for S-V), but this increase was not big. We can say that the stable structures of the carbon rings did not allow the electronegativity to change.

The different results were obtained for the chemical hardness and chemical softness values of the systems. The interaction of the glycine with the second carbon ring caused a decrease in the value of the chemical hardness of the structure. In this case it is possible to say that the interaction with the single carbon ring is more stable. So, in the interaction with the double rings, the chemical hardness showed a decrease, which means that the structure becomes more favorable to the reaction. Moreover, the interaction with the double rings increased both the electron affinity and the dipole moment of the system.

5. SUGGESTIONS

We can summarize the study as follows: The glycine, which are the building blocks of proteins and have an important place among the Carbohydrates, and interaction of it with carbon nano-ringing was calculated by using the DFT. The B3LYP method, which has proven itself in many studies, was chosen. As a result of calculations using the 6-311G base set, geometrical and chemical parameters of the glycine and were obtained. In addition, UV-Vis and IR analyzes were performed by the same method and basis set. The UV and IR analyzes were similarly performed after energy optimization in order to investigate the interaction of Glycine with the single Carbon ring. Later, similar processes were repeated to study the interaction of glycine with the double carbon ring. Finally, the obtained data were analyzed and interpreted.

As a result of the calculations, the dipole moment value of the glycine with the charge +1 was calculated to be twice as large as than charge neutral and -1. It was also found that C5-O1 have the shortest bond length in the charge +1 while the bond length is in the longest while having a charge of -1. For that reason, we can say the excess and lack of electrons in the system.

O1, O2 and N3 atoms of the M-II have increased in Mulliken charge densities compared to M-I and M-III, while charge densities are decreased on the carbon atoms C4. In the case of interaction of glycine with single and double carbon rings, the Mulliken charge densities of oxygen atoms, nitrogen atoms and carbon atoms were observed close to each other, whereas for two ring system, it was observed that the Mulliken charge density of the nitrogen-bonded hydrogen atom increased and the charge density of the oxygen-bonded hydrogen decreased.

Until now, many theoretical and experimental investigations have been carried out on the structure of amino acids and the conditions in different environments. Some studies have investigated the adhesion reactions of different amino acids onto carbon nanotubes. In these investigations, carbon nanotube interactions with some amino acids such as Glycine, Uracil, Guanine, Timin, L-alanine have been studied experimentally and theoretically [18-23]. In this context, the works on this subject have continued intensively, and it is aimed to reach to obtain the proteins which are the basis of the artificial organ construction in the laboratory conditions.

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