quarterly journal of new horizons in chemistry

Online ISSN: ۲۷۸۳-۱۱۵۹

Quantum Chemistry Calculations based on the Density Functional Theory on Diazinon Pesticides

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Abstract

In this research, to investigate the effect of organ phosphorus pesticides on serine amino acid, the quantum chemistry calculations based on the density functional theory on diazinon pesticides and its derivatives, as well as complexes of these derivatives with serine were also studied. The DFT quantum chemistry calculations were carried out using the B3LYP method and the 31-6G (d, p) basis set. Sustainable energy and dipole moment of the systems were measured. Enthalpy and Gibbs free energy of the diazinon complexes were all positive, indicating the endothermic and non-spontaneous nature of the formation of these complexes. The value of the band gap, which is calculated from the difference in the energy of the HOMO and LUMO orbitals, was close together in the diazinon complexes and about 5.7 electron volts. The dipole moment values of these complexes were in the range of 3.4 to 10.1 electron volts. Next, the quantum mechanical descriptors were examined and they were used in determining the best complexes. The lengths and angles of the bonds of compounds before and after the formation of the complex were calculated and compared and the change of angles and the general form of structures were separately evaluated. QTAIM data were

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studied and the nature of the existing bonds was explored. The nature of the bond was between serine amino acid and all of the electrostatic diazinon derivatives and intermolecular interactions exhibited the stability of these complexes.

Key words: Quantum Chemistry Calculations, Density Functional Theory, Organophosphate Pesticides (OPPs), Diazinon, DFT

1- Introduction

The use of pesticides is related to the history of Rome and ancient Greece. Someone named Homer referred to a fumigation poison caused by sulfur poisoning. Pleny (Italian researcher) recommended the use of arsenic against insects, as well as Soda and baking soda for seed modification. In the middle of 1970s-1980s, many new pesticides were introduced. They were completely established on the basis of biological and biochemical mechanisms and, in comparison with the older pesticides, most of them have been very effective at the lowest dose. In 1952, Diazinon was synthesized at Ciba-Geigy Company in Switzerland and introduced to the world. The diazinon poisoning was first used to control the cockroaches, fleas and ants, and was later used more widely in agriculture and horticulture. The fast and powerful effectiveness of this poison has led to continuous use of it in many parts of the world including Iran. Diazinon is dangerous to humans and mammals and the diazinon's toxicity degree is 214 mg/kg. Based on the type of their chemical structure, pesticides are classified into organophosphate, organochlorine, organizates (carbamate) and pyrethroid toxins [1]. Diazinon is one of the organophosphate pesticides whose mechanism of action is same as the other organophosphates, so that it causes the total inhibition of enzymes and mainly the acetylcholine enzyme [2]. These compounds with phosphorylation of the serine amino acid in the active site of the acetylcholinesterase enzyme will cause the inhibition of enzyme and the accumulation of acetylcholine will cause the high excitability of nicotinic and muscarinic receptors, which ultimately lead to occurrence of the cholinergic crisis of seizure, and, in severe cases,

brain injury and death [3-6]. Serine (Ser) is one of the amino acids used in the structure of proteins, including alcohol containing amino acids with an -OH group. Serine is very abundant in silk fibers and is also involved in the structure of lipids and compound proteins. Due to the presence of an alcohol group in the molecule, Serine creates hydrogen bonding with water molecules and can be easily dissolved in it.

Considering that carrying out of frequent tests in experimental research methods lead to the accumulation of unwanted chemicals and creating such chemical wastes is dangerous to the environment and its elimination also requires time and cost, the approach of chemists to use computational chemistry has been more in recent years. In computational chemistry, the behavior of unstable compounds can be also observed together and, using the data extracted, items on their behavior can be commented. Eventually, according to the results obtained, it is possible to perform final experimental tests with high confidence and make effective savings in time and cost. The proposed theories in computational chemistry are divided into two categories of classical theories and quantum theories. In this research, using Gaussian software, quantum chemistry calculations for the effect of organophosphate pesticides (diazinon and its derivatives) on the serine enzyme have been examined. The objective of this study was to evaluate the structure of diazinon derivatives and complexes formed by these derivatives with serine amino acids.

2- Computational Methods

In this study, the quantum computations carried out have been done using the density functional theory (DFT) with the help of Gauss View software [7-8]. The structure of the tautomer and the formulation of various compounds are designed and then, with the help of Gaussian software [9], is identified at the different theoretical and optimum levels, and the most stable tautomer of the molecule is determined. DFT calculations with B3LYP method and the standard basis set of 6-31 G (d, p) was conducted to evaluate the influence of

diazinon poisoning and its derivatives (dia 1- dia 6) on serine amino acid through hydrogen bonding in water solvent. The B3 symbol means the use of Beck's three-parameter electron exchange function [10] and the LYP represents the use of Lee-Yang-Parr's electron correlation function [11].

3- Discussion & Results

In the present study, various derivatives of diazinon poisoning (dia 1- dia 6) and their complexes with serine amino acid (dia-ser 1- dia-ser 6) have been investigated. The studied structures of diazinon poison derivatives are illustrated in Figure 1.

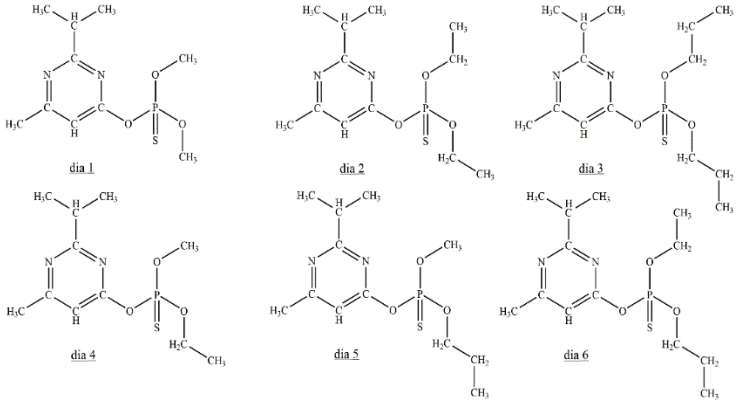


Figure 1- Structure of diazinon pesticides derivatives

4- Dipole Moment and Sustainable Energy:

Measuring the dipole moment of diazinon derivatives in water solvent was done by b3ly/6-31G (d). The dipole moment of the diazinon derivatives in the water solvent has a close values from 7.2 to 7.5 Debye. The dipole moment of the serine enzyme is 4.7 Debye. Given the results seen in Table 1, the order of dipole moment of the compounds and the sustainable energy of the diazinon-serine complexes have been presented. The results revealed that polarization

of diazinon derivatives in the water medium with the B3LYP method is for all close together and approximately close to 7.4 Debye. The polarity of Complex No. 1 and Complex No. 6 has increased in the diazinon complexes.

(μ): dia6 > dia3 > dia2 > dia5 > dia4 > dia1

(μ): dia-ser6 >dia-ser3 >dia-ser1 >dia-ser2 >dia-ser5 >dia-ser4

(ΔE): dia-ser3 > dia-ser6 > dia-ser2 > dia-ser5 > dia-ser1 > dia-ser4

In the diazinon complexes, the highest value of sustainable energy is related to complexes No. 3 and No. 6, and the lowest value of sustainable energy is related to complexes No. 1 and No. 4.

5- Thermodynamic Data:

According to the results available in Table 1, the values of ΔS, ΔH and ΔG of the diazinon complexes are such that the values of ΔG in the range from 8.6 to 11.7 kcal, the values of ΔH in the range from 0.5 to 1.3 kcal and the values of ΔS in the range from -0.025 to -0.035 kcal are, respectively. The highest value of G and H in diazinon and its derivatives is related to combinations No. 3 and No. 6, and the lowest value is related to combinations No. 1 and No. 4. The results are as follows:

(ΔG): dia-ser3 > dia-ser2 > dia-ser6 > dia-ser1 > dia-ser5 > dia-ser4

(ΔH): dia-ser3 > dia-ser 6 > dia-ser1 > dia-ser4 > dia-ser5 > dia-ser2

(ΔS): dia-ser3 = dia-ser2 > dia-ser6 > dia-ser 1> dia-ser5 > dia-ser4

In the diazinon complexes, the ΔG values are in the range from 8.7 to 11.4 kcal/mol that the highest value of ΔG is related to complexes No. 3 and No. 2, and its lowest value is for complexes No. 4 and No. 5. It is worth mentioning that ΔG of all complexes is positive, indicating non-spontaneous nature of the reactions. In the diazinon complexes,

the highest value of ΔH can be seen in complex No. 3 and the lowest value of ΔH in complexes No. 2, No. 4, and No. 5. It should be noted that ΔH of all complexes is positive, representing the endothermic nature of the reactions.

6- Natural Bond Orbital (NBO) Analysis and Energy Band Gap (EG) Analysis

The results of the calculations indicated that the band gap of diazinon derivatives are too close together and about 5.8 electron volts. The band gap of serine enzyme is 6.5 electron. As well as, the band gap values of the diazinon complexes are very close together, but they approximately exhibit up to 0.1 decline (Table 1).

(Bandgap): dia1 > dia4 > dia5 > dia2 > dia3 > dia6

(Bandgap): dia-ser6 > dia-ser3 > dia-ser1 > dia-ser4 > dia-ser2 > dia-ser5

Table 1- The calculated parameters of μ, ΔE, ΔG, ΔH, ΔS, Eg and bandgap of diazinon derivatives and its complexes with serine

ITEM		μ(debye)	ΔE (kcal/mol)	ΔG (kcal/mol)	ΔH (kcal/mol)	ΔS (kcal/k)	Eg (hartree)	Band Gaps (ev)
ser		4/6666					-0/2390	-6/5026
dia 1	m-m	7/2605					-0/2157	-5/8696
dia 2	e-e	7/5061					-0/2147	-5/8432
dia 3	p-p	7/5116					-0/2147	-5/8419
dia 4	m-e	7/2784					-0/2153	-5/8596
dia 5	m-p	7/2872					-0/2153	-5/8593
dia 6	e-p	7/5227					-0/2146	-5/8399
dia-ser 1	m-m	9/0892	-0/194	9/34	1/13	-0/276	0/2097	-5/7058
dia-ser 2	e-e	4/7685	-0/184	11/40	0/50	-0/366	0/2088	-5/6821
dia-ser 3	p-p	7/1185	0/024	11/78	1/30	-0/352	0/2113	-5/7499
dia-ser 4	m-e	4/3603	0/016	8/62	1/02	-0/255	0/2087	-5/6835
dia-ser 5	m-p	4/5109	-0/451	8/72	1/00	-0/259	0/2077	-5/6527
dia-ser 6	e-p	10/0768	0/015	10/44	1/24	-0/309	0/2118	-5/7646

7- Quantum-Mechanical (QM) Descriptors:

Using the quantum-mechanical descriptors, diazinon complexes were calculated and evaluated and they were used in determining the best complexes. According to the results derived from the calculations, the ionization (I) energy values of the diazinon derivatives is about 6.9 ev and the serine amino acid is 6.7 ev. Moreover, these values for the diazinon-serine complexes are very close together which shows about 6.7 ev, representing a reduction of about 0.2 ev compared to that of diazinon derivatives. Complexes No. 2 and No. 5 have the minimum values and complexes No. 1 and No. 4 with the maximum values of ionization energy. By examining the data, the electron affinity (A) is about 1.06 ev for diazinon derivatives, 0.18 ev for serine amino acid and about 1.05 ev for diazinon-serine complexes. The chemical potential (μ) values are approximately -4 ev for diazinon derivatives, -3.4 ev for serine amino acid and about -3.9 ev for diazinon-serine complexes, which have changes about 0.1 ev compared to the diazinon derivatives. The electronegativity (χ) values are about 4 ev for diazinon derivatives, 3.4 ev for serine amino acid and about 4 ev for diazinon complexes, which have changes approximately 0.1 ev relative to diazinon derivatives. The hardness (η) values are about 2.93 ev for diazinon derivatives, 3.25 ev for serine amino acid and about 2.55 ev for diazinon complexes, which have a decline about 0.07 ev relative to the diazinon derivatives. The electrophilicity values are about 2.72 ev for diazinon derivatives, 1.8 ev for serine amino acid and approximately 2.67 ev for diazinon complexes, which have a decline about 0.05 ev relative to the diazinon derivatives

The trend of variations for quantum-mechanical descriptors is as follows:

(I): dia-ser6 > dia-ser3 > dia-ser1 > dia-ser4 > dia-ser2 > dia-ser5

(A): dia-ser4 = dia-ser1 > dia-ser5 > dia-ser2 > dia-ser3 > dia-ser6

(μ): dia-ser5 > dia-ser2 > dia-ser4 >dia-ser1 > dia-ser3 > dia-ser6

(χ): dia-ser6 > dia-ser3 > dia-ser1 > dia-ser4 > dia-ser2 > dia-ser5

(η): dia-ser6> dia-ser3 > dia-ser1 > dia-ser2 > dia-ser4 > dia-ser5

(ώ): dia-ser1 > dia-ser4 > dia-ser6 > dia-ser3 > dia-ser5 > dia-ser2

Table 2- Quantum-mechanical descriptors of diazinon, diazinon complex, serine and its derivatives

ITEM		*I (ev)*	*A (ev)*	*μ (ev)*	*X (ev)*	*η (ev)*	*ώ (ev)*
ser		6/6849	0/1823	-3/4336	3/4336	3/2513	1/8131
dia 1	m-m	6/9415	1/0719	-4/0067	4/0067	2/9348	2/7350
dia 2	e-e	6/8944	1/0511	-3/9728	3/9328	2/9216	2/7010
dia 3	p-p	6/8942	1/0523	-3/9732	3/9732	2/9210	2/7023
dia 4	m-e	6/9301	1/0705	-4/0003	4/0003	2/9298	2/7310
dia 5	m-p	6/9257	1/644	-3/9961	3/9961	2/9296	2/7254
dia 6	e-p	6/8882	1/0482	-3/9682	3/9682	2/9200	2/6963
dia-ser 1	m-m	6/7676	1/0607	-3/9136	3/9136	2/8529	2/6843
dia-ser 2	e-e	6/7295	1/0485	-3/8896	3/8896	2/8411	2/6625
dia-ser 3	p-p	6/7894	1/0398	-3/9148	3/9148	2/8750	2/6653
dia-ser 4	m-e	6/7404	1/0610	-3/9001	3/9001	2/8391	2/6788
dia-ser 5	m-p	6/7077	1/0539	-3/8803	3/8803	2/8264	2/6636
dia-ser 6	e-p	6/8030	1/0387	-3/9210	3/9210	2/8823	2/6670

8- Bond Lengths and Angles Calculations:

Followed by the structural studies, using b3ly/6-31G (d) method, lengths and angles of bonding the compounds before and after the formation of the complex for diazinon-serine complexes in the water medium were calculated and compared, and the change of angles and the general form of structures were examined separately. In this case, three important electrostatic bonds of O5 ... H-O4, O5 ... H-C9, and S ... H-O4 can be seen. The plot and number of atoms in these complexes are presented in Figure 2. The results associated with the

lengths and angles of the bonds have been collected in Tables 3 and 4.

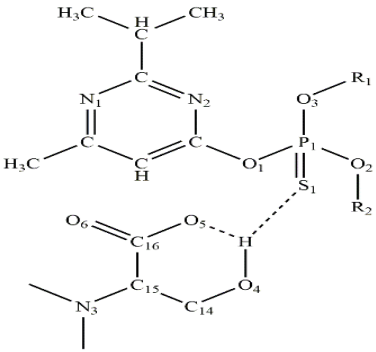


Figure 2- Structure and number of atoms in diazinon-serine complexes (dia-ser 1-6)

Table 3- Structural parameters of diazinon derivatives and serine amino acids

(Å) Bond Length	dia 1	dia 2	dia 3	dia 4	dia 5	dia 6	ser
O5…H-O4	2.25	2.37	2.28	2.37		2.15	
O5…H…S	2.54	3.48	2.50	3.58			
S…H-O4	2.78	2.71	2.84	2.69	2.66	3.10	
(°) Bond Angle							
O5…H-O4	92	88	93	41		46	
O5…H…S	14	71	79	47			
S…H-O4	106	93	105	107	91	106	
O1-P1-S1	116.02	115.86	115.85	115.76	115.76	115.87	
O2-P1-S1	117.65	117.53	117.59	117.55	117.49	117.51	
O3-P1-S1	113.40	113.51	113.42	113.55	113.59	113.45	
C14-C15-C16							109.98
C14-O4-H							105.14
C14-C15-H							107.66

Table 4- Structural parameters of diazinon and serine complexes

(Å) Bond Length	dia-ser 1	dia-ser 2	dia-ser 3	dia-ser 4	dia-ser 5	dia-ser 6
S-H	2.78	2.71	2.84	2.68	2.66	3.10

(°) Bond Angle						
O1-P1-S1	116.05	115.67	115.75	115.86	115.50	115.75
O2-P1-S1	117.91	117.73	117.72	117.67	117.44	117.97
O3-P1-S1	113.20	113.13	113.30	113.06	113.73	113.18
C14-C15-C16	110.19	110.26	110.18	110.41	110.28	109.98
C14-C15-H	108.32	108.42	108.38	108.28	108..53	107.66

9- Analysis of Atoms in Diazinon Complexes with Quantum Theory of Atoms in Molecules (QTAIM)

According to the results of Aim data, O5 ... H-C10 and S ... H-O4 and O5 ... H-O4 bonds in the dia-ser complex1, as well as O5 ... H-C10 and S ... H-O4 and O5 ... H-O4 bonds in the dia-ser complex2, O5 ... H-C10 and S ... H-O4 and C12-H ... N3 and O5 ... H-O4 bonds in the dia-ser complex 3, O4 ... H-C9 and S ... H-O4 and S ... O5 and O5 ... H-O4 bonds in the dia-ser complex 4, S ... H-O4 and O5 ... H-O4 bonds in the dia-ser complex 5 and finally, O4 ... H-C9 and S ... H-O4 and O5 ... H-O4 and N3 ... H-C9 N3 ... H-C11 bonds in the dia-ser complex 6, and also O6 ... H-O4 bond in the serine amino acid have low ρ (r) values and positive Laplacian and H (r) values; therefore, they have Ionic and electrostatic properties and the rest of the bonds (blue data) enjoy a covalent nature.

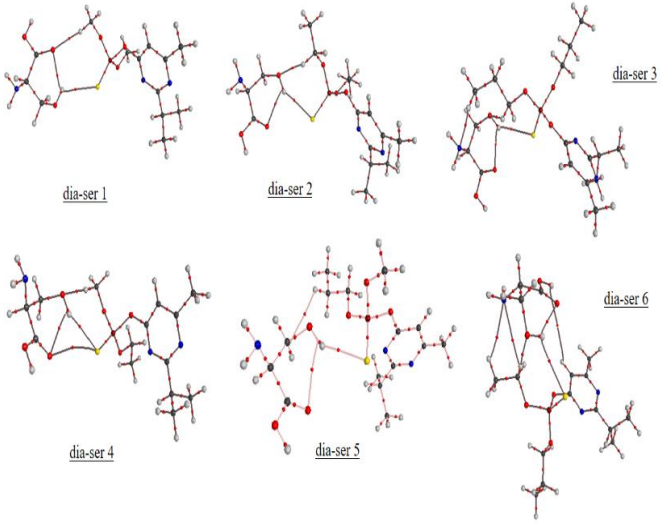


Figure 3- Hydrogen bonds in diazinon-serine complexes

10- Study of Electron Transfer (ET)

According to examining the uv-vis peak and electron transfers, the highest percentage of H-9 → L transfer was observed in the serine amino acid at a maximum wavelength of 106.75 nm (Figure 4). In the dia 1 derivative of diazinon, the highest percentage of transfer at maximum wavelength of 175.54 nm is related to H-5 → L and H-4 → H; as well as, the highest percentage of transfer at maximum wavelength of 181.12 nm is related to H-5 → H. In the dia 2 derivative, the highest percentage of transfer at maximum wavelength of 175.70 nm is related to H-5 → L; as well as, the highest percentage of transfer at maximum wavelength of 199.63 nm is related to H-4 → L. Furthermore, in the dia 3 derivative, the highest percentage of transfer at maximum wavelength of 175.70 nm is related to H-3 → L and H-4 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.83 nm is related to H-4 → L. In the dia 4 combination, the highest percentage of transfer at maximum wavelength of 175.82 nm is related to H-5 → L + 1; as well as, the

highest percentage of transfer at maximum wavelength of 181.50 nm is related to H-2 → L + 3. Studies of electron transfer in the dia 5 derivative show that the highest percentage of transfer at maximum wavelength of 175.77 nm is related to H-4 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.45 nm is related to H-4 → L + 1. And in the case of the dia 6 derivative, the highest percentage of transfer at maximum wavelength of 175.80 nm is related to H-4 → L + 1; as well as, the highest percentage of transfer at **m**aximum wavelength of 181.37 nm is related to H-4 → L.

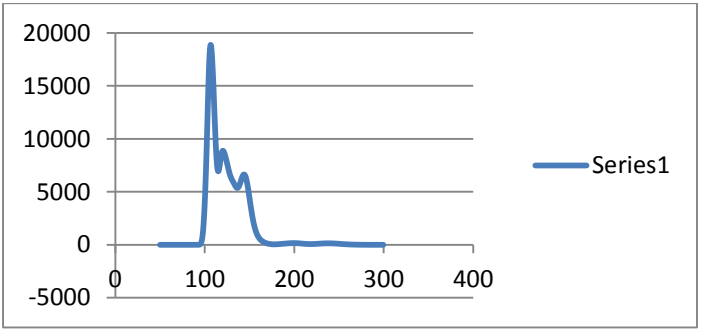


Figure 4- Uv-vis peak of the serine amino acid

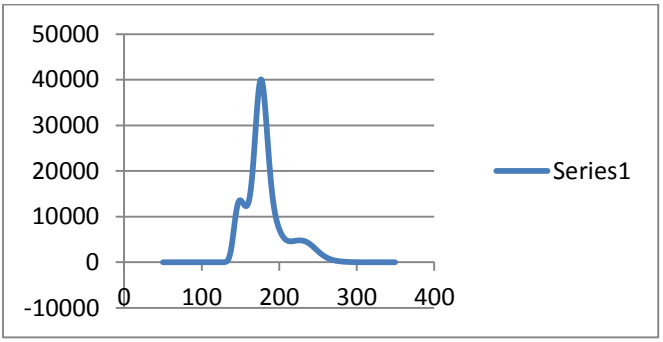


Figure 5- Uv-vis peak of the diazinon (dia 1)

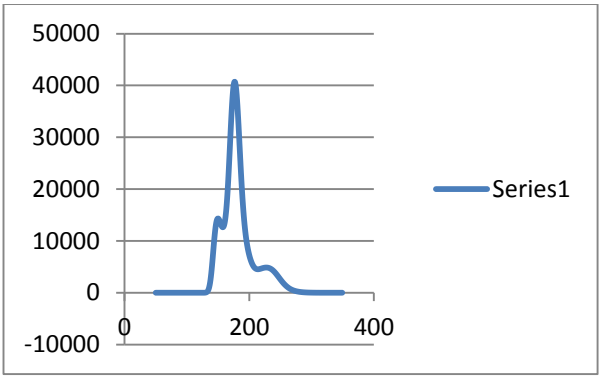


Figure 6- Uv-vis peak of the diazinon (dia 2)

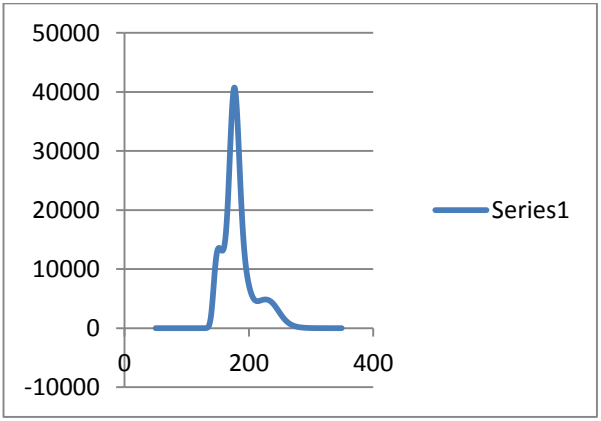


Figure 7- Uv-vis peak of the diazinon (dia 3)

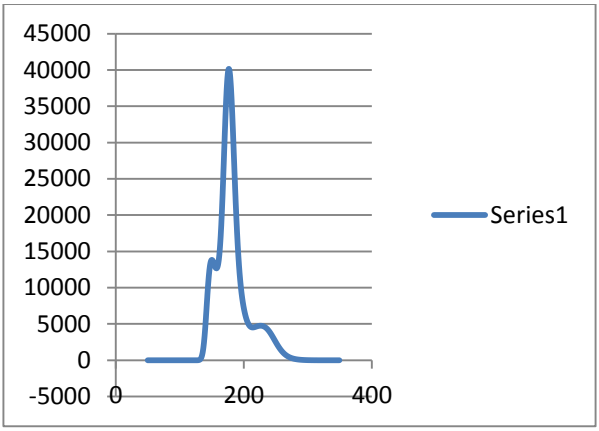


Figure 8- Uv-vis peak of the diazinon (dia 4)

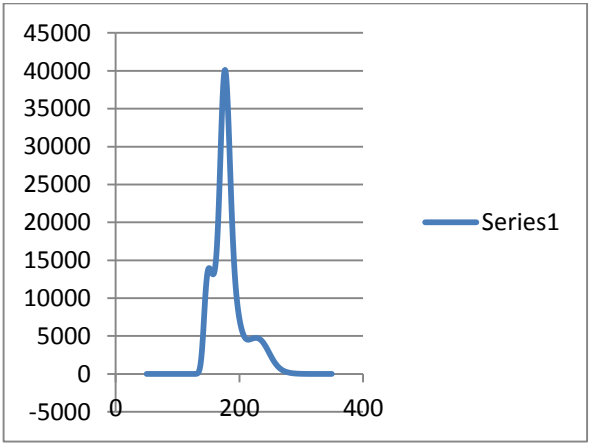


Figure 9- Uv-vis peak of the diazinon (dia 5)

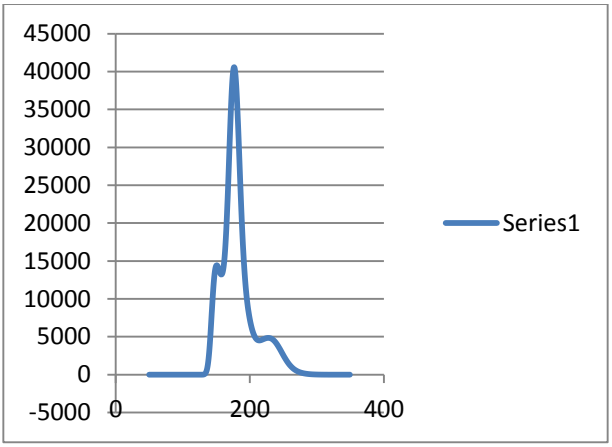


Figure 10- Uv-vis peak of the diazinon (dia 6)

In evaluating the electron transfers of diazinon-serine complexes, the results indicate that, in the dia-ser1 complex, the highest percentage of transfer at maximum wavelength of 175.62 nm is related to H-4 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 199.63 nm is related to H-4 → L. In the dia-ser2 complex, the highest percentage of transfer at maximum wavelength of 175.41 nm is related to H-7 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 180.95 nm is related to H-7 → L. The results of the electron transfer of the dia-ser3 complex show that the highest percentage of transfer at maximum wavelength of 175.63 nm is related to H-7 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.22 nm is related to H-7 → L. In the dia-ser4 complex, the highest percentage of transfer at maximum wavelength of 175.62 nm is related to H-7 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.10 nm is related to H-8 → L + 1. In the dia-ser5 complex, the highest percentage of transfer at maximum wavelength of 175.77 nm is related to H-7 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.26 nm is related to H-3 → L + 2. Finally, using computational data, it was

found that, in the dia-ser6 complex, the highest percentage of transfer at maximum wavelength of 175.91 nm is related to H-7 → L + 1; as well as, the highest percentage of transfer at maximum wavelength of 181.64 nm is related to H-7 → L.

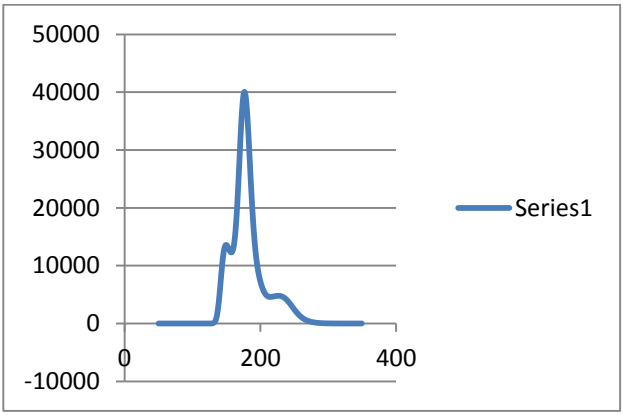


Figure 11- Uv-vis peak of the diazinon-serine complex (dia-ser 1)

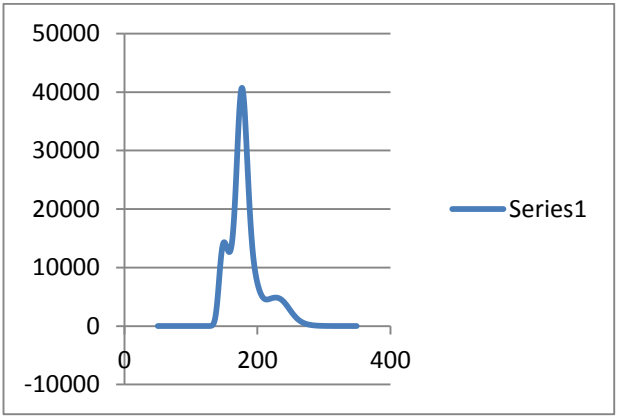


Figure 12- Uv-vis peak of the diazinon-serine complex (dia-ser 2)

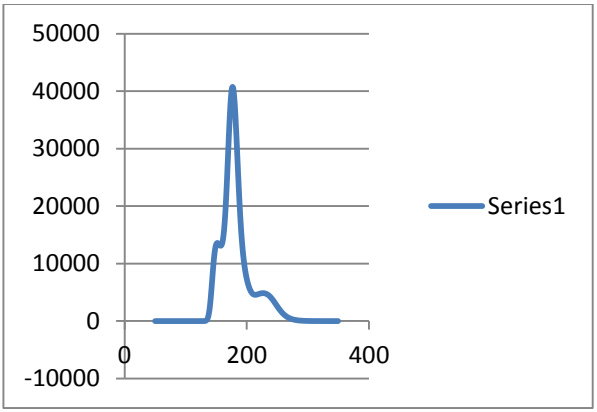


Figure 13- Uv-vis peak of the diazinon-serine complex (dia-ser 3)

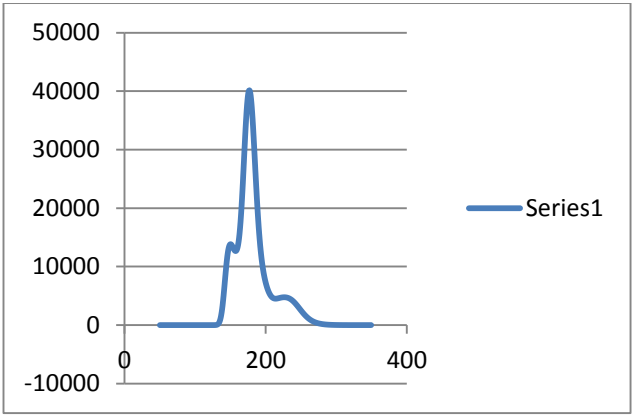


Figure 14- Uv-vis peak of the diazinon-serine complex (dia-ser 4)

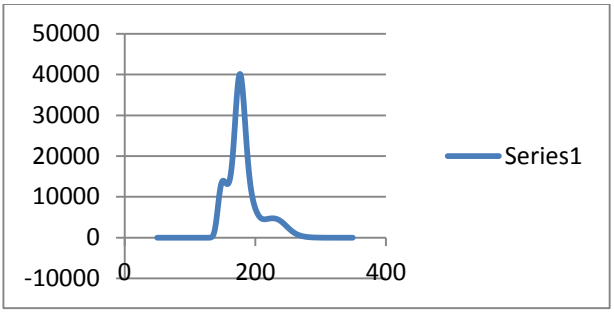


Figure 15- Uv-vis peak of the diazinon-serine complex (dia-ser 5)

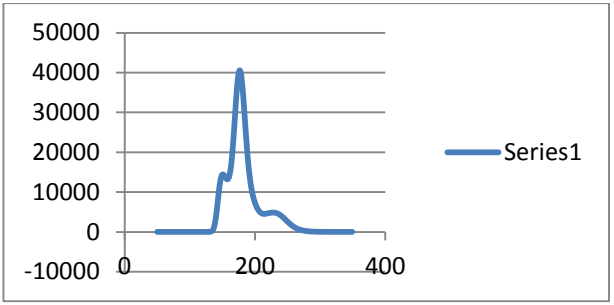
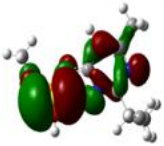
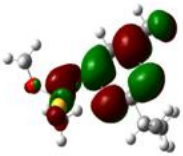
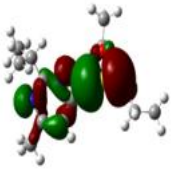
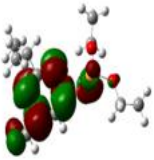
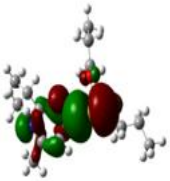
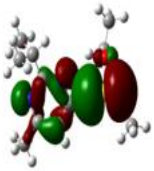
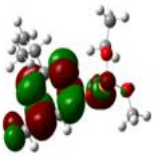
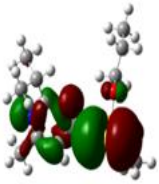
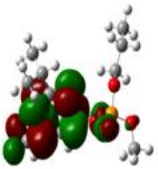


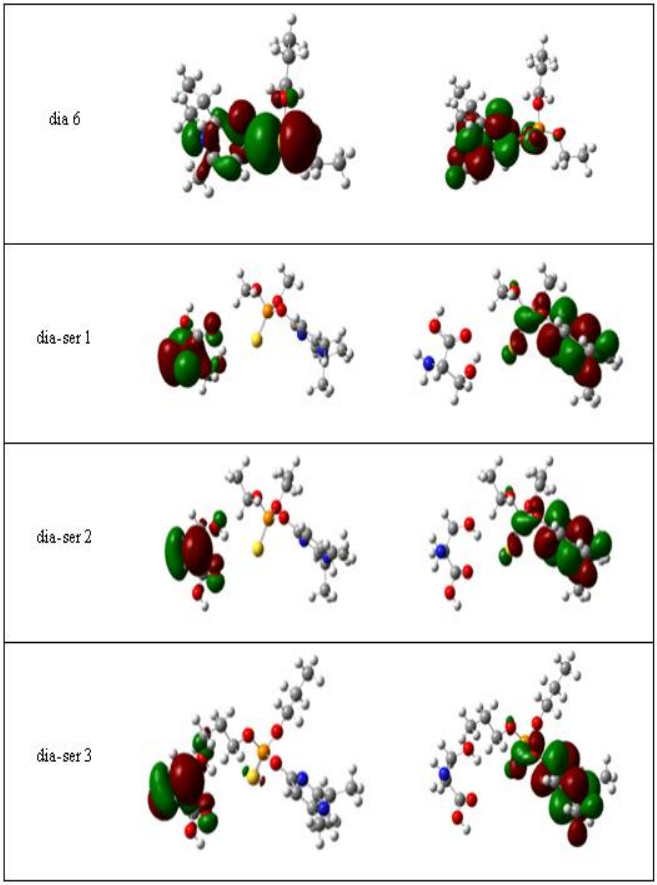
Figure 16- Uv-vis peak of the diazinon-serine complex (dia-ser 6)

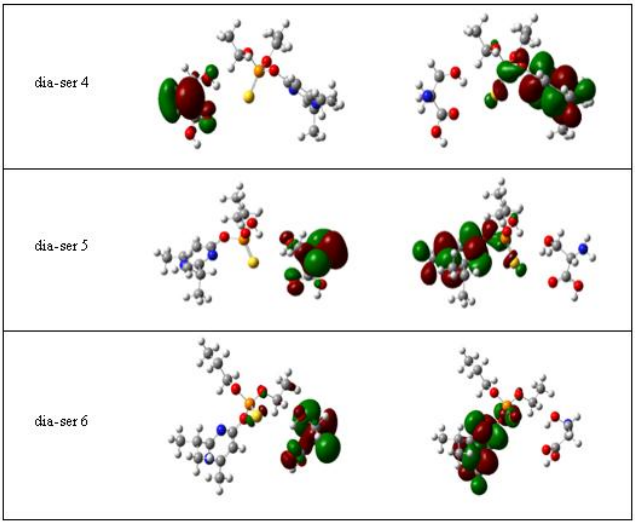
11- Evaluation of HOMO and LUMO Forms

Negatively charged wave functions (red) and positively charged wave functions (green) in the LUMO forms are focused more on the aromatic ring of diazinon and its derivatives and in the complexes on the aromatic ring of the diazinon-serine complex. The functions in the HOMO forms, in addition to the aromatic ring of diazinon and its derivatives, are focused on the phosphate esters of these compounds and in the complexes on the serine amino acid (Table 5).

Table 5- HOMO and LUMO forms in diazinon derivatives and diazinon-serine complexes

Item	homo forms	Lumo forms
dia 1		
dia 2		
dia 3		
dia 4		
dia 5		

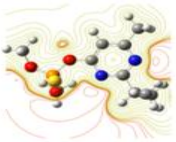
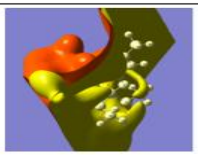
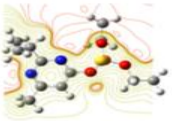
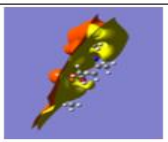
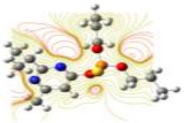
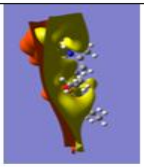
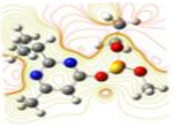

dia 6
dia-ser 1
dia-ser 2
dia-ser 3

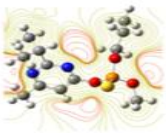
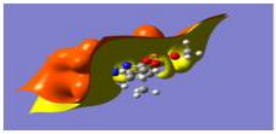
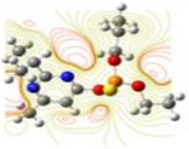
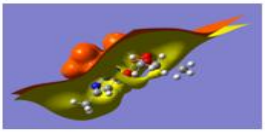
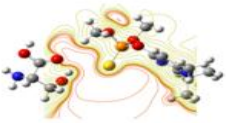
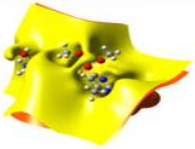
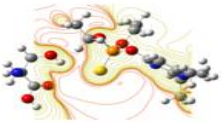
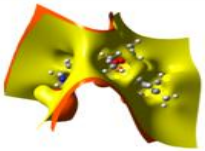


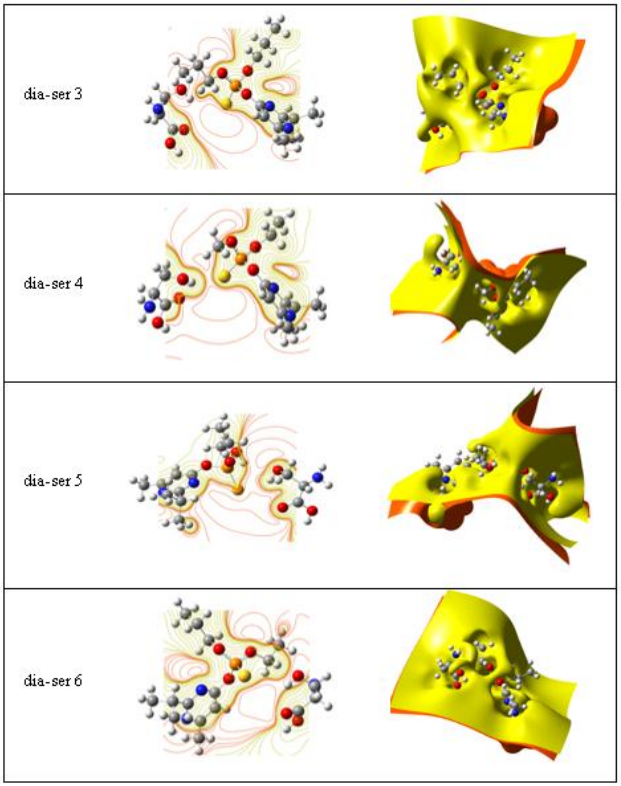
12- Examining the Surface Electrostatic Charge Potential and Contour Map Images

In the surface electrostatic charge potential forms, the negative charge density plate (red) is outside the molecule and the positive charge density plate (green) surrounds the molecule itself. In the contour forms, the negative charge lines (red) are around the molecule and the positive charge lines (green) circumvent within the molecule. Density plates and lines in contour maps in confirming the results of dipole moment calculations show that diazinon and its derivatives are not symmetrical. In the surface electrostatic charge potential and the contour map forms of diazinon complexes with serine amino acid, the asymmetry of all complexes is again evident. The dipole moment in complexes 2, 4 and 5 decreased relative to the individual combination and the dipole moment in complexes 1 and 6 increased relative to the individual combination. The changes in the positively charged lines and the negatively charged lines in relation to the individual combination in the contour map confirm this (Table 6).

Table 6- Images of surface electrostatic charge potential and contour map in diazinon derivatives and diazinon-serine complexes

Item	contour	Surface
dia 1		
dia 2		
dia 3		
dia 4		

dia 5		
dia 6		
dia-ser 1		
dia-ser 2		



13- Conclusion

In this project, to investigate the effect of diazinon pesticide and its derivatives on serine amino acid and detect the most stable diazinon complexes with serine, DFT calculations with B3LYP method and 6-31G (d, p) standard basis set were performed. The interaction of these compounds was demonstrated through the length of the bond between the surface of the HOMO and LUMO, electronic transfers, and quantum mechanical descriptors. The nature of the bond between serine amino acid and all derivatives of diazinon is electrostatic and intramolecular interactions indicate the stability of these complexes. The dipole moment of the diazinon derivatives and its complexes with

serine amino acids reveals that the dipole moments are close together and the dipole moment of complex No. 5 have had the greatest decline compared to its individual derivative. In the evaluation of thermodynamic data, the process of forming all reactions is non-spontaneous and thus endothermic. Gibbs free energy for diazinon complexes is in the range of 8.6 to 11.8. In examining the Energy Band Gap (EG) and the Natural Bond Orbital (NBO), the difference in energy between the highest occupied molecular orbital of HOMO and the lowest empty molecular orbital of LUMO that represents the electron conductivity was studied. Finally, in reviewing the data of the quantum-mechanical (QM) descriptor, it was found that diazinon complex No. 5 enjoys a favorable condition. Quantum chemistry calculations and thermodynamic data in this study will be effective in order to complete the research of experimental tests data, because they have identified the conditions for the synthesis of these complexes, and it is obvious that experimental tests with shorter time and less cost can be conducted. To complete the information in this area, it is recommended that an experiment regarding the effect of organophosphate pesticides with oxygen functional group on the phosphorus atom on the serine amino acid, as well as the effect of the pyrethroid pesticides (new generation of agricultural pesticides) on amino acids to be done in the future investigations.

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