



QSAR relationships The changes in the ratio of electrons to the natural charge of atoms in the complexes of glycine and alanine amino acids with intermediates

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Abstract

In this paper, the quantum chemistry calculations related to the structural parameter of the three anions and the resulting complexes with glycine and alanine have been performed. The calculations were carried out using the HF and DFT method and in the base series 6-31G *. Natural Transplantation Orbital (NBO), hybrid capacity for bindings and is obtained. The ratio of the internal electrons, Valance and Reedberg to the natural charge of atoms and its relation with complex stability have been considered.

Keywords: NBO, glycine, alanine, natural charge

1. Introduction

In the last 40 years, the presence of a small amount of chromium in human and animal nutrition has been known to be known. Chromium is present in more natural forms with chromium, and this form is much more stable than its form. The role of chromium in antioxidant activity and favorable effects on stability and nucleic acids are known. Although its most important metabolic effect is the increase in insulin activity due to the presence of chromium in an organic metal molecule, which is known as the factor of tumor growth factor. The structural details are unknown. But it seems that the factor consists of nicotinic acid, glutamic acid, glycine and cystine. In humans, chromium concentration in the lung tissue is highest. Molybdenum plays a key role in metabolic processes such as sulfur dioxide, purine catabolism, nitrate absorption and hormonal synthesis in plants. Chromium and molybdenum are intermediate elements of a periodic table group, both of which are both low but essential in nutrition because they play a key role in the metabolism of the body's chemical activities. Anion analysis of these compounds has been performed to compare the properties of the elements of the periodic table in a group of the periodic table.

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of glycine and alanine were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Fluoxetine on Fullerene were investigated through attachment to three different base positions. All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor.

In this report, all computations of quorum gas constituents in the gas phase have been performed. For calculations of chromium, molybdenum, the Lanl2DZ base series and for the 6-31G * base series are used for carbon and hydrogen, and nitrogen and oxygen. All compounds are initially optimized by the Hatter method and the density function theory. In this work, glycine and alanine are located around the chromite and molybdate ions. NBO normal orbital analysis was performed with the NBO key word. The values of the ratio of the electron ratios of the valence electrons and the additional electrons of each atom to the partial charge on that atom are obtained for the complexes studied by the NBO method in the 6-31G * series in both HF and DFT methods.

3. Results

In Fig. 1, the ratio of the electron beam to the atoms for the two complexes has been shown and there are completely two graphs in the negative loads, while in the positive loads the ratio of the electron-brain ratios to the charge for the complex is greater, which indicates that the stability of this complex is greater. Figure 2 shows the ratio of the ratio of the electrons to the load on the atom for and shown in the two diagrams in the negative load section on the atom, but in positive loads, the ratio of the electrons to the charge for a lower value, which indicates a higher stability than the ratio It is a complex. Figure 3 shows that, in the range of negative loads on the atom, the ratio of the excess electrons to the partial load (load / leaf reed) is greater than that, but this trend is reversed in the range of positive loads, that is, the ratio (load / leaf reed) is less than . For the range of negative loads, the ratio of total is shown in Fig. 4 for the range of negative loads, while for the total positive load ratio the total ratio is less than the HF and DFT methods, one is the one that indicates the general accuracy of the method and the method for doing these calculations and also The stability of the molybdenum complex is more than that. In Fig. 5, the ratio of the ratio of electron nuclei to the atomic mass in the complexes is in the range of negative bands, while the ratio of the electron cores to the atomic charge in the range of positive loads is greater than that which indicates the stability of the complex. Fig. 6 The ratio of the electrons to the load in the complexes and the lower ratio of the electrons to the load, which itself indicates a higher stability

than that. Fig. 7 shows the additional electron diagram of the charge on the atom for 2 complexes. Here, the curve in the boundary of the curve loads is greater than the ratio of the additional electrons to the charge for the complex, and in the range of positive loads, the ratio of the additional electrons to the charge is lower, indicating that its complex stability is greater than that.



Fig. 1 Characterization of the changes of the brain electrons to the partial charge of the atom in complexes and in the 6-31G* base series in two methods HF and DFT

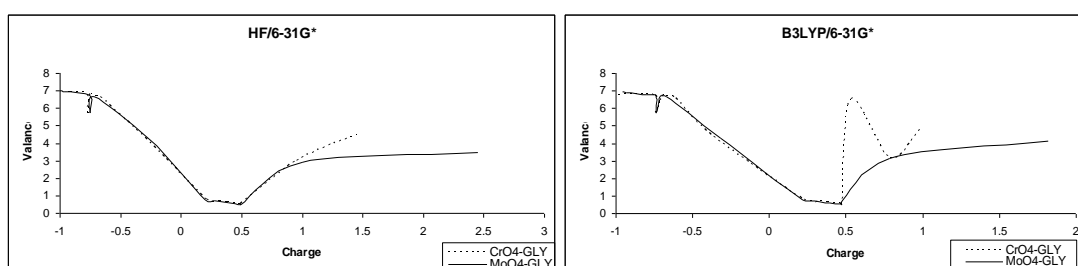


Fig. 2 Characterization of the changes in the thickness layer electrons to the partial load of the atom in the complexes and in the 6-31G* base series in two methods HF and DFT

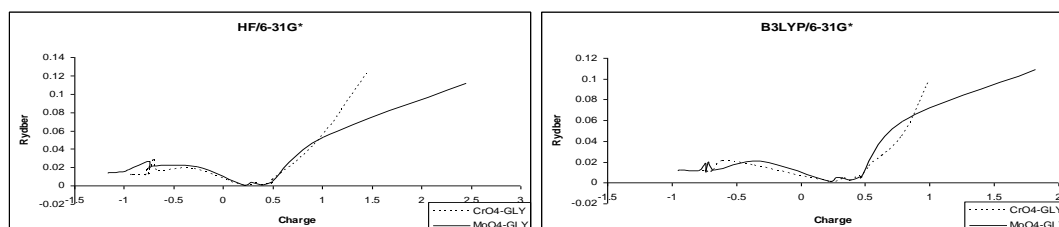


Fig3. Characterization of the changes of additional electrons to the partial charge of the atom in complexes, and in the 6-31G* base series in two methods HF and DFT

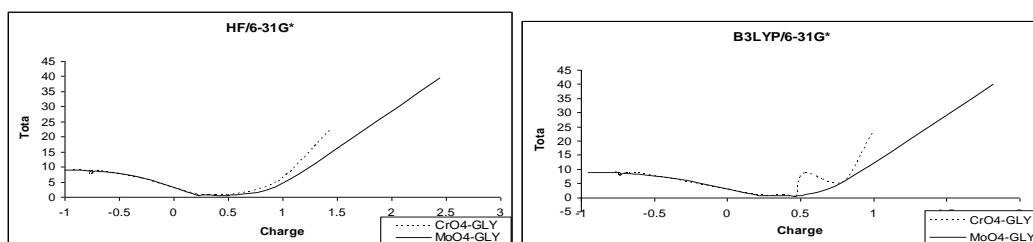


Fig4 shows the evolution of total electrons to the partial charge of the atom in complexes and in the standard series 6-31G * in both HF and DFT

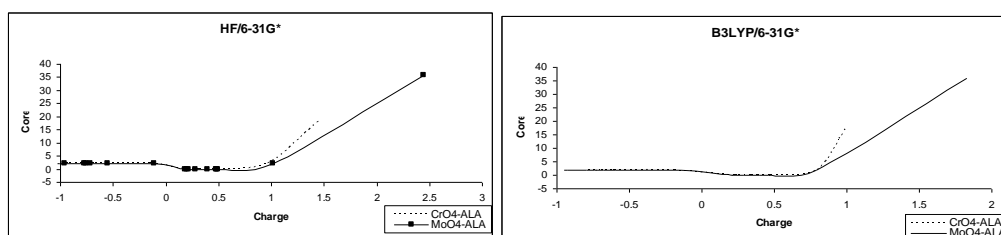


Fig. 5 Characterization of the changes of the brain electrons to the partial load of the atom in the complexes and in the standard series 6-31G * in two methods HF and DFT

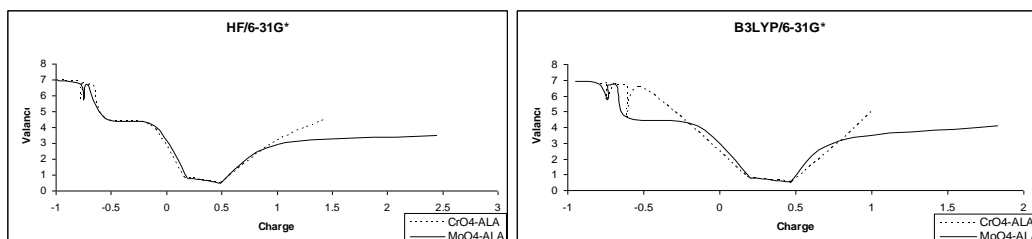


Fig. 6 Characterization of the variations of the electron layer thickness to the partial load of the atom in the complexes, and in the standard series 6-31G * in both HF and DFT

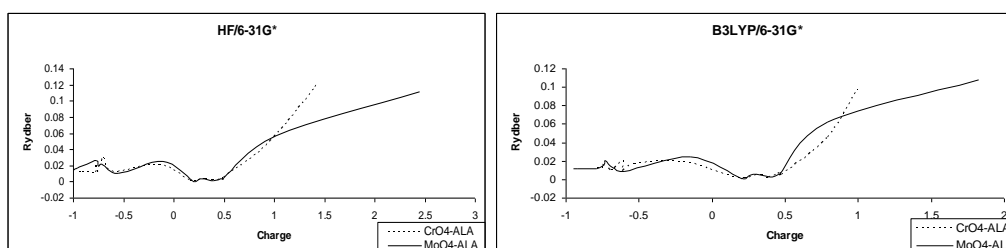


Fig. 7 Characterization of the changes of the additional electrons to the partial charge of the atom in the complexes and in the standard series 6-31G * in two methods HF and DFT

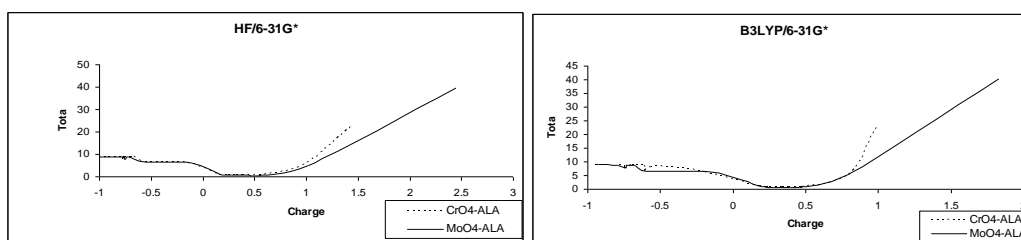


Fig 8. shows the evolution of total electrons to the partial load of the atom in complexes and in the standard series 6-31G * in both HF and DFT

In Table 2, the hybrid coefficients of all anionic bonds obtained from the NBO method in the 6-31G * base series are presented with two HF and DFT methods. Comparison of the bonds in these two compounds. It is stated that in molybdenum anion, the number of double bonds and (graft) bands according to both HF and DFT methods is more than chromite. In the HF method, the number of bonds in the anion is less than molybdenum until and when it occurs. However, in the DFT The number of bonds in anion is more molybdenum than the complex with glycine or alanine. In Table 1, the share of orbital (P & D) in complex links and calculated by NBO technique in the 6-31G * series series is presented with two HF and DFT methods. The share of orbital (P & D) in metal-oxygen bonds in anion. Complexes and differences do not show much difference, while the share of orbitals (P & d) in metal-oxygen bondings in anions. The complex is considerably more complex than the other. The results obtained from the HF and DFT method confirm the two cases.

Table 1. Percentage of orbital d and p in complex compounds, and by NBO method in 6-31G * series in both HF and DFT methods

bonds	$CrO_4^{2-}GLY(HF)$				$CrO_4^{2-}GLY(B3LYP)$			
	σ		π		σ		π	
	p	d	p	d	p	d	p	d
Cr-O ₂	2.83	0.3625	-	-	0.01	1.02	-	-
Cr-O ₃	3.17	2.043	21.13 1.00	1.72 1.51	3.068	1.59	0.6206 63.24	38.32 37.99
Cr-O ₄	2.56	1.302	99.99	39.23	3.24	1.22	-	-
Cr-O ₅	2.83	0.8475	-	-	3.31	1.02	-	-
bonds	$MoO_4^{2-}GLY(HF)$				$MoO_4^{2-}GLY(B3LYP)$			
	σ		π		σ		π	
	p	d	p	d	p	d	p	d
Mo-O ₂	1.93	0.7216	-	-	2.63	0.7879	-	-
Mo-O ₃	2.64	1.01	14.96 80.02	3.01 9.47	2.74	0.9519	74.22	9.26
Mo-O ₄	2.10	1.01	84.24	28.29	2.78	1.183	2.78	16.9185
Mo-O ₅	1.93	0.9602	82.42 17.95	25.40 26.53	2.23	0.9226	29.98 99.99	29.27 32.18

For anion, there is no link between Cr and oxygen atoms, while when Gly + or AIA + is placed side by side, a similar number of grafts is generated in the anion. For ionic state, the number of bands and multiple bands in the individual anions before the formation of the complex 4 were graft, whereas after the complexation with Gly + and AIA +, the number of bonds to 5 was multiple.

Table 2 Hybrid coefficients of all anionic links and its complex with Gly + and AIA + obtained from the NBO method in the 6-31G * series with two HF and DFT methods

Bond	HF(CrO_4^{2-})	B3LYP(CrO_4^{2-})
$Cr_1 - O_2$	$\sigma = 0.5587(sp^{0.01}d^{3.30})_{Cr_1} + 0.8294(sp^{7.09}d^{0.02})_{O_2}$	$\sigma = 0.4989(sp^{0.31}d^{2.30})_{Cr_1} + 0.8666(sp^{7.46}d^{0.02})_{O_2}$ $\pi = 0.3764(p^{6.73}d^{23.14})_{Cr_1} + 0.9265(p)_{O_2}$
$Cr_1 - O_3$	$\sigma = 0.5587(sp^{0.01}d^{3.30}f^{0.02})_{Cr_1} + 0.8294(sp^{7.09}d^{0.02})_{O_3}$	
$Cr_1 - O_4$	$\sigma = 0.5514(sp^{0.06}d^{3.49}f^{0.01})_{Cr_1} + 0.8342(sp^{7.46}d^{0.02})_{O_4}$	$\sigma = 0.5514(sp^{0.06}d^{3.49}f^{0.01})_{Cr_1} + 0.8342(sp^{7.46}d^{0.02})_{O_4}$ $\pi = 0.3871(sp^{5.60}d^{22.13}f^{0.33})_{Cr_1} + 0.9220(p)_{O_4}$ $\pi = 0.3724(sp^{9.26}d^{26.47}f^{0.53})_{Cr_1} + 0.9281(p)_{O_4}$
$Cr_1 - O_5$	$\sigma = 0.5587(sp^{0.01}d^{3.03}f^{0.02})_{Cr_1} + 0.8294(sp^{7.09}d^{0.02})_{O_5}$	$\sigma = 0.5166(sp^{0.18}d^{2.35}f^{0.02})_{Cr_1} + 0.8562(sp^{7.46}d^{0.02})_{O_5}$ $\pi = 0.3871(sp^{5.62}d^{22.15}f^{0.33})_{Cr_1} + 0.9220(p)_{O_5}$
Bond	HF($CrO_4^{2-}GLY$)	B3LYP($CrO_4^{2-}GLY$)
$Cr_1 - O_2$	$\sigma = 0.4840(sp^{0.23}d)_{Cr_1} + 0.8751(sp^{4.28}d^{0.01})_{O_2}$	$\sigma = 0.5243(sp^{0.01}d^{2.67})_{Cr_1} + 0.8515(sp^{5.37}d^{0.01})_{O_2}$
$Cr_1 - O_3$	$\sigma = 0.5679(sp^{0.02}d^{4.99})_{Cr_1} + 0.8231(sp^{5.34}d^{0.01})_{O_3}$	$\sigma = 0.5754(sp^{0.01}d^{3.84})_{Cr_1} + 0.8179(sp^{5.22}d^{0.01})_{O_3}$
	$\pi = 0.4560(sp^{0.26}d^{4.99})_{Cr_1} + 0.8900(sp^{31.82}d^{0.05})_{O_3}$	$\pi = 0.5278(p^{0.01}d^{99.99})_{Cr_1} + 0.8494(p^{1.00})_{O_3}$
	$\pi = 0.3926(sp^{1.00}d^{5.04})_{Cr_1} + 0.9197(sp^{1.00})_{O_3}$	$\pi = 0.5159(sp^{2.21}d^{99.99})_{Cr_1} + 0.8566(sp^{99.99}d^{0.65})_{O_3}$
$Cr_1 - O_4$	$\sigma = 0.5507(sp^{0.01}d^{3.26})_{Cr_1} + 0.8347(sp^{4.24}d^{0.01})_{O_4}$	$\sigma = 0.5386(sp^{0.01}d^{3.11})_{Cr_1} + 0.8425(sp^{5.32}d^{0.01})_{O_4}$
	$\pi = 0.3861(sp^{99.99}d^{99.99})_{Cr_1} + 0.9225(sp^{99.99}d^{13.80})_{O_4}$	
$Cr_1 - O_5$	$\sigma = 0.4869(sp^{0.23}d^{2.35})_{Cr_1} + 0.8735(sp^{4.28}d^{0.01})_{O_5}$	$\sigma = 0.5261(sp^{0.01}d^{2.64})_{Cr_1} + 0.8504(sp^{5.35}d^{0.01})_{O_5}$
Bond	HF($CrO_4^{2-}ALA^{1+}$)	B3LYP($CrO_4^{2-}ALA^{1+}$)
$Cr_1 - O_2$	$\sigma = 0.4814(sp^{0.22}d^{2.22})_{Cr_1} + 0.8765(sp^{4.27}d^{0.01})_{O_2}$	$\sigma = 0.4829(sp^{0.27}d^{2.40})_{Cr_1} + 0.8757(sp^{5.40}d^{0.01})_{O_2}$
$Cr_1 - O_3$	$\sigma = 0.5586(sp^{0.03}d^{5.58})_{Cr_1} + 0.8294(sp^{5.95}d^{0.01})_{O_3}$	$\sigma = 0.5749(sp^{0.02}d^{3.82})_{Cr_1} + 0.8182(sp^{5.27}d^{0.01})_{O_3}$
	$\pi_1 = 0.4640(sp^{0.32}d^{19.87})_{Cr_1} + 0.8858(sp^{21.91}d^{0.04})_{O_3}$	$\pi_1 = 0.4310(sp^{99.99}d^{99.99})_{Cr_1} + 0.9024(sp^{99.99}d^{10.02})_{O_3}$
	$\pi_2 = 0.3971(sp^{99.99}d^{99.99})_{Cr_1} + 0.9178(sp^{99.99}d^{2.74})_{O_3}$	$\pi_2 = 0.5149(sp^{3.11}d^{99.99})_{Cr_1} + 0.8572(sp^{99.99}d^{0.39})_{O_3}$
$Cr_1 - O_4$	$\sigma = 0.5479(sp^{0.03}d^{3.35})_{Cr_1} + 0.8365(sp^{4.37}d^{0.01})_{O_4}$	$\sigma = 0.5390(sp^{0.01}d^{3.08})_{Cr_1} + 0.8423(sp^{5.27}d^{0.01})_{O_4}$
	$\pi = 0.3909(sp^{24.65}d^{99.99})_{Cr_1} + 0.9204(sp^{99.99}d^{0.28})_{O_4}$	$\pi = 0.4213(sp^{99.99}d^{99.99})_{Cr_1} + 0.9069(sp^{99.99}d^{4.54})_{O_4}$
$Cr_1 - O_5$	$\sigma = 0.4888(sp^{0.23}d^{2.42})_{Cr_1} + 0.8724(sp^{4.26}d^{0.01})_{O_5}$	$\sigma = 0.4878(sp^{0.26}d^{2.44})_{Cr_1} + 0.8730(sp^{5.34}d^{0.01})_{O_5}$

n compounds containing Mo, the proportion of nuclear electrons to the natural charge of the atom is greater than this ratio in the same compounds, including Cr, while the ratio of valence and extracellular electrons on the atoms to Mo compounds is lower than that of Cr compounds (Table 3).

Table 3. Electron-to-Atom Ratio in Chromate and Molybdate Complexes with Glycine and Alanine Calculated by NBO Technique in Base Series 6-31G * in both HF and DFT

<i>HF^a, B3LYP^b (6-31G*)</i>				
	<i>Core Charge</i>	<i>Valence Charge</i>	<i>Rydberg Charge</i>	<i>Total Charge</i>
<i>CrO₄²⁻GLY</i>	12.3938 ^a	3.0945	0.08472	15.5730
	18.0059 ^b	4.9457	0.09893	23.0505
<i>MoO₄²⁻GLY</i>	14.6927	1.4290	0.04556	16.1673
	19.7552	2.2601	0.0600	22.0754
<i>CrO₄²⁻ALA</i>	12.4032	3.0976	0.0847	15.5850
	17.9778	4.9366	0.0986	23.0130
<i>MoO₄²⁻ALA</i>	14.6933	2.8882	0.0458	16.1680
	19.6850	2.2495	0.0592	21.9900

Conclusion

In the compounds containing Mo, the proportion of nuclear electrons to the natural charge of the atom is greater than this ratio in the same compounds, including Cr, while the ratio of valence and additional electrons to the atoms is related to Mo compounds less than Cr compounds. For anion, there is no link between Cr and oxygen atoms, while when Gly + or Ala + is placed side by side, a similar number of grafts is generated in the anion. For ionic mode, multiple bands and numbers, In its single anion, it was 4 before the formation of the complex 4 complex, while after the formation of the complex with Gly + and Ala +, the number of multiple bonds reached 5. The fact that after complex formation and with Gly + and Ala +, the number of multiple bonds within these anions increases. The stability of these complexes can be predicted from the initial anions, of course, and Kth values confirm this fact. The stability of most of the Mo compounds in relation to Cr compounds is related to the greater ability of Mo to form multiple bonds with the O atom.

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5. Conclusion:

Computational Quantum Mechanics at the theory level of B3LYP/6-31G on the structure of Fullerene and Fullerene Derivatives of Fluoxetine drug was done separately and only when the structure of Fluoxetine was attached to Fullerene and the results of this computation can be classified as follows:

- The investigation of all the parameters show that the attachment of Fluoxetine structure to Fullerene structure will influence the energy levels and dipole moment changes and these changes are able to be investigated in the electrical and chemical parameters of Fullerene Derivatives structure.
- The results showed that energy gap of FS is the highest and FFS (3) is the lowest. It should be noted that conductivity of FFS (3) is the highest and FS is the lowest.
- Chemical potential of FFS (3) is more than FS and after of them is FFS (1) and (2).
- Chemical hardness of FS is the highest and the lowest value is related to FFS (3).
- Dipole moment of FS is first and FFS (3) is the second.
- Bond length in FFS (3) in each bond is the most but bond of C1 and O in FFS (2) is the most.

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