



Comparison of Hartree Factor and Density Function Theory in Calculating Coating Constants and NMR Parameters of Chromate and Molecular Complexes with Alanine and Glycine

Vinod Nguyen*

Department of Chemistry, Faculty of Sciences, Ibn Zohr University, Agadir- Morocco.

*Corresponding Author e-mail Address: Vinod.nguyen.chem@gmail.com

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Abstract

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 chemical activity of the body. Anion analysis of these compounds in order to compare the properties of the elements of the periodic table in one The group is from the periodic table. In this paper, the quantum chemistry calculations related to the structural parameter of the two anions and the resulting complexes with glycine and alanine have been performed. The calculations have been done by HF and DFT methods and in the base series 6-31G *. NMR parameters and fixed tensors of coating and their changes have been considered. In this regard, the differences in the method in the accuracy of measurements have been considered.

Keywords: Chromium, molybdenum, HF , DFT methods.

1. Introduction

In this study, using quantum chemistry calculations, the anion structure and then the structure of the quorum (ionic complexes),, were optimized in the gas phase. The calculations were carried out for atoms with a standard 6-31G * base series and for metals in the standard lanL2Dz standard series. As the ions of the molecules were large molecules, the optimization was gradually and step-by-step, while completing the shape of the molecule from the smaller series to the larger. Since ions were quethritic molecules and there were electronic gravitational forces between cations and anions, and there was no coupling between two cation and anion components, for initial optimization, the dummy atom was used. Subsequently, NMR calculations were performed on them[1-5] .

2. Computational details

The NMR protection tensors obtained for the base series 6-31G * are presented in two hacker and hierarchical methods of density function (B3Lyp) (Table 1). In (Figures 1 to 4), the NMR protection tensor curve for anions and complexes is plotted. Figures show that in all cases the linear changes of anions in the complexes change to the curve. Which indicates the effects of complex formation on NMR protection tensors. In Fact's hartree method, the process is quite similar to the two complexes, so that the two curves correspond to each other, while in the DFT method, the distinction between the curve of two complexes is quite obvious In this case, the HF method is better. In Table 2, the calculated values for the anions and its complexes with glycine and alanine in the 6-31G * series are given in both HF and DFT (Fig. 5 to 7) The graphs of the calculated values for the anions of the oxygen are linear and for the oxygen species of the complexes obtained from this anion with glycine and alanine[6-10].

3. Results

Table 1 Comparison of Coefficient of Constant Constants for Anions and Its Complexes with Glazin and Alanine in the 6-31G *

Series by Two Methods of HF and DFT

		σ_{11}	σ_{22}	σ_{33}	σ_{iso}	σ_{aniso}
HF	Cr_1	-4686.6412	-4686.6412	-4686.6412	-4686.6412	0.0000
	O_2	-1264.6003	-1264.6003	223.3753	-768.6085	1487.9756
	O_3	-1264.6003	-1264.6003	223.3753	-768.6085	1487.9756
	O_4	-1264.6003	-1264.6003	223.3753	-768.6085	1487.9756

B3LYP	$CrO_4^{2-} GLY^{1+}$	O_5	-1264.6003	-1264.6003	223.3753	-768.6085	1487.9756	
		Cr_1	-6756.8945	-6340.6388	-5931.6481	-6343.0604	617.1185	
		O_2	-1408.1580	-640.5870	177.4253	-623.7732	1201.7979	
		O_3	-2475.2247	-1773.6225	84.8238	-1388.0078	2209.2474	
		O_4	-2282.3048	-1086.3657	159.5689	-1069.7005	1843.9041	
	$CrO_4^{2-} ALA^{1+}$	O_5	-1514.4273	-670.7814	180.2807	-668.3094	1272.8850	
		Cr_1	-6732.3859	-6389.2242	-5891.1986	-6337.6029	669.6065	
		O_2	-1290.2074	-606.9091	176.5612	-573.5184	1125.1195	
		O_3	-2490.5162	-1757.5068	90.0909	-1385.9774	2214.1024	
		O_4	-2318.1463	-1103.3732	156.3835	-1088.3787	1867.1432	
	B3LYP	CrO_4^{2-}	O_5	-1580.3484	-688.8079	176.3897	-697.5889	1310.9678
			Cr_1	-2329.4761	-2329.4761	-2329.4276	-2329.4599	0.0485
			O_2	-554.2738	-554.2698	-109.1927	-405.9121	445.0791
			O_3	-554.2738	-554.2698	-109.1927	-405.9121	445.0791
			O_4	-554.2738	-554.2698	-109.1927	-405.9121	445.0791
$CrO_4^{2-} GLY^{1+}$		O_5	-554.2738	-554.2698	-109.1927	-405.9121	445.0791	
		Cr_1	-393.5018	-333.1012	-279.6736	-335.4255	83.6279	
		O_2	-269.8512	-3.2210	256.4074	-5.5549	392.9435	
		O_3	-434.5604	-416.6409	145.3464	-235.2850	570.9470	
		O_4	-300.7515	-151.0836	-3.2380	-151.6910	222.6796	
$CrO_4^{2-} ALA^{1+}$		O_5	-300.1625	-16.1078	245.3304	-23.6466	403.4655	
		Cr_1	-4398.2934	-4155.1776	-4080.3452	-4211.2721	196.3903	
		O_2	-816.3977	-406.7214	-160.5314	-461.2168	451.0281	
		O_3	-1174.0195	-1022.2626	-419.1611	-871.8144	678.9799	
		O_4	-1060.7605	-557.6900	-276.2797	-631.5767	532.9455	
O_5	-951.5181	-442.0022	-210.3262	-534.6155	486.4339			

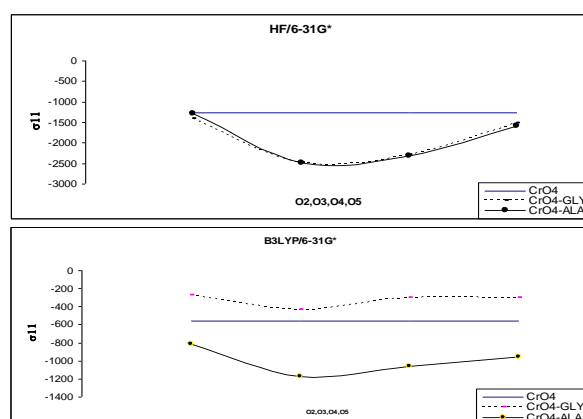


Fig1. shows the changes for oxygen atoms and in the base series in HF and DFT

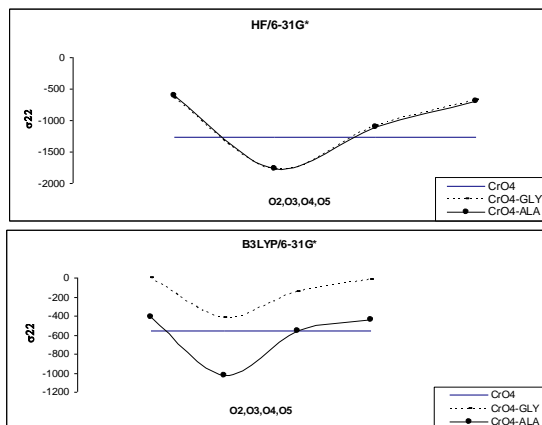


Fig. 2 shows the changes for oxygen atoms and in the base series in HF and DFT

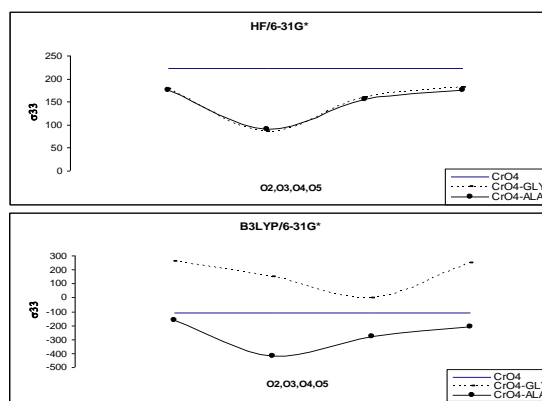


Fig. 3 shows the changes for the oxygen atoms and in the base series in the HF and DFT methods

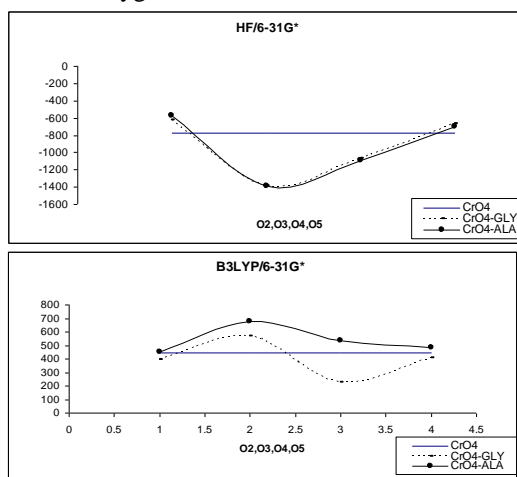


Fig. 4 shows the changes for the oxygen atoms and in the base series in the HF and DFT methods

Table 2 Comparison of the values for the anions and its complex with glycine and alanine in the base of 6-31G * in both HF and DFT

			η	δ	CSA	CSA_a
HF	CrO_4^{2-}	Cr_1	0	#DIV/0!	0	-3.72529E-09
		O_2	0	-2.54964	1487.976	861027.7778
		O_3	0	-2.54964	1487.976	861027.7778
		O_4	0	-2.54964	1487.976	861027.7778
		O_5	0	-2.54964	1487.976	861027.7778
	$CrO_4^{2-} GLY^{1+}$	Cr_1	-0.03391	-31.8355	617.1185	84134.83436
		O_2	-1.71967	-2.5571	1201.798	327836.4658
		O_3	-0.53838	-2.88482	2209.247	1442938.567
		O_4	-1.31403	-2.74038	1843.904	765933.5035
		O_5	-1.72868	-2.57511	1272.885	361104.4917
	$CrO_4^{2-} ALA^{1+}$	Cr_1	-0.02806	-29.394	669.6065	112492.764
		O_2	-1.72134	-2.52922	1125.119	294390.014
		O_3	-0.56564	-2.87793	2214.102	1432607.246
		O_4	-1.30341	-2.74873	1867.143	784161.1782
		O_5	-1.71056	-2.59635	1310.968	378120.6466
B3LYP	CrO_4^{2-}	Cr_1	0	-144240	0.0485	0.000914495
		O_2	-7.8E-06	-3.736	445.0791	77036.50861
		O_3	-7.8E-06	-3.736	445.0791	77036.50861
		O_4	-7.8E-06	-3.736	445.0791	77036.50861
		O_5	-7.8E-06	-3.736	445.0791	77036.50861
	$CrO_4^{2-} GLY^{1+}$	Cr_1	-0.0982	-13.0328	83.6279	1492.046291
		O_2	1.062896	-1.04241	392.9435	34009.14995
		O_3	-0.19924	-2.23629	570.9471	123399.9876
		O_4	-0.96604	-3.04362	222.6796	10974.2459
		O_5	1.281351	-1.17583	403.4656	35188.84811
	$CrO_4^{2-} ALA^{1+}$	Cr_1	-0.02932	-65.3301	196.3903	6472.083541
		O_2	-0.65891	-4.06777	451.0282	38497.74362
		O_3	-0.11755	-4.85202	678.98	147815.2725
		O_4	-0.55413	-4.5552	532.9456	52721.7399
		O_5	-0.68397	-4.29715	486.434	41853.6356

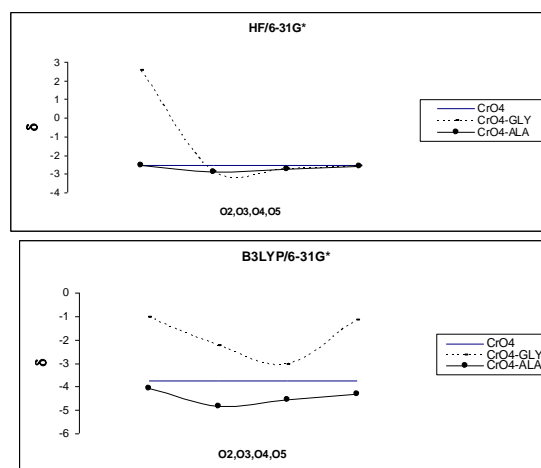


Fig5. shows the changes for oxygen atoms and in the base series in HF and DFT

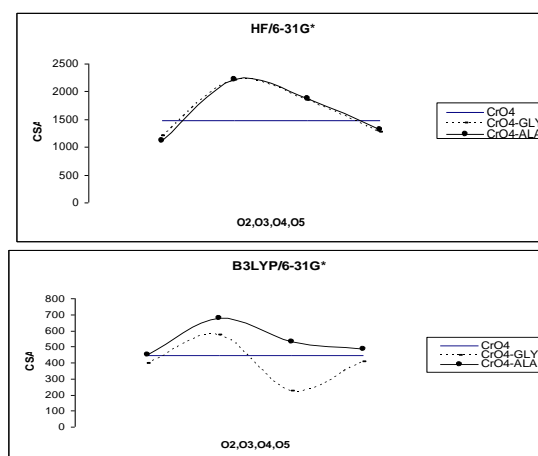


Fig6. shows the changes for oxygen atoms and in the base series in HF and DFT

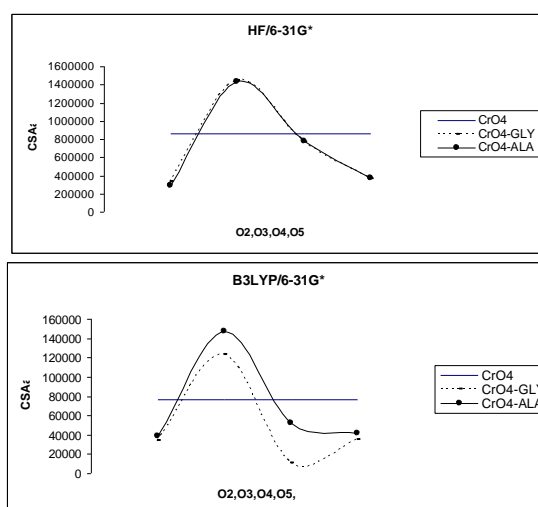


Fig7. shows the changes in the oxygen atoms and in the base series in the HF and DFT methods

Figures 8 to 15 show protection tensors and NMR parameters for anions and its complexes with glycine and alanine, as before, anionic oxide is linear and for oxygen complexes, where both the HF and DFT methods have the same trend for Two-component oxides show that this is the correctness of both methods in performing this type of calculation [11].

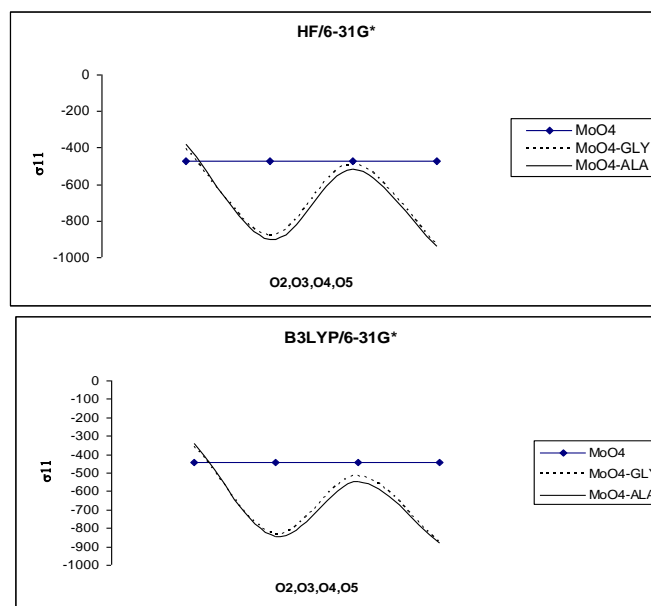


Fig. 8 shows the changes in the oxygen atoms and in the base series in the HF and DFT methods

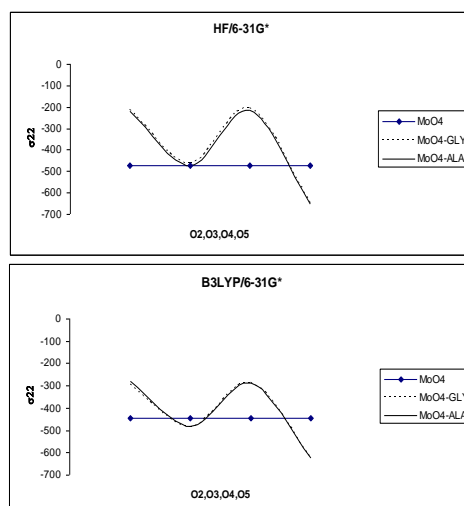


Fig9. shows the changes for oxygen atoms and in the base series in HF and DFT

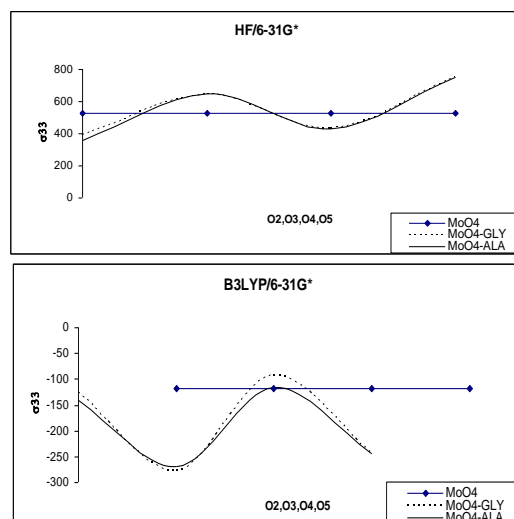


Figure 10 shows the evolution of the changes for oxygen atoms and in the base series in the HF and DFT methods

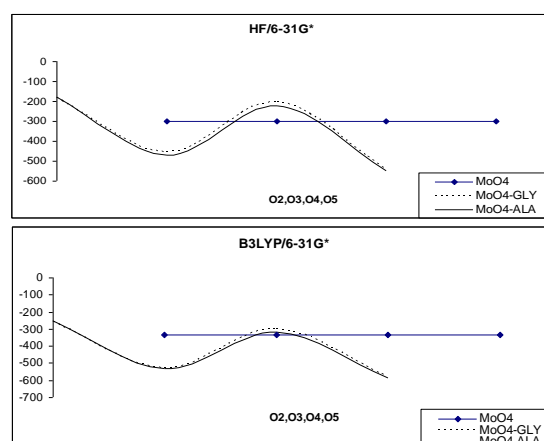


Figure (11) shows the changes for oxygen atoms and in the base series in the HF and DFT methods

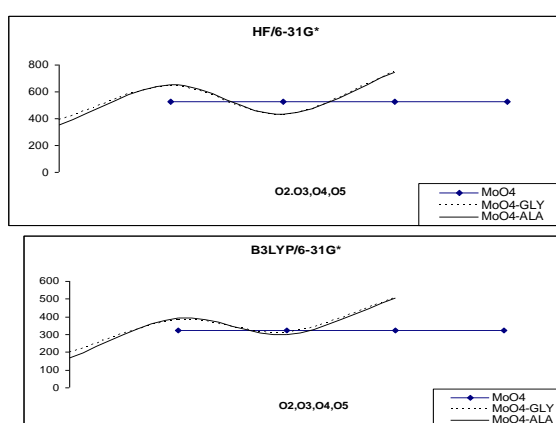


Fig. 12: Chart transformations for oxygen atoms and in the base series in HF and DFT

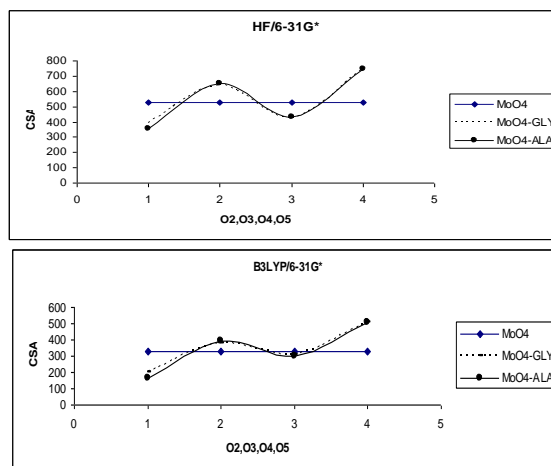


Fig. 13 shows the changes for oxygen atoms and in the base series in the DFT method.

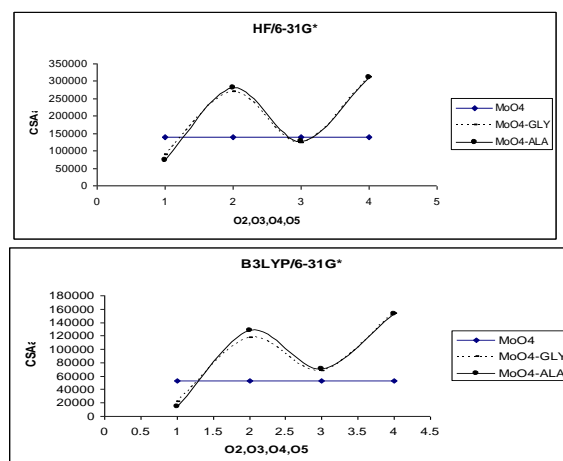


Fig14. shows the changes for oxygen atoms and in the base series in the DFT method

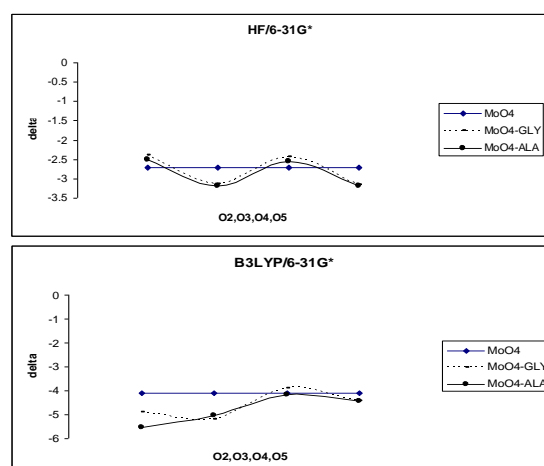


Figure (15) shows the changes for oxygen atoms and in the base series in the DFT method

4. Conclusion

The graphs of the calculated values of the conservation tensors and the NMR parameters for the anions oxides are linear and for the oxygen species of the complexes obtained from this anion with glycine and alanine, the curve shows that in the HF method, the curves of the complexes exhibit a coincidental process, while in The DFT is differentiated between complex curves, which seems to be a better HF method in computing. While for anions oxygen is a linear process for the oxygen of complexes, here both the HF and DFT methods show a similar trend for the two-component oxides, which indicates the correctness of both methods in performing this type of calculation.

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