



Thermodynamic-Biochemical Study of Complexes of Intermediate Elements with α -Amino Acids in Some Proteins with Active Site

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Abstract

In this paper, the quantum chemistry calculations related to the structural parameter of the chromite and molybdate anions and the complexes obtained from them with the glycine and alanine amino acids were performed. The calculations were carried out using HF and DFT methods and in the base series 6-31G *. Thermodynamic studies related to the formation of complexes have been considered and their equilibrium constant has been calculated. Finally, by comparing the thermodynamic factors, the stability of the complexes was determined relative to each other.

Keywords: Thermodynamic, Biochemical, molybdate anions.

1. Introduction

In this paper, the quantum chemistry calculations related to the structural parameter of the chromite and molybdate anions and the complexes obtained from them with the glycine and alanine amino acids were performed. The calculations were carried out using HF and DFT methods and in the base series 6-31G *. Thermodynamic studies related to the formation of complexes have been considered and their equilibrium constant has been calculated. Finally, by comparing the thermodynamic factors, the stability of the complexes was determined relative to each other [1-6].

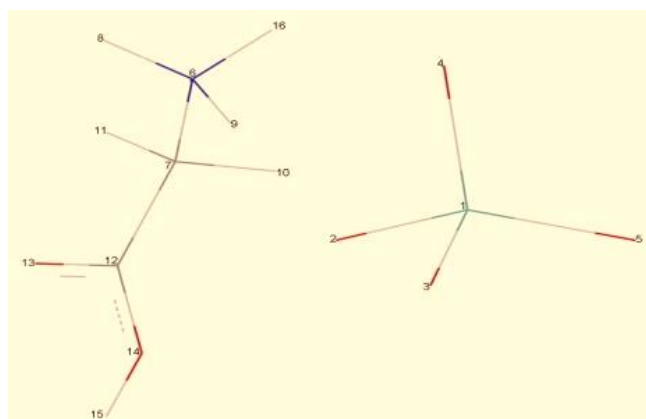
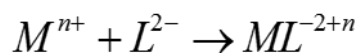


Fig 1. The structure of complexes with amino acid glycine after optimization

2. Computational details

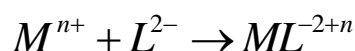
All Computations are performed by means of GAUSSIAN 03 packing [7-9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of molecules were designed primarily using of Gauss View 5.0.8 and nanotube The thermochemical properties of chromate and molybdate anions and the complexes resulting from the combination of these anions with glycine and alanine were performed using Gaussian 2003 and Gossive software. The compositions were first optimized with two hacker-factor and density functional theory in a 6-31G * series. Then IR studies were performed. All values were calculated at 298 and shown in Table 1. The quantities in the complex formation reactions are negative (Table 1). The negativity of the values is justified by the following reaction. This is evident because, in complex reaction reactions, it is accompanied by a decrease in irregularities and consists of two particles of a particle, hence entropy decreases:



The constant equilibrium values of all complexes are calculated and in Table 1, the comparison of constant equilibria shows that the molybdenum compounds have a lower equilibrium constant [10].

Table 1 shows the values at 298 calculated in the 6-31G * base series in two methods: ^a HF and DFT^b, based on (kcal / mol)

3. Results



The constant equilibrium values of all complexes are calculated and in Table 1, the comparison of constant equilibria shows that the molybdenum compounds have a lower equilibrium constant.

Table 1 shows the values at 298 calculated in the 6-31G * base series in two methods: ^a HF and DFT^b, based on (kcal / mol)

	ΔG°	ΔH°	ΔE°	ΔS°	$-\Delta G^\circ / RT$	K_{eq}
$CrO_4^{2-}GLY^{1+}$	-3.77128	0.009413	0.601773	-0.03572	0.565596	1.7604967
	-2.53259	-0.4016	0.188878	-0.04501	0.379825	1.4620287
$MoO_4^{2-}GLY^{1+}$	-1.47965	3.151305	3.743038	-0.04654	0.22191	1.2484590
	-3.09546	4.503568	5.095928	-0.04469	0.464241	1.5908063
$CrO_4^{2-}ALA^{1+}$	-3.67401	0.160013	0.753	-0.03554	0.551009	1.7350028
	-5.09216	-0.52083	0.072163	-0.03682	0.763696	2.1461939
$MoO_4^{2-}ALA^{1+}$	-1.13829	3.310063	3.90305	-0.04715	0.170714	1.1861515
	-1.9898	4.067455	4.659815	-0.04986	0.29842	1.3477277

Correct empirical data on the equilibrium geometries of the complexes of intermediate metal compounds are very limited in relation to the major group molecules. Table 2 shows some of the bond lengths of the anions and complexes studied in this study. These compounds are measured at HF and DFT levels. The results of the table indicating a general expansion. The length of these bonds in similar cases from Cr to Mo suggests that these studies in each HF and DFT method show a significant result, indicating that both methods have the same accuracy[11-13].

Table 2 Comparison of graft lengths and angles in anions and their complex formation states with glycine and alanine in a 6-31G* series with two standard methods of HF and DFT

Bond distance & Bond angle				
HF ^a , B3LYP ^b (6-31G*)				
	$M_1 - O_2$	$M_1 - O_3$	$M_1 - O_4$	$M_1 - O_5$
CrO_4^{2-}	1.5968 ^a	1.5968	1.5968	1.5968
	1.648 ^b	1.648	1.648	1.648
$CrO_4^{2-}GLY^{-1}$	1.64	1.5478	1.5838	1.6334
	1.6833	1.6044	1.6333	1.6761
$CrO_4^{2-}ALA^{-1}$	1.6464	1.548	1.5821	1.6293
	1.6892	1.6048	1.6523	1.6743
MoO_4^{2-}	1.7628 ^a	1.7628	1.7628	1.7628
	1.8072 ^b	1.8072	1.8072	1.8072
$MoO_4^{2-}GLY^{-1}$	1.7904	1.7313	1.7894	1.7342
	1.8497	1.7652	1.8242	1.768
$MoO_4^{2-}ALA^{-1}$	1.7935	1.7298	1.7859	1.7343
	1.8333	1.7643	1.8199	1.7681

Conclusion

The length of the bonds of both complexes of chromium and molybdenum complexes with amino acids shows that the molybdenum composition is larger than the composition of Cr, and also the zero point energy obtained and the magnitude and Kth for the same compounds of molybdenum and chromium, indicating the stability of the molybdenum ratio of the ratio To chromium compounds.

Reference

- [1] M. Outokesh, A. Tayyebi, A. Khanchi, F.Grayeli, G. Bagheri, *J. Microencapsulation*, 28(4), 248 (2011).
- [2] J.G. Lambardino, E.H. Wiseman, *J. Med.Chem.*, 17, 1182 (1974).
- [3] A. Puratchikody, M. Doble, *Bioorg. Med. Chem. Lett.*, 15, 1083 (2007).
- [4] M. Antolini, A. Bozzoli, C. Ghiron, *Bioorg.Med. Chem. Lett.*, 9, 1023 (1999).
- [5] L. Wang, K.W. Woods, Q. Li, *J. Med.Chem.*, 45, 1697 (2002).
- [6] M. Y.Pathan, V. V. Paike, P. R.Pachmase, S.P.More, S. S. Ardhapure, R. P. Pawar, *Arkivoc*, Part (xv), 205 (2006).
- [7] J.C. Lee, J.T. Laydon, P.C. McDonnell, *Nature*, 372, 739 (1994).
- [8] T. Maier, R. Schmierer, K. Bauer, U. S. Patent 4820335 (1989); *Chem. Abstr.*, 111, 19494 (1989).
- [9] R. Schmierer, H. Mildenerger, H. Buerstell, German Patent 361464 (1987); *Chem. Abstr.*, 108, 37838 (1988).

- [10] P. Wasserscheid, W. Keim, *Angew. Chem.Int. Ed. Eng.*, 39, 37872 (2000).
- [11] I. Satoru, Japn Kokkai Tokyo Koho JP 01, 117, 867, May 10, 1989; *Chem. Abstr.*, 111, 214482 (1989).
- [12] S. Samai, G.C. Nandi, P. Singh, *Tetrahedron*, 65, 10155 (2009).
- [13] S.A.A. Mansour, K.U. Sadek, *Chin. Chem. Lett.*, 20, 812 (2009).