International Journal of New Chemistry, 2017, 4 (2), 39-43
Published online January 2017 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

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

Olduz Tkach*

Department of Chemistry, School of Engineering, Presidency University, Bengaluru-560064, India.
*Corresponding Author e-mail Address: O.tkach@yahoo.com
Received 2 January 2017; Accepted 11 February 2017; Published 30 March 2017

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