



University of zabol
Graduate school
Faculty of science
Department of chemistry

**The Thesis submitted for the Degree of M. Sc
(in the field of physical chemistry)**

Title:

**Investigation of effects of metal cations on
intramolecular hydrogen bond interactions in
nitrogen-containing heterocyclic compounds**

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Abstract

Pyrazolo pyrimidine derivatives can participate in formation of intramolecular and intermolecular hydrogen bonds because they have nitrogen containing rings. It seems that these compounds could be able to remove metal ions from wastewater. First, initial structure of one of pyrazolo pyrimidine derivatives without and with intramolecular hydrogen bonding was optimized using quantum mechanical computations in this study. Then, interactions of these two class molecules with some metal cations were investigated and the best positions of interactions were distinguished. The optimized structures, energies, ring and bond critical points, electron charge densities and aromaticity of these compounds were surveyed using various computations. Finally, energy decomposition analyses were performed to corresponding components. Results show that these compounds have good ability for removal of metal ions from wastewaters. Therefore, it is possible to use intramolecular hydrogen bonds in planning similar compounds in future to increase efficiency of removal of metal ions.

Keywords: Intramolecular hydrogen bond, electron charge density, aromaticity, quantum mechanics