University of Zabol
Faculty of Science
Department of Chemistry

The Thesis Submitted for the Degree of Master of Science
(In the field of physical Chemistry)

Computational study of the interaction of heavy metal ions with adsorbents containing heterocyclic aromatic groups

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Abstract:

Heavy metals have various risks for human health and can cause disorders such as kidney damage, liver damage, dysfunction of the central nervous system, cancer and mutation. Usually, several methods are used to remove heavy metals from environment, such as ion exchange, chemical precipitation, complexation, liquid-liquid extraction, reverse osmosis, oxidation-reduction process, evaporation, separation and adsorption, which in many cases, these methods are costly and ineffective. Adsorption is one of the most economical and widely used methods for removing heavy metals from the water. As one of the most important and simple biopolymers, chitosan has significant applications in water purification as a metal chelating agent, and chemical modifications of chitosan will improve its absorption properties. In this research, , the structure of new chitosan derivatives containing aromatic groups was optimized by using quantum mechanical calculations. The results show that the two factors of effective nuclear charge and ionic radius play an important role in the interaction of heavy metals with these adsorbents, and these results can be used in the design of new derivatives with higher absorption capacity.