



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)

Investigating the interaction of some metal ions with pyrene derivatives and the effect of intramolecular bondings on it

Supervisor:

Dr. M. Sanchooli

Dr. P. Karimi

Adviser:

Dr. M. Poorsargol

Dr. H.Samare Delarami

By:

Raziye Safaei Moghadam

November.2023

Abstract

It is about the investigation of π -cation bond in the interaction of sodium and magnesium ions with some pyrene derivatives. These derivatives have substitutions with different number of π conjugate bonds. The second group of compounds are pyrenes with intramolecular hydrogen bonds with the same substitutions as before. The purpose of investigating the role of substitutions and intramolecular hydrogen bonding on the interaction with the mentioned ions is that by theoretical calculations at the M062x6-311++g** level, the effect of various factors on the binding energy of the complexes such as structural data, electronic data, data Electron charge density and charge transfer and aromaticity of rings are investigated. These compounds are susceptible to design for sodium and magnesium ion batteries. Therefore, identifying the best parent derivatives in terms of type and position of substitution is considered.

Keywords: *Cation- π interaction, Intramolecular hydrogen bond, Pyrene derivatives, Ion battery*