Abstract

In this project, quantitative structure property relationship (QSPR) analysis was carried out between molecular descriptors of 65 complexes derived from 1,4,7,10,13-pen-taoxacyclopentadecane ethers (15C5) and stability constants associated with sodium cation. The structure of the crown ethers was drawn and optimized using Gaussian98 and Hayperchem softwares. In this study, three different sets of quantum mechanical properties including charge, dipole moment, and orbital energy were calculated for quantum variables in the vacuum state. Dependence of stability constants of crown ethers on the parameters was evaluated using multiple linear regression. Results indicated a squared linear correlation coefficient of 0.519 for 65 crown ether molecules. In the current model, electronic charge variable has a significant contribution to the stability constant of the aforemenhoned.Although the obtain liner model interpret the mechanism of the 1,4,7,10,13 derivative stability in an excellent mammer, it suffers on low power of predict ability of stability constants. As a result, nonlinear variables tried to be modeled using neural networks in order to provide better correlations in the model. Neural network model suggests a squared linear order of 0.924 for all molecules. Developed models point out that stability mechanism of the complexes is mostly of colombic reaction type. Orbital overlaping is also observed to a limited extent. In this research, interesting results was obtained suggesting that the crown ether with sodium atoms are not involved in all electronegativity atoms of oxygens inside the ether ring but some of positive-charged carbon atoms also contribute in the stability of the complex with the mediation of solvent (water) molecules.

Key words : Stability constant; Crown ethers; Electronic discriptors; **QSPR**

University of Zabol

Graduate School

Faculty of Science

Department of Chemistry

The Thesis Submitted for the Degree of Master of Science

(In the field of Analytical Chemistry)

Determination of stability constants of 15-crown-5 complexes with sodium cation using electronic discriptors in QSPR method

:Supervisors

Dr. Massoud Nejati Yazdinezhad

Dr. Mahmoud Sanchooli

:Advisor

Dr. Mansour Ghaffari Moghaddam

:By

Mohsen Behzadi Far

January 2014