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(in the field of physical chemistry)

Title:

Theoretical study on effects of substituent and intramolecular hydrogen bonding interaction on the chelating ability of ١,١٠-Phenanthroine with metal ions

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Abstract

١, ١٠-Phenanthroline is a compound with rings containing nitrogen atoms and has a good potential to absorb heavy metal ions. In this research, the interactions of this ligand and its derivatives containing intramolecular hydrogen bonds in closed and

open configurations with some metal cations are studied. Energies, atomic charges, electron charge densities at critical points and aromaticity of these compounds have been calculated using different calculations on optimized structures. Also, the interaction energy analysis has been done into its components. The results show that these compounds have a good ability to absorb metal ions. Energy is a function of charge distribution. In addition, the distribution of electron charge density in the critical points of the rings and the change of the charge of their atoms affects the stability of the complexes. The functionalization of Phenanthroline leads to the creation of a new ring containing an intramolecular hydrogen bond in which the lower the aromaticity of this ring in the complexes, the higher the corresponding binding energies. Analysis of interaction energy analysis shows that the electrostatic and polarization energies play a key role in the stability of complexes that have formed by functionalized Phenanthroline in closed configuration and ions. Functionalization of the Phenanthroline is a method to adjust its sensitivity as a chemical sensor that can be useful for use in different environments.

Keywords: ١, ١٠-phenanthroline, Intramolecular hydrogen bond, electron charge density, aromaticity, sensor