International Journal of New Chemistry, 2018, 4 (4), 400-408.
Published online January 2018 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Investigating the Complexation of a recently synthesized phenothiazine with Different Metals by Density Functional Theory

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Received 19 November 2017; Accepted 20 December 2017; Published 27 march 2018

Abstract

In this research, the complexation of a new recently synthesized phenothiazine with 10 different metals was evaluated by Density functional theory. At the first step, the structures of 6,15-diazabenzo[a][1,4]benzothiazino[3,2-c]phenothiazine, cations and their complexes with the mentioned material were optimized geometrically. Then, IR calculations were performed on them to obtain the values of formation enthalpy and Gibbs free energy. The acquired results indicate that Cu^{2+} forms the most stable and strongest complex with 6,15-diazabenzo[a][1,4]benzothiazino[3,2- c]phenothiazine. Hence, this substance can be utilized as an outstanding ionophore or a potential ligand in the determination of copper by ion selective electrodes and different extraction methods respectively. All calculations were applied by Density functional theory in the level of B3LYP / 6-31G(d).

Keywords: 6,15-diazabenzo[a][1,4]benzothiazino[3,2- c]phenothiazine, Density Functional Theory, Complexation, Copper, Thermodynamic Parameters.