عنوان مقاله:

Evaluating the Performance of 2,3-dihydro-1H-phenothiazine-4(5aH)-one as an Ionophore in Construction of a Cation Selective Electrode by Density Functional Theory

محل انتشار:

فصلنامه شیمی نوین, دوره 5, شماره 1 (سال: 1397)

تعداد صفحات اصل مقاله: 10

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خلاصه مقاله:

In this study, the complexation of 2,3-dihydro-1H-phenothiazine-4(5aH)-one with 14 various cations were investigated by density functional theory. At the outset, the structures of the ligand, different cations and their derived complexes were optimized geometrically. Then, IR calculations were performed on them in order to acquire the formation enthalpy and Gibbs free energy values. The obtained results substantiate that 2,3-dihydro-1H-phenothiazine-4(5aH)-one forms the strongest and the most stable complex with Cr3+ cation. In addition, this ligand demonstrates an eminent selectivity toward chromium (III) ions. In this regard, it can be used as an electroactive sensing material in developing a Cr3+ selective potentiometric electrode. All calculations were applied by Density functional theory in the level of B3LYP / 6-31G(d).

کلمات کلیدی:

dihydro-1H-phenothiazine-4(5aH)-one, Density Functional Theory, Complexation, Chromium, Ionophore-2,3