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The study of electron-orbital properties of bipolar energy of complex (2,6-diaminopyridinium bis (4-hydroxy-pyridine-2,6,6-dicarboxylate) dihydrate chromate III))) with alteration of ligands by computational methods

Salvador Casagrande*

Department of Chemistry, College of chemistry, Universidade Federal de Mato Grosso do Sul, Brasil.

*Corresponding Author e-mail Address: Salvadir.C19937@gmail.com

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Abstract

In this report, using the ab initio method of stability and electron-orbital properties of the complex (2,66-diaminopyridinium bis (4-hydroxy-pyridine-2, 6-dicarboxylate) dihydrate chromate III) with a change of ligand at position 17 It has been studied with ligands such as F, Cl, Br,,, and. The results indicate changes in energy levels, bipolar moments, and sustainability rates due to these changes in these bonds.

Keywords: (2,6-diaminopyridinium bis (4-hydroxy-pyridine-2,6,6-dicarboxylate) dihydrate chromate III))).