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Original Research Article

Investigation of the Conversion Process of Verdoheme Hydroxyl Iron (II) to Biliverdin Iron (II): Theoretical Study

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ABSTRACT

Heme oxygenase (HO) is an enzyme that breaks down heme and as a result iron is recycled in most organisms, including the human body. This enzyme produces bilirubin, divalent iron, and carbon monoxide. Heme Oxygenase was first described in the late 1960s [1-3]. Study of the reaction of the peripheral substituents on the heme ring with verdohemes offers models that are not very well known. In this project, a computational study of destruction reaction of verdoheme iron (ii) was carried out and the role of lateral substitution on its hydrolysis process was investigated. Theoretical calculations show that the rate of hydrolysis reaction is slower for complexes containing peripheral substitutions. On the other hand, hydrolysis of verdohemes non-environmental is a convenient parameter for energy. To better understand this process, theoretical calculations were performed using the DFT method. Calculations of the stability energy of the compounds showed that the higher the intermolecular interactions of hydrogen, the greater the stability of the compound. Also, the highest stability energy is related to compound D, which has more intermolecular interactions from type of the hydrogen bonds.

Keywords: Hydrolysis verdohemes, DFT calculation, Hydrogen bond, Keq

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