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Investigation of Spin-Charge-Structure in Human Verdoheme Using The DFT Method

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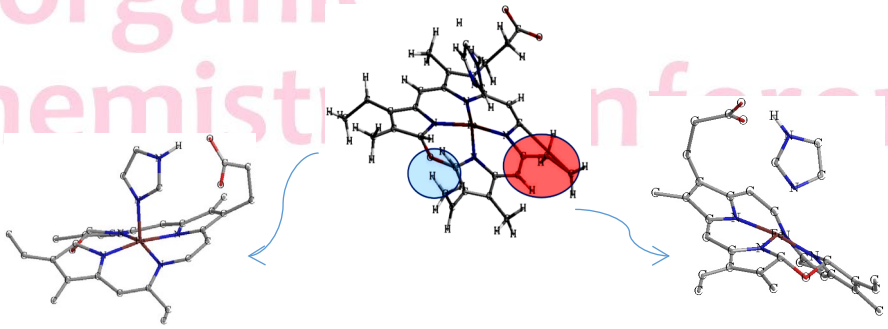
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The enzyme heme oxygenase (HO) plays an essential role in the destruction of heme molecules. Heme oxygenase uses dioxygen to open the specific orientation of the porphyrin ring at the position of the α-meso carbon. This enzyme catalyses the degradation of heme to biliverdin IXα through three distinct intermediates, α-hydroxyheme, α-verdoheme and ferric biliverdin–Iron chelate, at the expense of O_2 and electrons. To elucidate the mysterious mechanism of the oxygenation steps, the atomic-resolution structure of the verdoheme–HO complex has been needed. In this work the structure of Iron verdoheme in complex with Human Heme Oxygenase according to the structure of verdoheme that was solved by Lad et all (PDB Id: 1TWN) (figure 2), was studied by density functional theory based B3LYP method and 6-31G basis set. Herein we regard the central metal of the five coordinated human verdoheme as ferrous (Fe2+) and ferric (Fe3+). Many parameters such as charge of verdoheme and Iron as central metal, electron distribution, spin multiplicity of the molecule and proximal substituents effect on the verdoheme ring stabilization and their arrangement were discussed

Keywords: Verdoheme, Human, Density Functional Theory, structure optimization



Input and calculated human verdoheme structures

References:

[1] H. Tasharofi, P.R.Jmaat, and M. Daghighi Asli, *Journal of Porphyrins and Phthalocyanines*, **2022**, 26, 889.