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Theoretical Kinetics and Thermodynamics study peripheral substituent effects on the hydrolysis of verdoheme

Shahryar Sarabi[a], Parisa Rajabali Jamaat [a]

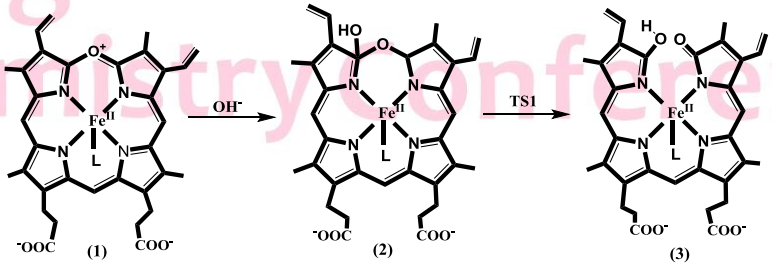
[a] *Department of chemistry, Faculty of Science, East Tehran Branch of Islamic azad University, Tehran, Iran*

[*] *E-mail: sh.sarabi41@yahoo.com*

[*] *E-mail: Parisa.Jamaat@iau ac.ir*

The heme oxygenase enzyme is a free heme protein that binds to heme in the body. Heme acts as both a substrate and a cofactor in this enzyme. The heme oxygenase enzyme (HO) plays a key role in destroying heme molecules. Studies of the reaction of 5-oxaporphyrin iron complexes (verdohemes) with peripheral substituent on the heme ring have been undertaken to provide models and largely unknown for the initial step in hydrolysis of verdohemes. In this work a theoretical kinetics and thermodynamics study of degradation reaction of verdohemes was performed, and calculations show that $\Delta G_{Reaction}$ in hydrolysis of verdohemes non- peripheral substituent is more negative than hydrolysis of verdohemes with peripheral substituent. In the other words, hydrolysis of verdohemes with non- peripheral substituent is more energy efficient than verdohemes with peripheral substituent. The equilibrium constant calculation shows that hydrolysis of verdohemes non- peripheral substituent is much faster than verdohemes with peripheral substituent, which it is due to more convenient nucleophilic attack to cationic ring than anionic. In order to obtain a better molecular understanding of peripheral substituent effects on the hydrolysis of verdoheme inhibitory role of have been studied using DFT method.

Keywords: Heme oxygenase, peripheral substituent, DFT method, Hydrolysis, Ring Opening of Verdohemes.



The studied mechanism in verdoheme hydrolysis References

References:

[1] S. Sarabi, P.R.Jmaat, and H. Djahaniani, *Journal of Porphyrins and Phthalocyanines*, **2020**, 24, 1233.