

**NON-HEME METAL COMPLEXES- A  
VERSATILE DESIGN FOR PHARMACEUTICAL  
REACTION, ENVIRONMENTAL POLLUTANTS  
AND CHEMICAL WARFARE DETOXIFICATION:  
A QUANTUM MECHANICAL STUDY**

***THESIS SUBMITTED FOR THE AWARD OF THE DEGREE OF***

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## ABSTRACT

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The enzymes have important biological functions. Metalloenzymes have metal as cofactor bound to proteins. The metal ions in active site of enzymes allow it to perform redox reactions. Metals were used in most developed civilizations since ages in therapeutic purposes but the mechanism was not known properly. With advent of computer, the theoreticians could compute structures and reaction pathways within reasonable time. The quantum mechanical methods have been of great help in devising competing methods for explaining involved phenomena. With advancement in technology, these theoretical results were validated by experimentalists as well. Hence both began working in close collaboration. Their concerted efforts have helped develop highly benchmarked computational methods that produce reliable results. Now modeled structures have grown in size and complexity.

Metalloenzymes may be broadly classified into heme and non-heme enzymes. While former have been well documented, latter is in growing phase but has immense potential for exploring various reaction pathways that may further be fine-tuned. In this work, iron(IV)-oxo species have been studied in great detail. Reaction pathways have been proposed that closely match with experimental results. Aliphatic hydroxylation catalysis reactions by synthetic models of variously ligated complexes have been considered that exhibited low activation barriers compared to known efficient catalysts. Also, comparative study between iron(IV)-oxo versus iron(V)-oxo complexes has been attempted for the first time. In another work, alkane synthesis by intramolecular methyl and hydrogen atom transfer has been studied and reaction mechanism has also been deduced.