

*Dedicated*

*to*

*AAMA AND BABA*

## DECLARATION

I declare that the thesis entitled "**Exploration of Catalytic Activities of Some Transition Metal Borates for Green Synthesis of Nitrogen Containing Heterocyclic Compounds**" has been prepared by me under the supervision of Dr. Biswajit Sinha, Professor, Department of Chemistry, University of North Bengal and Dr. Dhiraj Brahma, Assistant Professor, Department of Chemistry, St. Joseph's College, Darjeeling. No part of this thesis has formed the basis for the award of any degree or fellowship previously.

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## Preface

*With the development of the idea of Green Chemistry as given by Prof.P.T.Anastas, solvent free multicomponent reactions are becoming very popular in the present days. Keeping this theme in mind and also with an enthusiasm of exploring the catalytic activity of some selected transition metal borates, this research work is carried out by the author under the joint guidance of Dr.Biswajit Sinha, Professor, Department of Chemistry, University of North Bengal and Dr. Dhiraj Brahman, Assistant Professor, Department of Chemistry, St. Joseph's College, Darjeeling.*

*While going through the literatures it was observed that there were numerous applications of transition metal borates in various fields, however, it was observed that the catalytic activity of these borates were very poorly explored. Therefore, this encouraged us to explore the catalytic activity of these borates in some famous organic reactions involving the synthesis of 2,4,5-triaryl imidazoles, 3,4-dihydropyrimidine-2[1H]-ones, 1-hydroxy-2-arylimidazole-3-oxide and 2-substituted benzimidazoles and 1, 2-disubstituted benzimidazoles. Looking at the diverse applications of these Nitrogen Containing Heterocyclic Compounds, the synthesis of these compounds in a cleaner and milder way following the principles of Green Chemistry with the transition metal borates as catalysts may evolve as an attractive field of research in the field of chemical sciences.*

*Transition metal borates have been used profoundly in glass industries and have tremendous applications in lithium-ion batteries, glass electrodes, non linear optical devices and optical communication devices. Taking inspiration from the famous scientists like Hawthorne, Grimes and Braunschweig who have done various works in the field of borates, the present dissertation was undertaken for exploring the catalytic activity of some selected transition metal borates, namely Copper Borate, Iron Borate and Nickel Borate for the green synthesis of Nitrogen Containing Heterocyclic Compounds and the results of this work are quite promising.*

*Density Functional Theory (DFT), Molecular Docking, Computer Aided Drug Design (CADD) are widely used now-a-days for investigating the physical properties as well as for identification of suitable and specific drug target molecules. An attempt has been made to study the theoretical properties and drug likeliness of some of the selected synthesized compounds using DFT and Molecular Docking Studies and some of the theoretical parameters have also been compared with experimental results to get into a deep insight into the structures of the selected compounds.*

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