Density Functional Theory Approach towards Electronic Structures, Formation of High Valent Metal Species and Metal Mediated C-H/O-H Bond Activation

Thesis Submitted to the Central University of Haryana for the partial fulfillment of the Degree of

Doctor of Philosophy

in

Chemistry

By Monika



Department of Chemistry Central University of Haryana Mahendergarh-123031 Haryana, India

January 2022