PREFACE

The work in this thesis entitled 'C-H Bond Activation by Transition Metal Complexes' was initiated from an attempt to explore the possibility of activation of different types of C-H bonds by using known or newly designed metal complexes. Selective activation of C-H bond was attempted following (i) stoichiometric and (ii) catalytic routes. Another objective of the present work was to develop efficient catalytic system capable of oxygenating hydrocarbons at ambient condition.

The thesis consists of six chapters. A brief review of major advances in the title area has been made in Chapter I with emphasis on stoichiometric C-H bond activation and catalytic hydrocarbon functionalization relevant to bioinorganic chemistry. Current challenges in this area and the purpose of the present investigation are also outlined in the chapter.

Chapter II deals with the selective C(naphthyl)-H bond activation by palladium(II) and isolation of resulting cyclopalladates. All the cyclopalladates have been characterized by spectral data and X-ray diffraction. The theoretical electronic structure of the organometallates was deduced on the basis of 'Time Dependent Density Functional Theory' (TDDFT).

The regiospecific C(naphthyl)-H bond activation by platinum(II), isolation of resulting cycloplatinates, their spectral and structural characterization constitute the core of chapter III. The reactivity of platinum(II) cyclometallates has also been examined.

The activation of C(naphthyl)-H bonds by rhodium(I) constitute the subject matter of chapter IV. Different C(naphthyl)-H bonds *viz.* C(1)-H, C(2)-H, C(3)-H and C(8)-H have been found to be activated by Wilkinson's catalyst, $[Rh(PPh_3)_3Cl]$. The isolation, characterization, X-ray crystallographic analyses and TDDFT study of the resultant cyclometallates have been described.

Chapter V deals with room temperature oxygenation reactions of alkanes and alkenes catalyzed by chiral iron(III)-salen and manganese(III)-salen complexes. The electronic properties of the metallosalens have been tuned by the incorporation of electron donating and electron withdrawing substituents in the salen frame. A comparative study between the iron(III) and manganese(III)-salens as catalysts has been presented in this chapter.

The catalytic hydroxylation of alkanes (C-H → C-OH) by an electron deficient iron(IV)corrole complex (*meso*-tris(pentafluorophnyl)corrolatoiron(IV)chloride [(F_{15}TPC)FeCl]) with *m*-CPBA or t-BuOOH is the major theme of Chapter VI.

The present work was initiated in October 2004 at University of North Bengal, under the supervision of Dr. P. Bandyopadhyay, Department of Chemistry.

In keeping with general practice of reporting scientific observations, due acknowledgement has been made whenever the work described as based on the findings of other investigators. I must take the responsibility of any unintentional oversight and errors, which might have crept in spite of precautions.

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