ABSTRACT

N-heterocyclic carbenes (NHCs) have emerged as appropriate replacements for phosphines in transition metal-catalyzed cross-coupling chemistry. The advantages of NHCs over phosphines including ease of handling, minimal toxicity, stability and powerful electron donating properties. Improvement of catalytic processes has become increasingly relevant in light of prospective applications of organic transformations in industry as well as in synthetic laboratories.

N-heterocyclic carbene (NHC) ligands have become ubiquitous ligands in the preparation of metal complexes with new catalytic applications. Mainly due to their application in C-C bond formation reactions, a plethora of novel palladium-NHC complexes has been described, and a large number of review articles describing their chemistry have been published.

This dissertation focuses on the development of complexes involving *N*-heterocyclic carbene ligated with palladium metal and their applications in organic transformation. This dissertation is divided into four chapters.

The **Chapter–I** describes the general introduction of *N*-heterocyclic carbenes (NHCs) and the development of palladium-*N*-heterocyclic carbine complexes. In this chapter, various methods for the synthesis of Pd-NHC complexes have been described and the Pd-NHC catalyzed reactions are also illustrated.

The **Chapter–II** deals with the synthesis of benzimidazole-based *N*-heterocyclic carbene complexes with palladium metal. Two different Pd-NHC complexes have been synthesized (marked as **Catalyst A** & **Catalyst B**), characterized by spectroscopic analysis and finally their structures were established by single-crystal X-ray analysis. Both the catalysts were examined for their catalytic activity in the Suzuki-Miyaura cross-coupling reaction. Excellent catalytic performance was observed with Catalyst A and extended to a variety of aryl halides (I, Br, Cl) and aryl boronic acids. Apart from the Suzuki-Miyaura cross-coupling reaction, Pd-NHC catalyzed cross-coupling reaction between aryl acid chlorides and aryl boronic acids has also been performed successfully.

The **Chapter–III** depicts a convenient way to functionalization of aryl moiety at the 6-position of 4-quinolones *via* selective bromination and subsequent arylation by Suzuki-Miyaura cross-coupling reaction. Pd-NHC complex has been used as the catalyst for Suzuki-

Miyaura coupling reaction under microwave irradiation to achieve highly functionalized 4-quinolones - an important class of biologically active compounds.

In the **Chapter–IV**, Heck coupling reaction catalyzed by our newly developed palladium-*N*-heterocyclic carbene complex has been described. An efficient one-pot protocol for easy access of structurally diverse 4-aryl-2-quinolones *via* domino-Heck/cyclization reaction has also been presented in this chapter.