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Title of the Thesis: "**Synthetic and Mechanistic Investigations on Copper Mediated C-N Bond Formation in Arylation Reactions**"

Abstract

Copper mediated C-heteroatom coupling have been developed as cheaper substitute of expensive Pd/ligand system. Conversely to Pd-mediated cross coupling reactions, mechanism of these reactions are poorly understood and cheaper arylchlorides are extremely poor substrates. Moreover, Deactivation of copper catalyst during course of reaction are not well understood. However, uncertainty about the behavior of copper/ligand system and awaiting activation of cheaper aryl chlorides restricted the wider applications of copper catalyzed reactions.

In the first phase, in-situ spectroscopic (FTIR and Uv-Vis) experiments were designed to find the Cu(III) intermediate species. Observations indicate, carbonate and phosphates which are considered as base, actually are second ligands and octahedral Cu(III) species are intermediate in the reactions. In second phase of studies, detailed DFT studies were conducted to investigate deactivation of copper catalyst, it was found that ligation of carbonate base to active copper species is actual reason for deactivation. In third phase of studies, a normal and facile protocol has been developed for arylation of imides, amides and amines, using cheaper aryl chlorides and catalytic cycle has been proposed on the basis of DFT calculations.

This PhD thesis is expected to helpful for further investigation on mechanistic and synthetic aspects of these reactions. Current protocol opens scope for C-S, C-O and C-N couplings using aryl chlorides.

List of publications

- [1] K. K. Gurjar, R. K. Sharma, *ChemCatChem* **2017**, 9, 862–869. (Impact factor-4.8)
- [2] K. K. Gurjar, R. K. Sharma, *Ajchem* **2018**, 30, 1401–1404.
- [3] Gurjar KK, Sharma RK , Activation of C(aryl)-Cl bond activation in Ullmann C-N coupling; is under review in *Journal of Catalysis*, Elsevier. (Impact factor-6.9)
- [4] Total Presentations at National Conferences- **03**