



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Studies Toward Chelation Assisted *Ortho*-Selective C-H Bond Functionalization of Arenes
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SHORT ABSTRACT

The chapter 1 describes the literature survey of the transition-metal-catalyzed cross-coupling, C-H activation, chelation-assisted C-H functionalization and their mechanisms.

Chapter 2 demonstrates Pd-catalyzed *ortho*-halogenation of *N*-aryl ring of *N*,1-diphenyl-1*H*-tetrazol-5-amines via chelation assisted C-H functionalization utilizing *N*-halo succinimide (NXS) as halogen source and CF₃SO₃H as an additive at moderate temperature.

Chapter 3, presents a room temperature Cu-catalyzed chemo- and regioselective nitration of arenes using Fe(NO₃)₃·9H₂O as a nitro source. Here, 5-aminotetrazole and 3-amino-1,2,4-triazoles serve as the chelating groups. The directing group can be cleaved to give 2-nitroanilines in good yields. The mechanistic aspects have been illustrated based on kinetic isotope studies, ESI-MS and radical scavenger experiments.

Chapter 4, focuses on Cu-mediated regio-selective cross-dehydrogenative coupling (CDC) approach for the *N*-arylation of azoles under basic conditions. The reaction of pyrroles, indoles, pyrazoles and carbazole has been included. The kinetic studies show that the C-H bond cleavage takes place in the rate determining step.