

Abstract

The thesis entitled “**Cobalt and Copper Catalyzed Atom Economical Carbon-Carbon and Carbon-Nitrogen Bond Formation Reaction under Aerobic Condition**” is primarily an effort towards the first-row transition metal, specifically cobalt and copper-catalyzed new sustainable and atom-economical methodology development for carbon-carbon and carbon-nitrogen bond formation under aerobic conditions. The thesis has been divided into six chapters.

Chapter I describes a few important carbon-carbon and carbon-nitrogen bond formation strategies based on transition metal catalysts. Cross-coupling, nucleophilic substitution, cycloaddition, allylation, and alkylation reactions promoted by cobalt and copper compounds are briefly described. Cobalt and copper-catalyzed hetero cross-coupling, hydroamination, and N-alkynylation reaction methods for C-N bond construction also described here.

Chapter II illustrates the particular of the instruments used for characterization and structural evaluation of the catalyst, reaction intermediate, and new products. Here, $[\text{Cp}^*\text{Co}(\text{CH}_3\text{CN})_3](\text{SbF}_6)_2$ catalyst synthesis procedure has been described.

Chapter III describes a new approach for atom economical 1,3-dicarbonyl compound addition to the unactivated terminal alkyne using $[\text{Cp}^*\text{Co}(\text{CH}_3\text{CN})_3](\text{SbF}_6)_2$ (**I**) under mild neutral reaction condition having good to excellent yield. For the diketone system, it produces Markovnikov's addition product, while for the β -ketoester system, it produces tetra-substituted benzene products via cycloaddition between two equivalent terminal alkyne and enol-ester compound. *In situ* LCMS measurements were carried out of the corresponding reaction mixture at different time intervals for investigating the reaction mechanism.

Chapter IV presents the $[\text{Cp}^*\text{Co}(\text{CH}_3\text{CN})_3](\text{SbF}_6)_2$ (**I**) catalyzed atom-economical direct regio-selective monoallylation of the active methylene compounds with allylic alcohols under additive-free conditions. Here, the product conversion rate was tested by modifying the leaving group of the allylic substrates. Here, to find out the reaction mechanism *in situ* ^1H NMR and some control experiments were carried out. Based on the reports, and *in situ* ^1H NMR and the control experiments, we suggest that the reaction of allylic alcohols proceeds through two pathways, one η^3 - π -allyl complex formation and subsequent enolization of the diketones, followed by the

