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N-Heterocyclic Carbene Based Dearomatized Iridium Complex as an Efficient Catalyst towards Carbon-Carbon Bond Formation via Hydrogen Borrowing Strategy

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Abstract : The search for atom-economical and green synthetic methods for the synthesis of functionalized molecules has attracted much attention. Metal ligand cooperation (MLC) plays a pivotal role in organometallic catalysis to activate C−H, H−H, O−H, N−H and B−H bonds through reversible bond breaking and bond making process. Towards this goal, a bifunctional N–heterocyclic carbene (NHC) based pyridyl-functionalized amide ligand precursor, and corresponding dearomatized iridium complex was synthesized. The NMR and UV/Vis acid titration study have been done to prove the proton response nature of the iridium complex. Further, the dearomatized iridium complex explored as a catalyst on the platform of MLC via dearomatzation/aromatization mode of action towards atom economical α and β–alkylation of ketones and secondary alcohols by using primary alcohols through hydrogen borrowing methodology. The key features of the catalysis are high turnover frequency (TOF) values, low catalyst loading, low base loading and no waste product. The greener syntheses of quinoline, lactone derivatives and selective alkylation of drug molecules like pregnenolone and testosterone were also achieved successfully. Another structurally similar iridium complex was also synthesized with modified ligand precursor where a pendant amide unit was absent. The inactivity of this analogue iridium complex towards catalysis authenticated the participation of proton responsive imido sidearm of the ligand to accelerate the catalytic reaction. The mechanistic investigation through control experiments, NMR and deuterated labeling study, authenticate the borrowing hydrogen strategy.

Keywords : C-C bond formation, hydrogen borrowing, metal ligand cooperation (MLC), n-heterocyclic carbene
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