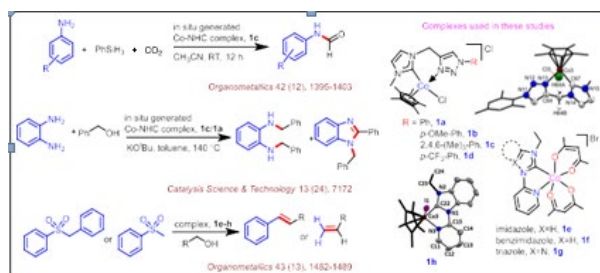


Systematic approach towards C-C/N bond formation using carbon dioxide and alcohol by employing cobalt-NHC complexes

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In the domain of metal-based catalysis, a comprehensive understanding of the structure of the metal-ligand complex is essential for assessing its catalytic performance. In this context, the steric and electronic properties of the ligands are important, as they significantly influence the complex's overall reactivity and stability. In this line we have conducted a comprehensive study on the C-C/C-N bond formation with cobalt centers using CO₂ and alcohol. Initially, we synthesized cobalt complexes with a heteroditopic NHC ligand and Cp* as an auxiliary ligand. At room temperature, these complexes were employed for the effective N-formylation of amines with CO₂ but exhibited limited catalytic activity for sterically demanding substrates. Subsequently, when the same catalytic system was applied for the selective alkylation or cyclization of 1,2-phenylenediamine, the corresponding products were generated under relatively harsh reaction conditions. It was observed that the inert Cp* auxiliary ligand might impede the access of these substrates to the active cobalt centers. Consequently, we replaced the Cp* ligand with structurally labile acetylacetonate (acac) ligands and synthesized the Co-NHC complexes to evaluate their performance with structurally demanding substrates. Our findings revealed that the Co-NHC complexes with the acac ligand exhibited superior performance compared to Cp* for ortho-substituted anilines. Furthermore, these acac-containing Co-NHC complexes demonstrated efficacy in the olefination of alcohols using sulfone.



Biography

Misba Siddique is a research scholar pursuing her doctoral studies (PhD) under the supervision of Prof. Arnab Rit. She joined the Department of Chemistry, at IIT Madras in July 2020. Her research focuses mainly on the synthesis of organometallic complexes and their catalytic activity in various transformations.

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