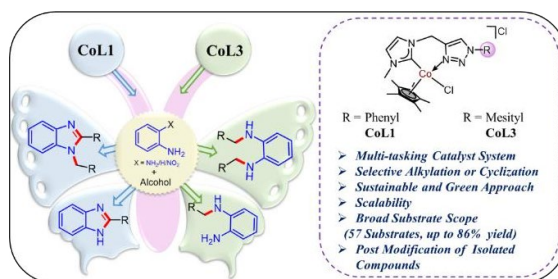


Control over borrowing hydrogen and acceptorless dehydrogenative coupling process for the Co (III)-NHC catalyzed chemoselective alkylation and cyclisation of 1,2-phenylenediamine with alcohols

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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. On the other hand, one-pot methodology offering either alkylation or cyclisation of 1,2-phenylenediamine using alcohol exploiting a single catalyst system remained unexplored. Herein, we report the chemoselective effective alkylation and cyclisation of 1,2-phenylenediamine with alcohol by simply switching the substituent on the supporting NHC ligand of cobalt(III) complexes. This varying catalytic behaviour of the complexes under consideration towards the selective formation of different products was fairly understood by analyzing their electronic properties based on NMR, electrochemical, and DFT studies. Further, the present protocol is compatible with a wide range of structurally diverse substrates offering ample variations of both amines as well as alcohols producing four different types of products starting from 1,2-phenylene diamine. Finally, an array of control experiments including the deuterium labeling and the identification of different intermediates assisted in establishing the proposed mechanism.



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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