



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI  
SHORT ABSTRACT OF THESIS

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Programme of Study : Ph. D.  
Thesis Title: "Ipso Nucleophilic Substitution on Electron Deficient Arene Systems"  
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**SHORT ABSTRACT**

The thesis entitled, "Ipso Nucleophilic Substitution on Electron Deficient Arene Systems" mainly focused on the development of greener and transition metal free methodologies for various alkylation reactions. The contents of the thesis have been divided into five chapters based on the results of experimental works performed during the research period.

**Chapter I**, the introductory chapter of the thesis, represents an overview of alkylation reaction of amine, thiol and active methylene compound, which constructs C-N, C-S, and C-C bond, respectively. Also, this chapter briefly describes the importance of the products achieved by alkylation reaction including application in pharmaceuticals, natural products, drugs and agrochemicals. Finally, the shortcomings related to the existing methods have been discussed. **Chapter II** demonstrates the alkylation of active methylene compounds on electron deficient benzene sulfonic acids with the construction of C-C bond through ipso nucleophilic substitution in transition metal free condition. **Chapter III** describes the development of an efficient, cost-effective method for synthesizing 2,4-dinitroaryl thioether derivatives by ipso nucleophilic substitution of an aromatic sulfonic acid with thiol to construct a new C-S bond in transition metal free mild condition. **Chapter IV** illustrates an efficient protocol for N and S-alkylation on 2,4-dinitrobenzenesulfonyl chloride which produces Smile rearrangement product via intermolecular ipso aromatic nucleophilic substitution. A series of control experiments and time dependent  $^1H$  NMR experiments have been demonstrated to elucidate the plausible reaction mechanism. **Chapter V** provides the strategy of alkylation on aryl benzotriazolyl derivatives by amine, thiol and active methylene compound. The desmotropic nature of aryl benzotriazolyl derivative has been demonstrated with DFT study.

Each of these chapters comprises of introduction, objective, results and discussion, mechanism, application, characterization data, and references. Synthesized compounds have been characterized with the help of modern techniques such as, HRMS, ( $^1H$ ,  $^{13}C$  &  $^{19}F$ ) NMR, IR and SC-XRD. Few of the NMR spectra and ORTEP diagram of representative compounds have been pictured in the last four chapters. Finally, the future possibilities the work have been discussed.