

# Structure/Activity Relationships in Catalytic C-H and C-X Functionalisation Reactions

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## Abstract:

The use of catalysis to construct bonds, particularly between aryl units, has made the synthesis of bi-aryl (and poly-aryl) compounds routine. New methodology using nickel or ruthenium catalysis has the potential to provide us with new, more economical, and more efficient reactions, but there are still many drawbacks to these. In this presentation, recent experimental and theoretical studies of two topics will be presented. Firstly, we have explored the relative rate of oxidative addition to nickel(0) of commonly-encountered aryl electrophiles. Secondly, we have developed a 'directing group scale' that allows us to predict site selectivity of two classes of ruthenium-catalysed C-H functionalisation reactions by conducting series of competition experiments. Both of these studies have delivered important understanding about these reactions, and we hope that these will enable the development of the synthetic processes of the future.