

Although asymmetric phase transfer catalysis has been known and practiced for over 25 years, the fundamental issues of what constitutes reactive and selective phase transfer catalysts are still unknown. This disparity is actually not surprising because phase transfer reactions are dominated by non-covalent interactions, solvation and interfacial process that are much harder to study than the influences and interactions of covalently bonded species.

This project succeeded in learning the “rules” that govern rate and enantioselectivity for simple phase transfer catalyzed alkylation reactions. The approach involved the creation of different chiral scaffolds for quaternary ammonium salts by implementation of the [4+2] cycloaddition and tandem [4+2]/[3+2] cycloaddition of nitroalkenes. The rigid, polycyclic amine scaffolds were embellished with a variety of different functional substituents in a convergent region of space using parallel synthesis methods to generate large libraries of ammonium ions.

The chiral ammonium salts were evaluated for their catalytic potential by standard kinetic and analytical methods. Next, a Quantitative Structure-Selectivity Profile was developed to explain the roles of the different substituents so that the most important controlling features can be systematically identified and their properties incorporated in designs for more reactive and selective catalysts.

