

Relationship between nucleophilicity/electrophilicity indices and reaction mechanisms for the nucleophilic substitution reactions of carbonyl compounds

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Theoretical electrophilicity and nucleophilicity scales, defined in terms of electronic reactivity indices, were tested for the reaction of a series of carbonates with neutral and charged reagents of varying nucleophilicity. The electrophilicity and nucleophilicity scales were used to rationalize some mechanistic aspects developed by these reacting systems: the greater the electrophilicity/nucleophilicity difference, the more concerted the reaction mechanism will be. Conversely, a small electrophilicity/nucleophilicity gap will in general be associated with a stepwise reaction mechanism. © 2004 John Wiley & Sons, Ltd.