Quo Vadis Chemie

A Quantitative Approach to Polar Organic Reactivity

kterou přednese

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Abstrakt:

For the construction of a comprehensive nucleophilicity scale, benzhydrylium ions (Aryl2CH⁺) and structurally related Michael acceptors (quinone methides, benzylidene-malonates) have been defined as reference electrophiles, which presently cover a reactivity range of more than 30 orders of magnitude. By studying the kinetics of their reactions with π-nucleophiles (alkenes, arenes, allylsilanes, enol ethers, etc.), n-nucleophiles (carbanions, amines, pyridines, phosphines, alcohols, etc.) or σ-nucleophiles (hydride donors) it was possible to directly compare nucleophiles which differ widely in reactivity using the correlation log k₂₀°C = sₙ (E+N), where electrophiles are characterized by one (E) and nucleophiles are characterized by two, solvent dependent, parameters (N, sₙ).¹,² A thermodynamic counterpart to this kinetic approach was developed analogously.³

(1) Database: http://www.cup.uni-muenchen.de/oc/mayr/DBintro.html