Applications of the Intrinsic Electrophilicity and Nucleophilicity Indices

Eduardo Chamorro, Mario Duque-Noreña, and Patricia Pérez

e-mail: echamorro@unab.cl

The suitability of intrinsic (i.e., electronic) relative indices for quantifying electrophilicity and nucleophilicity responses [1-5] is critically examined. Theoretical results are discussed within the framework of experimental reactivity categorization based on the linear free energy methodology developed by Mayr and coworkers [6-11]. The polar nucleophilic/electrophilic activation (as measured through simple descriptors) is shown to be a key factor driving the initial rate-determining steps of the electrophile-nucleophile coupling.

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