Integral Encounter Theory of Photochemical Transfer Reactions. Edition No. 1

Description: Non-Markovian (memory function) chemical kinetics formalism -Integral Encounter Theory (IET) is a common approach to study the kinetics of chemical reaction beyond conventional mass-action formalism. This work summarizes a general formalism of IET and its application to study two types of photochemical reaction systems. For the first application, the biexcitonic photoionization with short lived (singlet) excitations, the non-Markovian kinetics derived from IET was shown to be more accurate and detailed than its oversimplified Markovian analog. Only for long lived (triplet) excitations the non-Markovian and Markovian results are similar, provided that the rate constants are properly defined. For the second application, photooxidation competing with energy quenching was studied. We obtained the stationary concentration of the free carriers, with account of their geminate recombination before separation, as well as the stationary rate of singlet oxygen generation, affected by preliminary quenching of nearest excitations in the course of ionization.


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