Kinetics and Energetics of Chemical Reactions Through Intermediate States

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We analyze the kinetics of chemical reactions proceeding via an intermediate state. Two approaches are used. The first one is a mesoscopic description in which the system undergoes a diffusion process along a reaction coordinate in a tristable potential, modelled by considering boundary conditions and the detailed balance principle. The second consists of a quasi-static approximation in which the reaction flux depends only on time and not on the reaction coordinate. The probability distribution function is obtained numerically as a solution of the Fokker-Planck equation. The resulting reaction flux and entropy production (lost work) in the process depend significantly on the nature of the intermediate state, unstable or metastable. We compare the values of the flux and of the lost work obtained in both approaches finding that they differ especially at the first stages of the reaction or for large chemical potential differences and low energies of the intermediate state. The theory proposed is applied to organic, biochemical, and enzymatic reactions.