Information entropy for transformation of molecular structure

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There are two processes for transformation of molecular structure: a high-temperature transformation (Arrhenius dependence) and molecular tunneling (low-temperature plateau). Calculation of information entropy for these processes gives us some useful information, namely probabilities of occurrence of the reactions under considerations, their efficiency and mean-square fluctuations of the distribution function parameters. Essentially, this investigation is an evolution of Perrin’s radiation hypothesis proposed in 1919. Almost one century has passed…And now a fuller picture of the elementary activation act for unimolecular chemical reaction begins to emerge. Arrhenius dependence with low-temperature plateau.

Recent Publications:


Biography

Anatoly Stepanov has received his graduation of the BSU in 1976 and post-graduate studentship in the BSU 1983 - 1986.1997 up to the USSR disintegration: WATOC member; 1997 - 2000: NYAS member. Current research activity - there are a few problems in physics and chemistry that are in interest for me: an elementary activation act in solid state diffusion and chemical transformation; compensation effect in chemical kinetics; adiabatic and non-adiabatic approximation in molecules physics; dynamic properties of protein mobility; IR multi-photon absorption and photodissociation; molecular structure; molecular tunneling; prebiotic evolution; Einstein coefficients for activation barrier; low-temperature equilibrium fluctuations and functionally important motions in a globular protein; information entropy for activation process and molecular tunneling.

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