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Information entropy for transformation of molecular structure

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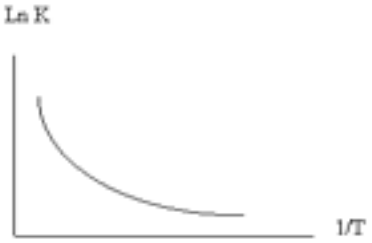
There are two processes for transformation of molecular structure: a high-temperature transformation (Arrhenius dependence) and molecular tunneling (low-temperature plateau). Calculation of information entropy for these processes gives us some useful information, namely probabilities of occurrence of 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:

1. Stepanov A.V., Stepanov M.A. (2018) Information entropy of molecular tunneling. Proceedings 2:151-162.
2. Stepanov A.V. (2015) Information entropy of activation process: Application for low-temperature fluctuations of a myoglobin molecule. International Journal of Modern Physics B 29:1550016-1-18.
3. Stepanov A.V. (2011) Modeling of metamaterials: a globular protein as a metamaterial prototype for electromagnetic-acoustic conversion at low temperatures. Proc. of SPIE 8070:807013-1-13.
4. Stepanov A.V. (2007) Activation process model: Einstein coefficients for activation barrier. Journal of Molecular Structure: THEOCHEM 805:87-90.
5. Stepanov A.V. (2002) Interaction model of thermal radiation with molecule at low temperatures: molecular tunneling. Journal of Molecular Structure: THEOCHEM 578:47-61.

Biography

Anatoly Stepanov has received his graduation of the BSU in 1976 and post-graduate studentship in the BSU 1983 - 1986.1989 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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