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Information Entropy of Molecular Tunneling

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Abstract: Molecular tunneling process has been considered by means of radiation theory. The formula for information entropy calculation has been derived by means of interaction model of thermal equilibrium radiation with a molecule at low temperatures. The physical meaning of information entropy for low-temperature plateau of unimolecular chemical reaction has been determined. It is a measure of conversion of thermal radiation energy to mechanical energy that moves atoms in a molecule during elementary activation act. It is also a measure of uncertainty of this energy conversion. The conversion takes place at a temperature when the average energy of the elementary activation act is equal to a part of zero energy of the transforming molecule. Two unimolecular reactions have been investigated. These are Fe-CO bond recombination in β-hemoglobin and double proton transfer in benzoic acid dimer for sequential deuteration of hydrogen bond and various hydrostatic pressures. Using the information entropy formula it is possible to calculate its value in energy units of measurements for low-temperature plateau. Probabilities of occurrence of the reactions under considerations, their efficiency and mean-square fluctuations of the distribution function parameters have also been determined.

Keywords: Shannon entropy; information entropy of molecular tunneling; thermal equilibrium radiation; interaction model of thermal radiation with a molecule at low temperatures; Fe-CO bond recombination in β-hemoglobin; double proton transfer in benzoic acid dimer.

Results and Discussion

1. The formula for information entropy of molecular tunneling has been derived.
2. Arrhenius dependence for molecular tunneling process is caused by information entropy change. In addition, information entropies for low-temperature plateau and for the beginning of the activation part of Arrhenius dependence are equal.
3. Efficiency comparison has been made for Fe-CO bond recombination in β-hemoglobin and double proton transfer in benzoic acid dimer. The first reaction is more effective at low temperatures, while the temperature dependence of the second one is the opposite.

Conclusions

Essentially, this investigation is an evolution of Perrin's radiation hypothesis proposed in 1919. Almost one century has been passed... And now a fuller picture of the elementary activation act for unimolecular chemical reaction is beginning to emerge.

Supplementary Materials

Links:

https://en.bntu.by/information-technologies-and-robotics-faculty/departments/engineering-physics

http://ozone.bsu.by

https://www.researchgate.net/profile/Anatoly_Stepanov/

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