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A mathematical model of molecular processes: spectra and chemical transformations

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Abstract

General questions of modeling objects of the molecular world are discussed. The existence of several stable geometric structures for a group of atoms in a limited region of space allows us to consider a wide well with high vertical walls and with a bottom in the form of a multiminimum surface as the most natural choice of the shape of the potential. The appearance of observed molecular formations can be considered as spontaneous transitions from stochastic states from levels with higher energy (undefined structures in the form of a cluster of atoms) to states with a specific geometry at lower levels of potential wells.

It is shown that an inverted Gaussian function can be one of the possible variants for choosing the shape of potential wells. This kind of potential makes it possible to explain physically the transition from the stochastic region to the region of localized states, since the zero energy value is at the lower level of the stochastic state and a gap appears between the energies of these states. In the region of the potential minimum, the shape of the wave functions is close to harmonic, and when the energy levels corresponding to the bound states are approached to the edges of the well, the distances between them decrease. Potentials in the form of a sum of several Gaussian functions are easily transformed, and mixed eigenfunctions appear to be different from zero both in the wells and in the gap between them, which leads to structural transformations.

It is shown that one can construct a mathematical model based on the basic principles of the theory of molecular spectra for describing complex, time-varying molecular objects without involving empirical parameters. A step-by-step algorithm for constructing such *ab initio* model is formulated and it is shown that the field of its applicability is not limited only to intramolecular processes, but also covers chemical transformations. The proposed approach opens up opportunities for analyzing the kinetics of chemical transformations, forecasting the development of processes and their optimization based on computer experiments.

An example of a general system of differential equations describing a complex multistage process of transformations, including structural transformations, decomposition and addition reactions, is given. The parameters of the system of equations calculated by means of the theory of spectra are the values of energy levels, the probabilities of transitions between them and the frequencies of quantum beats. The result of solving this system of equations is shown.

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