Nature of Compensation Law and “Exotic” Arrhenius Parameters in Denaturation of Proteins

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Proteins possess unique functionality in their native states operating in the cells of all known organisms. These native states are assembled by the folding of the protein chain into a secondary, tertiary or even quaternary structure. Denaturation of proteins provided by unfolding of this structure results in the loss of their functionality which can be followed by the death of the cells and organisms. The current work is devoted to theoretical investigation of the nature of two experimentally established phenomena in proteins denaturation provided by heating: Compensation Law behavior and “exotic” values of the Arrhenius parameters. Exotics of Arrhenius parameters can be illustrated by the fact that the preexponential factor A for the rate constants of these processes is almost always more than 10^{25} s^{-1} and can reach values up to about 10^{130} s^{-1} [1,2]. These numbers differ drastically from the values of about 10^{13}-10^{14} s^{-1} typical for unimolecular reactions of the different types of organic molecules [3]. In spite of the spread in values the changes of Arrhenius parameters E_a and A in a wide manifold of studied proteins compensate each other demonstrating so-called Compensation Law (CL) behavior [1,2,4]. Many hypotheses were suggested for explanation of CL behavior [4] but this behavior is still not understood.

In the presented work the unfolding of proteins is modeled by dissociation of the dimers of polypeptides (polyglycine) of varied length into the monomeric chains. The “loose” transition state model is suggested which allows one to calculate the rate constants and Arrhenius parameters for dissociation of these dimers within Transition State Theory (TST). The results obtained allow us to explain the “exotic” values of Arrhenius parameters and to conclude that the CL behavior is the intrinsic property of the protein denaturation process in a dry or hydrated shape of protein.

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