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A Study of Physical and Chemical Transformation of Mutated Gene Molecules Using Thermodynamic and Computational Analysis YOONJEONG KWON, ANDREW KYUNG, Choice Research Group — In this paper, a spontaneous DNA mutation was thermodynamically observed to determine whether the chemical or biological transformation can locally lower or increase the enthalpy of the system. An example of spontaneous DNA mutation is deamination of cytosine, in which cytosine turns into uracil through hydrolysis, mutating the DNA molecule while releasing ammonia under a certain condition. But in case of any endothermic reactions, in which heat energy becomes chemical potential energy, the reactions increase the chemical potential energy on the final products. Since the DNA does not exists in isolation but neatly packed together in tight coils, the study of physical stabilization of the DNA molecule after DNA mutation is not easy. In this paper, using computerized medicine and biomedical engineering, the possible methods to analyze and to study the stabilization and kinetics of the DNA mutation are shown. This research uses computational chemistry to calculate the thermodynamic stability of the gene molecules. To determine whether the DNA molecule is locally destabilized by a spontaneous DNA mutation, physical and chemical computational softwares is used to further display the optimized geometry energy levels and calculate each compound models theoretical values.

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