## Quantum-chemical modeling of the solvatochromic effect of the denaturation and mutation effect of DNA

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The influence of the environment on the proton transfer between nucleotide bases is of crucial importance for denaturation and mutation processes in DNA. For quantitative description of these processes, activation ( $\Delta E^*$ ) and reaction ( $\Delta E$ ) energies of the proton transfer as well as lactam-lactim ( $K_T^{LL}$ ) and amineimine ( $K_T^{AI}$ ) tautomeric equilibrium constants calculated by the quantum-chemical DFT (Density Functional Theory) method were used. It is shown that an increase in the environment polarity ( $E_r$ ) due to mixing of ethanol with water (solvatochromic effect) leads to a decrease in the activation energy of the proton transfer and to an increase of the mutation frequency ( $v_m$ ) and at the same time to the tendency of DNA to denaturation. Hence, energy and kinetic characteristics of the proton transfer may be used for quantitative description of a solvatochromic effect in DNA. The validity of the solvatochromic effect is confirmed by the bathochromic shift of the DNA absorption band in the UV spectrum.



## References:

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