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DNA melting and energetics of the double helix

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Highlights

- Studying melting and energetics of the DNA double helix has been one of the major topics of molecular biophysics over the past six decades. The main objective of the review article is to overview the current state of the field and to emphasize that there are still serious gaps in our understanding of the issue. We start our paper with a concise description of the commonly accepted theoretical model of the DNA melting. We then concentrate on studies devoted to the comparison with experiment of theoretically predicted melting profiles of DNAs with known sequences. For long DNA molecules, such comparison is significant from the basic-science viewpoint while an accurate theoretical description of melting of short duplexes is necessary for various very important applications in biotechnology. Several sets of DNA melting parameters of the nearest neighbor model will be compared and analyzed. The analysis leads to a conclusion that in case of long DNA molecules the consensus set of nearest neighbor parameters describes well the experimental melting profiles. Unexpectedly, for short DNA duplexes the same set of parameters hardly yields any improvement as compared to the default model, which completely ignores the effect of heterogeneous stacking. We will discuss the possible causes of this striking observation.
- The issue of separation of base-pairing and base-stacking contributions into the double helix stability will be reviewed for the first time. Recent experimental attempts to solve the problem will be extensively analyzed. It is concluded that the double helix is essentially stabilized by stacking interaction between adjacent base pairs.
- In the final section of the article, the kinetic aspects of DNA melting phenomenon will be discussed. The main emphasis will be on the hysteresis effects often observed in melting of long DNA molecules.

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