

## **Hydration and stabilization of structures and conformational states of DNA macromolecules**

Barbara Lubas

Basing on a general consideration of molecular mobility in the systems biopolymers - water the interaction of DNA macromolecules with water and its influence on the DNA structure and stability are reviewed and discussed. It is emphasized that studies of DNA hydration carried out by various techniques and by theoretical approach indicate considerable heterogeneity in the hydration shells or centers which differ in affinity to molecular subunits of DNA and in molecular mobility. On this background, basing on own experimental measurements of magnetic relaxation times in aqueous DNA solutions in function of a temperature general semiempirical model of DNA hydration is proposed and discussed. For description of the movement of heterogeneous hydration shells of DNA the log-normal distribution function, with parameters  $\beta$  and  $\tau_m$  being the half - width of the distribution and the most probable correlation time respectively was introduced. Subsequently, the systems of nonlinear parametric equations with empirical coefficients and unknown values ( $\beta$ ,  $\tau_m$ ) were derived, for solving of which by use of computer techniques numerical methods were developed and applied. The parameters ( $\beta$ ,  $\tau_m$ ) were then quantitatively compared under various conditions for DNA in the native, denatured and partially denatured states and also during thermal helix-coil transition. It led to the following characteristics of nonrotational hydration shells of DNA:

- 1) in the native state at higher ionic strength they are relatively uniform, homogenous and very limited in movement,
- 2) in the premelting regions, during helix-coil transition and at lower ionic strength in the native state they seem to be splitted into the homogenous and limited in movement fractions  $\chi$  and the strongly heterogeneous and much mobile as  $\chi$  fractions  $Y$ .

It was also proved that dehydration of DNA during denaturation is rather selective whereas rehydration of denatured DNA is much more statistical. The dynamic phenomena involving a mechanism of large rearrangements in the hydration shells of DNA during helix-coil transition are discussed in terms of the participation of water dipoles from the hydration shell of  $Na^+$  cation in the total hydration of DNA.