

STRUCTURIZATION OF COUNTERIONS
AROUND DNA DOUBLE HELIX: A MOLECULAR
DYNAMICS STUDY

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S u m m a r y

The structurization of DNA counterions around the double helix has been studied by the molecular dynamics method. A DNA dodecamer d(CGCGAATTCGCG) in a water solution with alkali metal counterions Na⁺, K⁺, and Cs⁺ has been simulated. The systems have been considered in the regimes without excess salt and with different added salts (0.5 M of NaCl, KCl, or CsCl). The results have shown that the Na⁺ counterions interact with the phosphate groups directly from outside of the double helix and via water molecules at the top edge of the DNA minor groove. The potassium ions are mostly localized in the grooves of the double helix, and the cesium ions penetrate deeply inside the minor groove, being bonded directly to atoms of the nucleic bases. Due to the electrostatic repulsion, the chlorine ions tend to be localized at large distances from the DNA polyanion, but some Cl⁻ anions have been detected near atomic groups of the double helix, by forming electrically neutral pairs with counterions already condensed on DNA. The DNA sites, where counterions are incorporated, are characterized by local changes in the double helix structure. The lifetime of Na⁺ and K⁺ in the complex with DNA atomic groups is less than 0.5 ns, while it can reach several nanoseconds in the case of cesium ions. On this time scale, the Cs⁺ counterions form a structured system of charges in the DNA minor groove that can be considered as ionic lattice.