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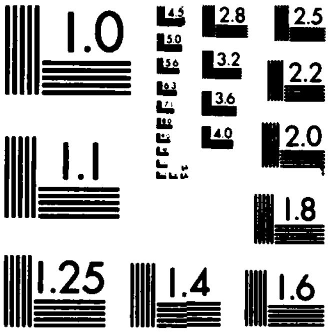

MICROCOPY RESOLUTION TEST CHART
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Response of DNA in Aqueous Solution to Microwave Irradiation

M.E. Davis & L.L. Van Zandt
Department of Physics
Purdue University
W. Lafayette, Indiana 47907

We have calculated the expected absorption of microwave radiation in the gigaHertz frequency range by fixed length DNA polymer molecules disolved in saline solution. While the effects of counterions and solvent dynamics have been accounted for in detail, the features of the absorption are completetly dominated by the interaction between the charged polymer molecule and the so-called first hydration layer, that is, the nearest layer of solvent water molecules not actually bonded to the polymer. The relevant parameters of this interaction are the strength of the water-to-polymer coupling and the average persistence time of individual water-to-polymer bonds. These are presumably hydrogen bonds to the oxygen atoms of the backbone phosphate structure. Using the best available estimates of the system parameters, we can obtain structured absorption corresponding to compressional wave phonon excitations on the polymer, "organ pipe" modes, such as have been claimed to be seen by Edwards, Davis, Swicord & Saffer. These modes are now well known in much drier sample materials. We have examined the effects of varying solvent salt concentration and the system temperature. In both cases, the effects are virtually nil, in the former because of the Manning condensation phenomenon that preserves a remarkably constant polymer environment over a wide range of bulk ionic strength, and in the later case because of a fortuitous competition between effects of bulk viscosity and persistence time changes with temperature. Hence, any effects seen in the experimental variation of temperature or salinity could be wholly attributed to their modification of the hydration layer properties.

The Effect of Propeller Twist on Phonon Dispersion in DNA

L. L. VanZandt and W. K. Schroll

Department of Physics
Purdue University
West Lafayette, Indiana 47907

We have developed a high accuracy software package for calculating a complete phonon dispersion spectrum for any DNA polymer configuration utilizing classical dynamics via a dynamical force constant matrix. These routines permit us to treat a variety of related physical systems with a minimum of attention to computing detail. As an example we have varied selected mean helix parameters over their allowed experimental ranges and then determined the particular values which yield a Helmholtz free energy minimum. A purine-pyrimidine base pair has a propeller twist angle defined as the angular displacement between the planes of the two bases when they are rotated in opposite directions about a common axis determined by the nitrogen-carbon bond joining each base with its associated sugar. This paper deals with the optimization of the propeller twist angle, ς, for B-configuration Poly(dG)·Poly(dC) DNA, which has an X-ray experimental uncertainty of $\pm 4.8^\circ$. We show a marked variation in phonon frequencies at zone center for the lower optical modes over the 9.6° variance permitted experimentally. This is to be expected because the two acoustic modes are mediated by the bulk structure of the polymer rather than the particular atomic positions. The highest optical modes are unaffected since these high frequency phonons generally correspond to oscillations of relatively localized atomic coordinates. We evaluate these various configurations and determine that a minimum in the Helmholtz free energy corresponds to a propeller twist angle 2.20° less than that quoted as the equilibrium value. Further applications of this algorithm package for DNA structure parameter determination will include baseroll, base inclination and B to Z conformational change.

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