Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Molecular mechanical studies of hydrated B-DNAs: conformation and counterions CHARLES CLEVELAND, UZI LANDMAN, Georgia Institute of Technology — We examine through molecular mechanics the fully hydrated DNA duplex 5'd(AAACCTAAACCTAATAT)3' and a similar structure where four sugars near the G-C base pairs are modified by adding isopropyl groups which intrude into the minor groove. Attention is paid to the distributions of water molecules and sodium counterions and the conformation of the duplexes. Apart from the effects of the chemical modification we are interested in the degree and kinds of correspondence between temporal variations of counterion positions and variations in the duplex conformation as expressed through structural parameters such as the width of the major and minor grooves, base-pair parameters such as roll, twist, and buckle, and such.

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Date submitted: 06 Dec 2004 Electronic form version 1.4