Meeting: 1002, Pittsburgh, Pennsylvania, SS 6A, Special Session on Mathematical Modeling of Nonlinear Phenomena in Biology and Mechanics

1002-74-217 **David Swigon*** (swigon@pitt.edu), Department of Mathematics, University of Pittsburgh, 301 Thackeray Hall, Pittsburgh, PA 15260, **Wilma K Olson** (olson@rutchem.rutgers.edu), Piscataway, NJ 08854, and **Bernard D Coleman** (bcoleman@jove.rutgers.edu), Piscataway, NJ 08854. *Influence of intrinsic curvature and coupling on configurations of DNA minicircles.*

Recently developed mesoscale theory of sequence-dependent DNA elasticity and methods for calculating configuration of DNA segments subject to imposed constraints make it possible to study the influence of intrinsic curvature and roll-twist coupling on configurations of DNA minicircles that are subject to binding of untwisting ligands. For minicircles formed from intrinsically straight DNA it was found that the distribution of roll-twist coupling strongly affects the dependence of the total elastic energy on the amount of imposed untwisting, and that dependence can be far from quadratic. A minicircle formed from intrinsically curved DNA can undergo large deformation with localized untwisting and bending at remote steps. The presence of coupling can amplify these configurational changes to the point where there can be first-order transition between two distinct stable configurations. (Received September 14, 2004)