

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Oxidative Damage to DNA¹ ROBERT N. BARNETT, Georgia Institute of Technology, CHARLES L. CLEVELAND, UZI LANDMAN, GARY B. SCHUSTER — The initial stage of the reaction of a guanine radical cation with water is investigated using ab-initio methods coupled with molecular mechanics. We explore the influence of the sugar- phosphate backbone, the complementary cytosine base, the adjacent base pairs in the B-DNA double strand, the state of hydration, and finally the distribution of counter-ions on the barrier and reaction path leading to 8-oxo-G.

¹Supported by US DoE and National Science Foundation

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Date submitted: 30 Nov 2004

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