DAMOP05-2005-000037
Abstract for an Invited Paper
for the DAMOP05 Meeting of
the American Physical Society

Theory of Damage to DNA by Low-energy Electrons

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Stimulated by the observations of Boudaiffa et al that low-energy electrons can induce strand breaks in DNA (probably via core-excited resonance states) and knowing of the work of Burrow et al on resonances in DNA bases, we explored the possibility that even lower-energy shape resonances could cause such damage. In a series of publications, we employed stabilization-type electronic structure methods and potential energy landscape exploration techniques to address this question. The systems we examined included small fragments of DNA each of which included at least one base, one sugar, and two phosphate units. We found that electron attachment to form a low-lying π^* shape resonance of a base unit could cause a sugar-phosphate C-O bond to be rendered susceptible to fragmentation over barriers ranging from 5 to 25 kcal mol^{-1} but only when the phosphate group has a counter cation nearby. The rates of C-O bond rupture can be as high as 10^{10}s^{-1} which, considering the ca. 10^{14}s^{-1} detachment rates of the π^* resonance, suggest a yield of one strand break in 10^4 attached electrons.