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Low energy electrons induced damage to selected DNA fragments

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We have theoretically and computationally investigated the mechanism of low energy electron (LEE) induced DNA damages such as single strand breaks (SSBs) and glycosidic bond cleavage in some selected DNA fragments (Fig. 1) viz., 2'-deoxycytidine-3'-monophosphate (3'-dCMPH) [Fig. 1(a)], 2'-deoxycytidine-5'-monophosphate (5'-dCMPH) [Fig. 1(b)] and sugar-phosphate-sugar (SPS) [Fig. 1(c)]. In this regard, we have used electronic structure theory and our newly implemented local complex potential based time dependent wave packet (LCP-TDWP) approach. Results from our calculations show that in 3'-dCMPH and 5'-dCMPH DNA fragments SSB predicted near 1 eV whereas in SPS moiety it appears around 0.6 eV. Further, in case of SPS moiety there are two dissociation channels namely 3' C-O and 5' C-O bond lesions. Our calculations show that the activation energy barrier for 5' C-O bond dissociation is less than of 3' C-O bond dissociation pathway. It has also been found that the metastable anion formed after electron attachment to SPS moiety is more long lived (~40-55 fs) than that to 3'-dCMPH and 5'-dCMPH fragments (~18-20 fs). On the other hand, the glycosidic bond cleavage in 3'-dCMPH moiety [Fig. 1(d)] requires higher activation energy than of the SSB in the same fragment and thus least preferred channel compared to SSB.

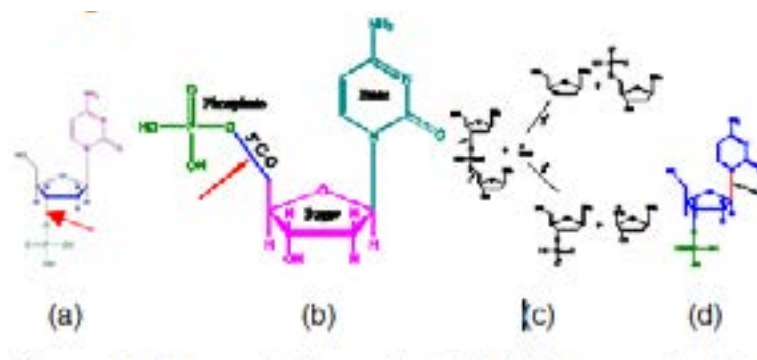


Figure 1: Some of the selected DNA fragments. For each fragment bond susceptible for cleavage is marked with an arrow.

Biography

Manabendra Sarma received his BSc and MSc degrees in the year 2000 and 2002 respectively from Goalpara College and Indian Institute of Technology Guwahati, Assam, India. After completing his MSc degree, he moved to Indian Institute of Technology Bombay, Mumbai, India in 2002 to pursue his PhD under Professor Manoj K. Mishra. He completed his PhD in 2008 and subsequently joined the Department of Chemistry at Indian Institute of Technology Guwahati, Assam, India as a Senior Lecturer in the same year. In the year 2011, he received the prestigious BOYSCAST Fellowship of India to work with Professor Lorenz S Cederbaum of University of Heidelberg, Germany for a year. His current research interests include development of new theoretical approaches to laser assisted control of chemical reactions and resonances in electron-molecule scattering. Currently he is an Associate Professor in Chemistry at Indian Institute of Technology Guwahati, Assam, India.

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