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Dynamical (e,2e) Studies of Bio-Molecules

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Declaration

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Joseph D. Builth-Williams,
March 1^{st}, 2012

Research is what I'm doing when I don't know what I'm doing.

$\sim$ Wernher Von Braun (1912-1977)

Abstract

As the basis of life, deoxyribonucleic acid (DNA) is an extremely important molecule and though, in many ways, it is a stable molecule, even the slightest damage can lead to potentially disastrous results. One such source of damage is high-energy ionising radiation and while this high-energy radiation can cause significant damage by directly interacting with DNA, a significant amount of damage is also caused by the low-energy secondary electrons it generates through ionisation. Previous attempts to model the effects of ionising radiation on DNA have been limited by the experimental data available at the time, and so have used water as a model for the biological medium. Thus a need to understand how these secondary ionising species, in particular electrons, interact with biomolecules exists.

In this thesis I report on original relative Triple Differential Cross Section (TDCS) measurements for the electron impact ionisation of pyrimidine, α-tetrahydrofurfuryl alcohol, tetrahydrofuran, tetrahydropyran and 1,4-dioxane. The TDCSs provide the probability that a bio-molecule will eject an additional electron, of a particular energy and at a particular angle, after being struck by an incident electron (that is subsequently scattered from the target molecule, at a specific angle and energy). In each case the Highest Occupied Molecular Orbital (HOMO) was probed, specifically the $7b_2$, $28a$, $9b + 12a'$, $15a'$ and $8a_g$ orbitals for each respective molecule listed above. In addition, some measurements were also made on the $10a_1$ orbital of pyrimidine. Furthermore, all these TDCS measurements are compared to results from calculations using the Molecular Three-Body Distorted Wave (M3DW) model. Fair agreement is typically found between the M3DW results and the experimental data. All the present results were measured using coplanar asymmetric kinematics.

Physics is imagination in a straight jacket.
$\sim$ John Moffat (1932-present)

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