Elastic electron scattering from the DNA bases: cytosine and thymine

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Abstract. Relative elastic differential cross sections for elastic scattering from cytosine and thymine have been measured using the crossed-beam method. The measurements have been performed at two electron energies of 500 and 100 eV, and cover the angular range of 10°-130°. Calculations of elastic differential cross sections have been performed via the screen corrected additivity rule method, and agreement is quite good with the present experimental results. The results obtained are important for the modelling of energy deposition in living tissue.

1. Introduction

Ionizing radiation is widely used in medicine as a diagnostic probe in radiology and as a palliative treatment in radiotherapy. It is now known that it is not just the primary ionizing particle that is responsible for cell and tissue damage, a significant amount has been shown to be due to secondary species that arise from the primary particle [1]. Upon entering the body, the primary particle thermalizes quickly through various scattering processes, liberating large numbers of low energy (0-20 eV) secondary electrons. These electrons can then interact with different biological molecules, and have been shown to cause significant damage to DNA via dissociative electron attachment [2, 3]. This leads to single or double DNA strand breakage, either directly or via the formation of free radicals.

Due to the difficult nature of reliable measurement or calculation of cross sectional data for electron scattering from large molecules, there is limited information on species of biological relevance. However, there is great interest in electron scattering data from large biological molecules such as the pyrimidine bases as an input for studying the effects of radiation damage via Monte Carlo based charged particle track structure simulations. Experimentally, elastic differential cross sections (DCS) for electron scattering from water have been around for some time [4], while data has only
recently appeared concerning formic acid [5], variations of the tetrahydrofuran ring [6, 7], alanine [8] and pyrimidine [9]. Due to the difficulties in handling these sorts of targets, theoretical calculation for the large biomolecules is actually preceding experimental investigation. Theoretical studies concerning electron scattering from the DNA bases have been performed by Możejko and Sanche [10] and Blanco and García [11, 12] who have calculated elastic cross sections for all of the DNA and RNA bases, differential in energy as well as in angle. An interesting outcome of both of these studies was the realization that the angular distribution at a given energy for any one of the DNA bases can be related quite accurately to the others by the ratio of their molecular weights or the number of electrons in the target.

The present study reports the first experimental cross sections for the elastic scattering of electrons from two of the DNA bases; cytosine and thymine. Angular distributions are presented for 500 and 100 eV incident electrons, and for angles between 10° and 130°. Theoretical cross sections calculated by the screen-correction additivity rule (SCAR) method are also presented for cytosine and thymine under the same conditions (see [11, 12] for details of the calculation). The measured elastic scattering cross sections are relative, and are only attributed an absolute scale by normalization to theory. Comparison is made with the existing theoretical results by Możejko and Sanche [10]. Due to the structural similarities between the two DNA bases and pyrimidine (see figure 1), cross sections are also compared to the previous experimental study of Maljković et al. [9]

2. Experiment

This study has been conducted in a conventional (e, 2e) spectrometer, which has been described previously in the literature [13]. As such only the elements pertinent to the present study shall be documented here.

The elastic differential cross sections are measured via the crossed beam method. Electrons from a conventional electron gun are crossed perpendicularly with the gas target before being energy selected via a hemispherical analyser and detected by a channel electron multiplier. Angular distributions are measured by varying the in-plane detection angle of the elastically scattered electrons whilst maintaining a fixed incident electron energy. As the normal mode of operation for the apparatus is to measure electron impact ionization via coincidence techniques, there is no provision in the experiment for the use of the relative flow technique to establish absolute values for the cross sections.

Both cytosine and thymine are powders at room temperature, and gaseous cytosine and thymine are produced in a molecular beam oven, centrally located in the spectrometer. Through the use of two independent Thermocoax heating elements temperatures in excess of 220°C are achievable with good stability. To avoid deposition of the target materials on elements inside the spectrometer, target gases are trapped via a cold finger that has been installed in the chamber, concentrically mounted above the interaction region. Manufactured from 310-stainless steel with an OFHC copper collection disk at the finger’s end, the cold finger is able to be filled externally with liquid nitrogen, and has been observed to be quite effective in the trapping of the DNA bases.
Figure 2. (Colour online) Relative DCS for electron scattering from cytosine (circles) at energies of (a) 500 eV and (b) 100 eV. The present data is attributed absolute value via normalisation to the SCAR calculations (solid line). Also shown are the IAM calculations [10] (dashed line) and the data for pyrimidine [9] (squares). The error associated with the experimental data is less than 10%.

Figure 3. (Colour online) DCS for electron scattering from thymine (circles) at energies of (a) 500 eV and (b) 100 eV. The present data is attributed absolute value via normalisation to the SCAR calculations (solid line). Also shown are the IAM calculations [10] (dashed line) and the data for pyrimidine [9] (squares). The error associated with the experimental data is less than 10%.
3. Results
Relative DCS’s for elastic scattering from cytosine and thymine are presented in figures 2 and 3 respectively, for 500 eV (panel (a)) and 100 eV (panel (b)) incident electrons. The data is presented alongside other available experimental and theoretical cross sections.

In figure 2, comparison is made between the present cytosine experimental data and the SCAR calculation. Absolute values are assigned to the measured relative cross sections via normalization to the SCAR calculation. Excellent agreement is seen between the calculated and measured data sets, particularly with regard to the depth and location of the minimum in the 100eV angular distribution (panel (b)). Perhaps the one failing of the SCAR calculation is the underestimation of the shoulder feature in the 100 eV DCS around 60°. The present results are also compared to the published independent atom method (IAM) calculation of Możejko and Sanche [10]. Good agreement is also seen with the IAM calculation; although it tends to overestimate the size of the cross section at backward angles. In contrast to the SCAR method, the IAM results overestimate the size of the shoulder around 60°. The measured cytosine distributions are finally compared to previous absolute experimental data for pyrimidine of Maljković et al. [9] at 100 eV (panel (b)). Clearly, the shape of the pyrimidine cross section mimics the recently measured cytosine distribution quite well. The absolute magnitude of the cytosine cross section, assigned by the SCAR calculation, is slightly greater than the pyrimidine cross section, particularly around the DCS’s minimum, which can likely be attributed to the previously mentioned difference in molecular weight [11].

Figure 3 compares the present thymine experimental data with the results of the SCAR calculation, with absolute values attributed to the experimental data via normalization to the theory. The SCAR calculation is again quite successful at reproducing the measured cross sections; however the issue with regards to the underestimation of a shoulder in the cross sections at 60° is again present. The thymine results are also compared to the IAM calculation [10], and again good agreement is observed, however the predicted cross sections are still overestimated at backward angles. The IAM results reproduce the shoulder in the cross sections near 60° slightly better in the thymine case. We again compare to the previously published experimental cross sections for pyrimidine [9], for 100 eV incident energy (panel (b)). The shape of the presently measured thymine cross section again correlates quite well with the pyrimidine data; however it is worth noting that the strength of the shoulder near 60° is more pronounced than for both cytosine and pyrimidine. The absolute magnitude of the thymine cross section, as assigned by the SCAR calculation, is greater than both the cytosine and pyrimidine cross sections, which is expected due to its greater molecular weight.

There is a greater difference between the SCAR and IAM calculations for both cytosine and thymine at 100 eV than at 500 eV. As is discussed in detail in ref [11] the IAM does not take into account interactions of the incident electron with more than one atom at a time and ignores geometrical screening corrections for each atom from the rest of the molecule. These are incorporated in an approximate way in the SCAR calculations through the screen corrected additivity rule. At larger electron incident energies atomic cross sections become smaller and the overlapping corrections become smaller. Hence, the inclusion of screening effects becomes less important at higher incident electron energies.

4. Conclusions
The present study reports experimental relative DCS’s for elastic electron scattering from cytosine and thymine, at incident electron energies of 500 and 100 eV. Theoretical cross sections produced via the SCAR method are also presented with the experimental cross sections, which are in good agreement with each other, and are also used to attribute absolute scale. Reasonably good agreement is also seen with the theoretical cross sections of Możejko and Sanche [10]. As has been found previously in theoretical studies [10, 11], the relative angular distributions of thymine and cytosine are very similar in shape and they also appear similar to the recent experimental cross sections of Maljković et al. [9] on pyrimidine. A shoulder in the angular distributions is shown to be present at approximately 60°,
and observed to be stronger for thymine than it is for cytosine. This likeness in the angular dependence of DCS values may be expected due to the similarities in the molecular structures of pyrimidine, thymine and cytosine.

Cross section values for electron impact ionization of DNA are needed for the modelling of radiation damage in biological systems. The present data can be used for energy deposition modelling in biological tissue and studies of radiation damage to biological systems. Further investigation into other incident energies is currently under way.

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