Excitation functions for positively charged fragments produced by electron impact on thymine

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Excitation functions for positively charged fragments produced by electron impact on thymine

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Synopsis Fragmentation of thymine in the gas phase is studied using low-energy electron impact. Positive ions have been detected using a reflectron time-of-flight mass spectrometer. Mass spectra have been measured as a function of electron impact from the ionization threshold to 400 eV, and excitation functions of most of the positively charged fragments have been extracted.

Recent research has shown that low-energy electrons are very effective at inducing single and double strand breaks in DNA. When ionizing radiation passes through a biological medium, it produces secondary particles along the radiation tracks, including a large amount of low-energy electrons. It is because of this that electron impact induced fragmentation of thymine is important for understanding radiation damage on the molecular scale.

To generate a molecular beam of thymine, it is placed in a resistively heated oven in powder form. The oven is mounted in an expansion chamber, and the forward section of the beam effusing from a capillary in the oven passes through a skimmer into the collision chamber. The beam is then crossed by a pulsed electron beam produced by an electron gun that consists of four electrostatic lens elements and a deflection system for steering the beam.

A reflectron time-of-flight mass spectrometer is used to detect and mass resolve the positively charged fragments. Individual time-of-flight spectra are acquired by a multichannel scaler. LabView code is used to accumulate time-of-flight spectra as a function of electron impact energy.

An overview of the experiment can be found in [1]. The pulsed valve used in [1] for the generation of molecular clusters has been replaced by the resistively heated oven.

The work we have done on thymine is based on two sets of mass spectra. In the first set the electron impact energy was increased from 0.5 to 100 eV in steps of 0.5 eV, whereas in the second set the energy was increased from 5 to 400 eV in steps of 5 eV.

For both sets of mass spectra the yields of the fragment ions were determined by fitting groups of adjacent peaks with a sequence of normalized Gaussians. Using a LabView program written for this purpose, the fitting was done automatically for all electron energies in succession. In this way, excitation functions for most of the positively charged fragments have been determined.

Tests of the electron beam current have shown that the current is constant above about 15 eV, but decreases at lower energies. Because all excitation functions are generated from a single dataset, and assuming that the detection efficiency of the reflectron mass spectrometer is mass independent, above 15 eV the yields of all fragments are on the same relative scale and are comparable.

In all our measurements we have found that the intensity of the thymine beam remained constant for about 6 – 10 hours and then decreased, even though enough thymine remained in the oven. The excitation functions have been acquired from a dataset collected before appreciable depletion of the thymine beam occurred, and a small correction has been applied to the excitation functions.

Mass spectra and excitation functions will be presented at the conference and will be compared with other research on thymine.

References

[1] G. Barrett and P. J. M. van der Burgt 2008 *J. Phys. Conf. Ser.* **101** 012008

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