Positive ion mass spectrometry for fragmentation of 5-fluorouracil by low energy electron impact

M. A. Brown* and P. J. M. van der Burgt* [1]

* Department of Experimental Physics, National University of Ireland Maynooth, Maynooth, Co. Kildare, Ireland

Synopsis. Fragmentation of 5-fluorouracil in the gas phase has been studied using low energy electron impact. Positive ions have been mass resolved and detected using a reflectron time-of-flight mass spectrometer. Mass spectra have been measured as a function of electron impact from 5 to 100 eV, and ion yield curves and appearance energies for most of the positively charged fragments have been extracted.

The halo-uracils are important in radiation treatment therapy as radiosensitizers, because cancer tissues doped with these sensitizer molecules will be destroyed preferentially under exposure with ionizing radiation. Because secondary electrons formed along the tracks of the ionizing radiation play an important role in radiation damage processes on the molecular scale, low-energy electron impact studies of radiosensitizers are of relevance [1, 2].

We have measured mass spectra of positive ions for electron impact on 5-fluorouracil, with electron energies ranging from 5 to 100 eV in steps of 0.25 eV. A beam of 5-fluorouracil was generated by a resistively heated oven mounted in an expansion chamber, and the forward section of the beam effusing from a capillary in the oven passed through a skimmer into the collision chamber, where the beam was crossed by a pulsed electron beam (0.5 μs, 8 kHz). Ions have been mass resolved and detected using a reflectron time-of-flight mass spectrometer. LabVIEW based data acquisition techniques have been used to accumulate mass spectra as a function of electron impact energy. Details about the experiment and the data analysis can be found in [3-5], which present results obtained for electron impact on cytosine, thymine and adenine.

Ion yield curves for most fragment ions of 5-fluorouracil have been obtained by fitting groups of adjacent peaks in the mass spectra with sequences of normalized Gaussians. Appearance energies have been determined by fitting a threshold function of the form $f(E) = c(E - E_0)^p$ (for $E > E_0$) to the ion yield curves. This function is convoluted with a Gaussian to account for the electron beam energy resolution.

Mass spectra, ion yield curves and appearance energies will be presented at the conference and will be compared with other research on uracil and the 5-halo-uracils (see e.g. [6-8]).

References

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[1] E-mail: peter.vanderburgt@nuim.ie