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Low energy electron-induced break-up of the tetrahydrofuran molecule: An (e, 2e+ion) study

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Synopsis We study the low energy electron impact-induced ionization and fragmentation of the tetrahydrofuran molecule using the reaction microscope. All three charged final state particles, two outgoing electrons and one fragment ion are detected in coincidence. The binding energy spectra and fully differential ionization cross sections for different fragment species are determined. As result detailed insight into the ionization mechanisms can be gained and track structure simulations for the investigation of radiation action can be supported.

For the interaction of energetic ionizing radiation with biological tissue it is well known that a large number of slow secondary electrons are produced which efficiently induce single- and double-DNA strand breaks [1]. Here, we investigate the ionization and fragmentation of the tetrahydrofuran (THF) C_4H_8O molecule as a surrogate of deoxyribose in the DNA backbone by low energy (35 eV) electron impact with the (e, 2e+ion) triple coincidence method [2]. The measured mass spectrum of THF cations is shown in figure 1. We can directly identify the cations of $C_4H_8O^+$, $C_4H_7O^+$ and CH_3^+. From comparison with a high resolution mass spectrum [3] the peaks labeled by X^+, Y^+ and Z^+ can be assigned to cations which contain 2, 3 and 4 heavier elements (either C or O), respectivly.

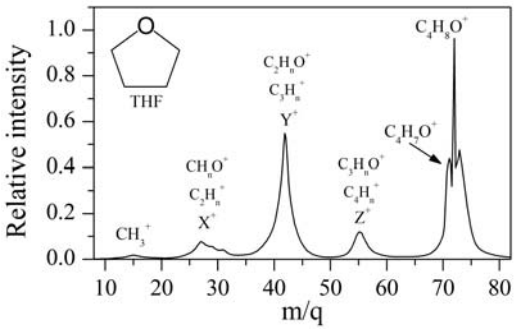

Figure 1. The mass spectrum of cations of tetrahydrofuran molecule for 35 eV electron impact.

In order to get information about the fragmentation mechanisms we measure the binding energy (BE) spectra for different fragments. We define the BE as the initial projectile energy minus the sum energy of the two final state electrons. As one example, the BE spectrum for the $C_4H_8O^+$ ion is presented in figure 2. The spectrum is analyzed with a multi-peak Gaussian fitting procedure. It is shown that the dominant contribution for $C_4H_8O^+$ ion production is ionization of the HOMO orbital. Presently we are commissioning a new photo-cathode electron gun in order to obtain an improved BE resolution. This will enable us to significantly extend existing studies [4, 5] by obtaining up to triple differential ionization cross sections for individual molecular orbitals and product ions even for projectile energies below 20 eV.

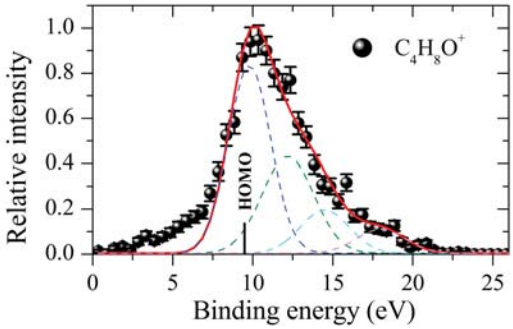

Figure 2. Binding energy spectrum for the $C_4H_8O^+$ ion of tetrahydrofuran for 35 eV electron impact. The solid symbols represent the experimental data. The dashed lines are the fitted Gaussian peaks and the solid line is the sum of the fits.

References

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