100 keV proton irradiation of Halo-Uracils in the gas phase: Specific fragmentation channels revealed by coincidence measurements.

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The ubiquitous role of ionizing radiations, on one hand used in medical treatments but on the other hand known as having potential harmful long term effects puts them at the confluence of several disciplines such as physics, chemistry, biology and medicine.

5-Halo-Uracil molecules (5XU, X = F, Cl, Br, I) are used in treatment of cancer as chemotherapy agents and they also act as radio-sensitizer in concomitant radio- and chemotherapies. Radio-sensitization is an increase of the macroscopic biological effect (tumoral cells death due to DNA mutations and breakages) of the ionizing radiation (X rays or high energy protons) on the targeted tissues. Surprisingly, although the advantages of radio-sensitizing substances is established, there is little knowledge on the microscopic fundamental physical and chemical mechanisms underlying radiosensitization and, more generally, on the interaction between ionizing irradiation and molecular systems.

We have undertaken a study of the direct effects (ionization, fragmentation, molecular rearrangement) of 100 keV proton irradiation on 5XU in the gas phase. The energy potentially deposited into the target molecules being very high, it could be expected that all dissociation pathways are statistically open and that these molecules, differing one to another by one atom only, should lead to similar fragmentation patterns. Interestingly, our experiments relying on a coincidence detection of the fragments have enabled the disentanglement of complex sequential dissociation pathways and specific pathways have been revealed. For instance, ion products of mass 38, 39 and 40 amu are associated to the transient formation of the de-halogenated uracil cation and their intensities are very sensitive to the nature of the primarily ejected halogen. It suggests that specific de-hydrogenation states are explored while these fragmentations occur. We will present these results as well as the latest results obtained from a similar experiment where energy controlled electrons are used as irradiation source to better appreciate the amount of energy absorbed by the parent molecules.

