PROTON BIOMOLECULE COLLISIONS

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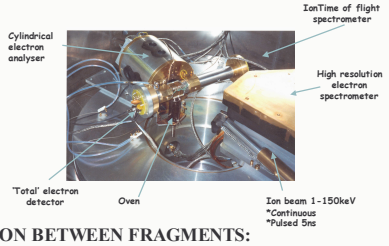
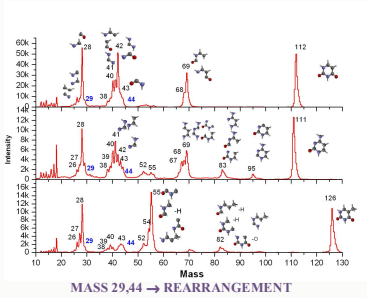
Damages induced by ionizing radiation can directly be linked to alteration of the DNA molecule. In this work, we have investigated interactions of 25 to 100 keV energy protons with DNA bases in gas phase gas, the pyrimidines: uracil, cytosine and thymine. The 100 keV energy corresponds to the maximum Linear Energy Transfer in biological medium, i.e. to the Bragg peak used in proton-therapy.

Experimental method:
- **Electron spectroscopy**
- **Multistop time of flight**



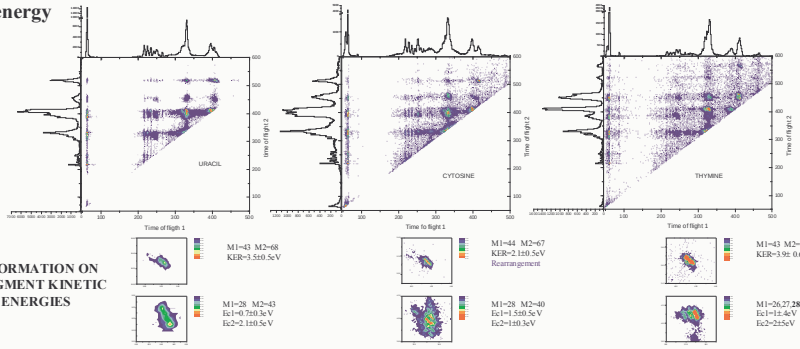
A - Direct effects: molecular fragmentation
Multistop time of flight technique

Formation of new small molecule with kinetic energy



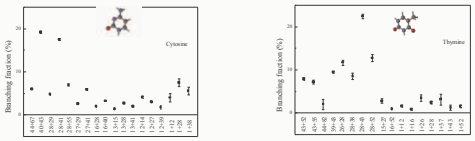
MASS 29,44 → REARRANGEMENT

CORRELATION BETWEEN FRAGMENTS:



INFORMATION ON FRAGMENT KINETIC ENERGIES

CORRELATED MASS BRANCHING RATIOS



B - Indirect effects: secondary electron emission
Electron spectroscopy

Damages induced by secondary electron depend on kinetic energy:

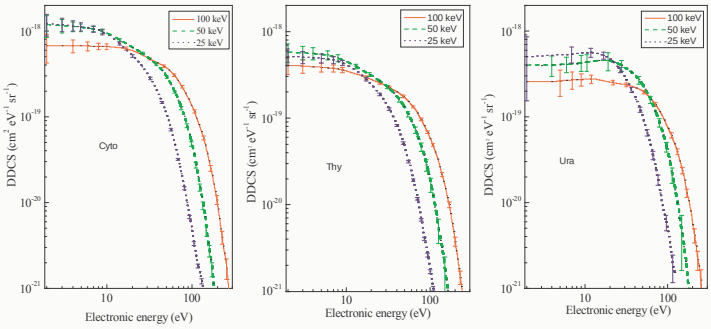
Low energy (<20eV): dissociative attachment

High energy(>20eV): ionization,fragmentation

Need to know energy spectrum of the emitted electrons

ELECTRON SPECTRA IN ABSOLUTE SCALE

(normalisation of cross section through 90° elastic scattering of projectiles)



Classical Trajectory Monte-Carlo calculations

Classical description of the trajectories of an electron initially bound in a uracil molecule and perturbated by an incoming proton : numerical integration of the trajectory by taking into account the electron/molecule - evaluated with ARGUSLAB 4.0.1 (www.arguslab.com) - and electron/proton interaction potentials.

$$\sigma_{(E,\theta)} = \frac{N_v N_{e(E\pm\Delta E/2,\theta\pm\Delta\theta/2)}}{N_{shot}} \frac{S_{ref}}{2\pi \sin\theta \Delta\theta \Delta E}$$