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Electron spectroscopy in H^+ to dry DNA, RNA collisions in the 25 – 100 keV energy range

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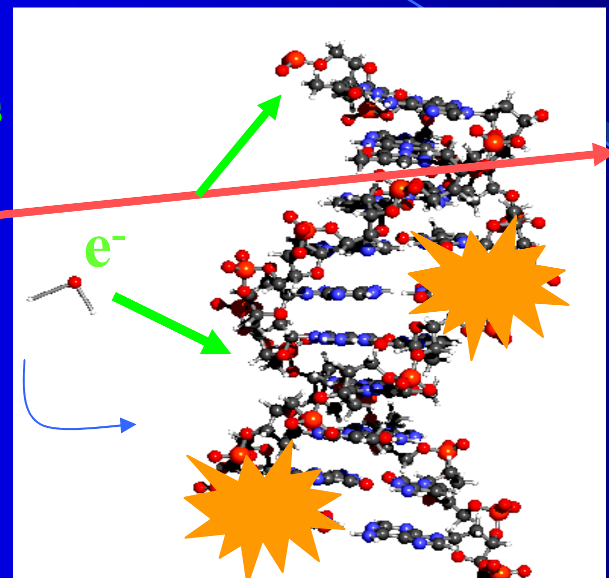
RADAM Groningen
6-9th june 06

Target : DNA …

Fragmentation, ionisation

Emission of secondary electrons

Ionising projectile



Water radiolysis H, HO

Single and double stand breaks

Characteristic times :

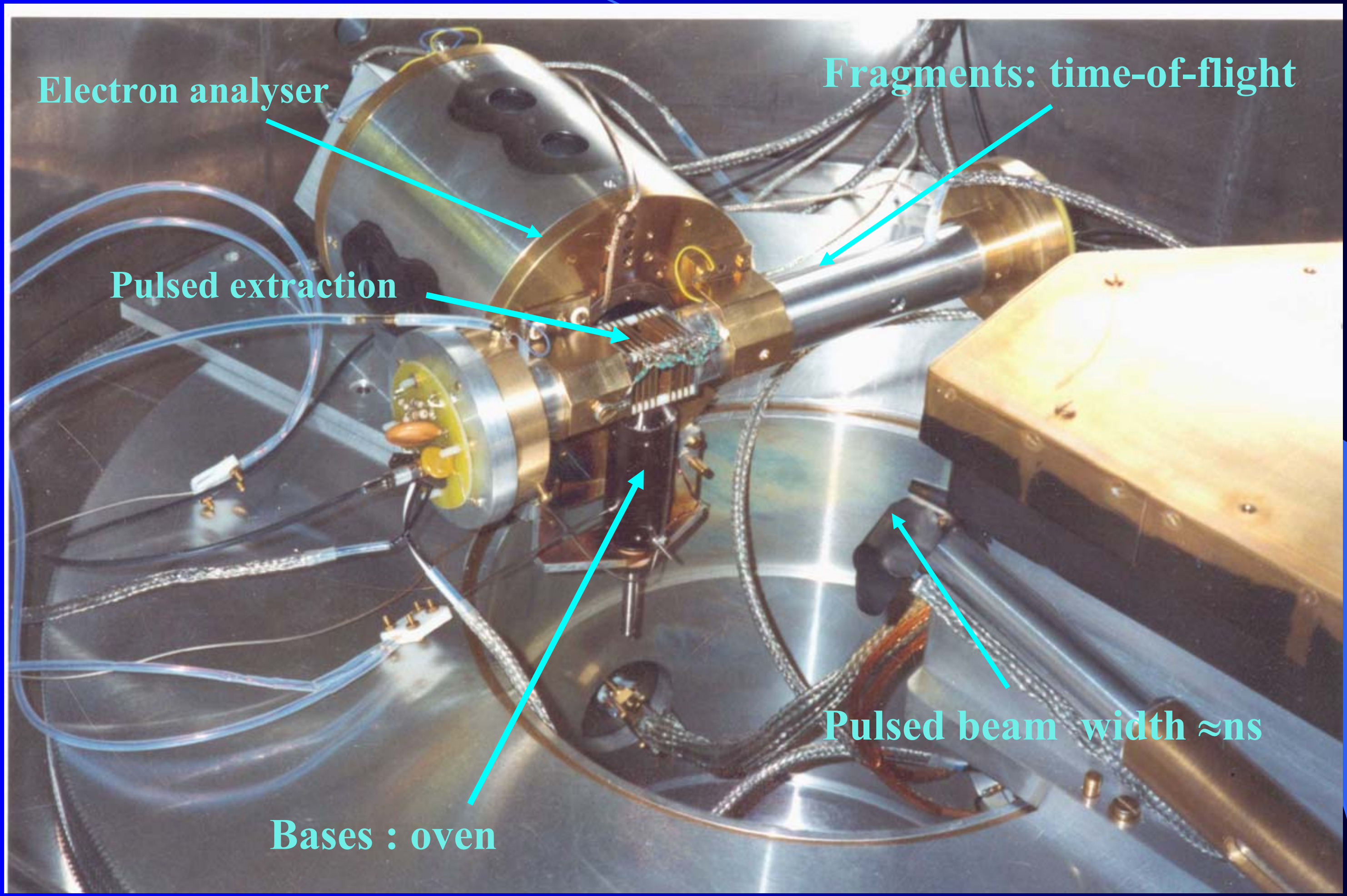
Physical	10^{-15} - 10^{-8} s	ionisation, excitation
Chemical	10^{-13} - 10^{-9} s	damages due to free radical
	10^{-3} s - hours	chemical repair

…what could we bring to this field ?

Experimental technique :

- Ion accelerator
- Production of gas phase biomolecules : sublimation of commercial powders by means of an oven (120-150°C)
- Analysis of the fragments by time-of-flight spectroscopy + « multistop » : correlations between fragments
- Electron spectroscopy by means of an electrostatic analyser (‘cylindrical mirror)

Experimental setup …



Multicorrelation analysis : event by event

Electronic emission

DOUBLE DIFFERENTIAL CROSS SECTION IN AN ABSOLUTE SCALE
(angle and energy)

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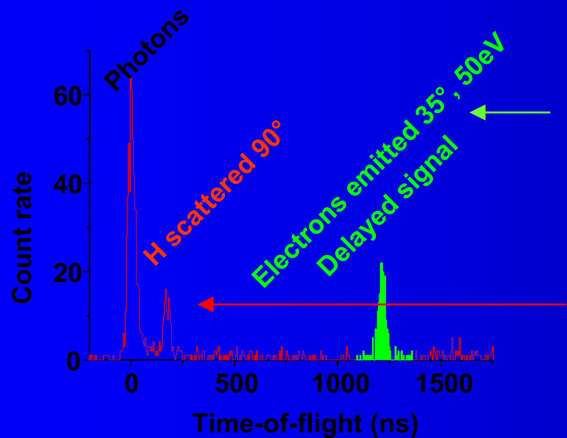
Normalisation of the cross-sections

Measurements of the number of electrons at 50eV **AND** of the number of scattered projectiles at 90°

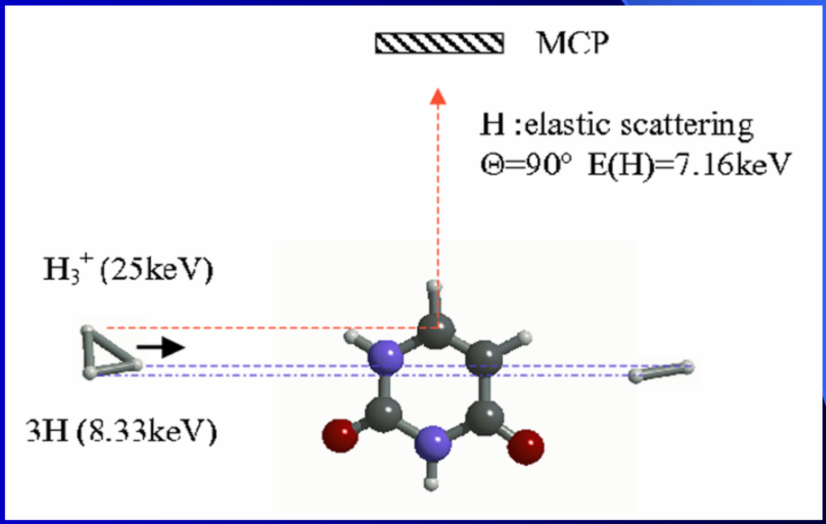
AIM :to account for the UNKNOWN projectile density and for its fluctuations



$$N_e = \frac{\partial^2\sigma_e}{\partial\Omega_e\partial E_e}(35°,50eV)[n.\ell.\Delta\Omega]_e\,\Delta E_e.\eta_e.N_{proj}$$

$$N_i = \frac{\partial\sigma_i}{\partial\Omega}.[n.\ell.\Delta\Omega]_i.\eta_i.N_{proj}$$

Number of scattered ions



Use of H_3^+, instead of H^+, since 2 antagonistic effects on the projectile energy E :

- E^{-2} Rutherford dependence on the elastic scattering cross sections.
- Large decrease of the ionic current with the energy.

The two combined equations :

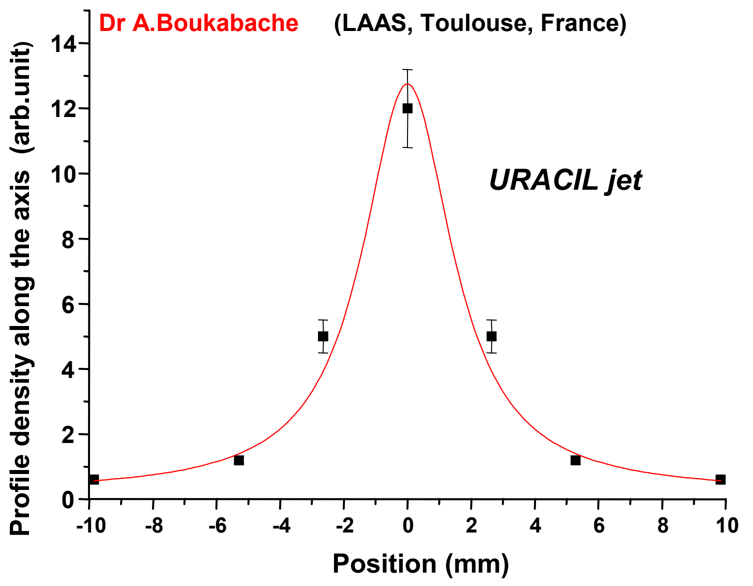
$$\frac{\partial^2 \sigma_e}{\partial \Omega_e \partial E_e} = \frac{N_e}{N_i} \cdot \frac{\partial \sigma_i}{\partial \Omega_i} \cdot \frac{[n.\ell.\Delta\Omega]_i}{[n.\ell.\Delta\Omega]_e} \cdot \frac{1}{\Delta E_e} \cdot \frac{\eta_i}{\eta_e}$$

Elastic scattering cross sections (10^{-21}cm²/sr)

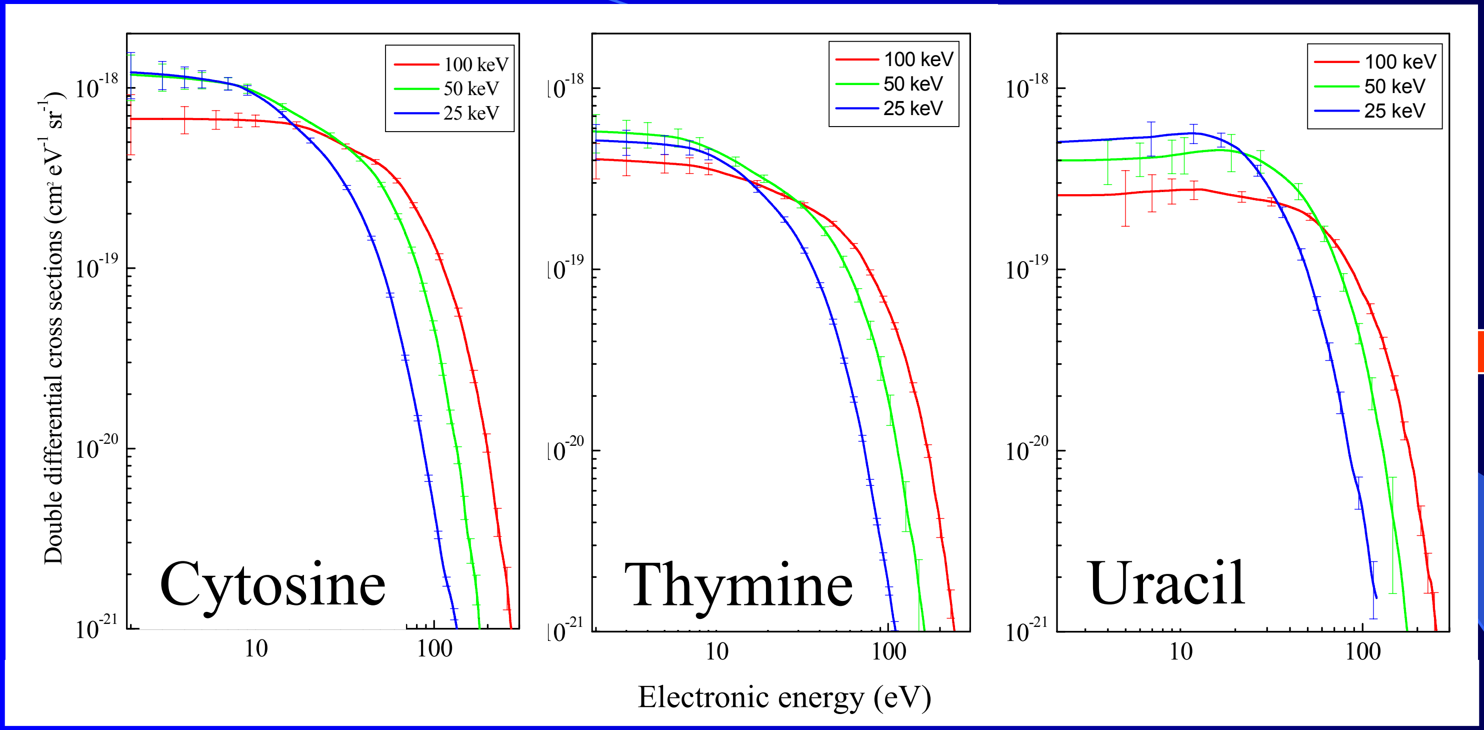
H (8.33keV) scattered at 90°

	C	N	O
P.Caffareli's calculations			
ZBL	2.45	3.26	4.32
Bohr	2.57	3.46	4.70
Molière	2.37	3.29	4.26
Pot.PMC	2.76	3.51	4.49
Us	2.72	3.70	4.81

Monte-Carlo simulation for the density profile



THE RESULTS :



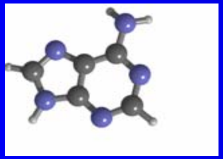
Léon Sanche happy !

Findings :

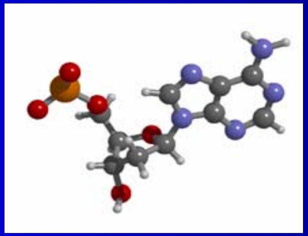
- No low energy peak but rather constant and sizeable cross sections (no centrifugal barrier like for the central potential C_{60}),
- No energy dependence E for the proton projectiles,
- At larger energies, exponential decay according to the Bethe-Born approximation – dominance of the dipolar interaction term,
- No lines arising from the Auger KLL electrons.

PERSPECTIVES

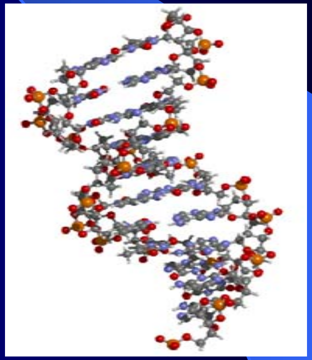
- **Angular distributions of the electrons, correlation electrons / fragments**
- **Solvated molecules (in collaboration with M et B. Farizon IPN, Lyon)**
- **Step forward to complexity :**



Base (adenine)



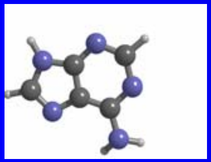
Nucleotide (hydrated or not)



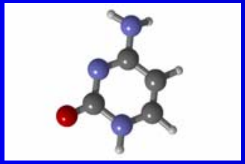
- **Radiosensitive molecules (5FU)**
- **Surfaces !?**

…and the targets so far !

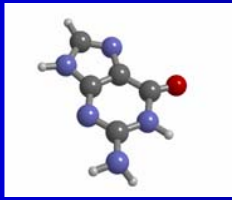
Adenine



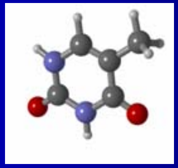
Cytosine



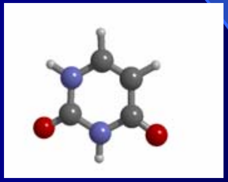
Guanine



Thymine



Uracil



5FU (fluorouracil)