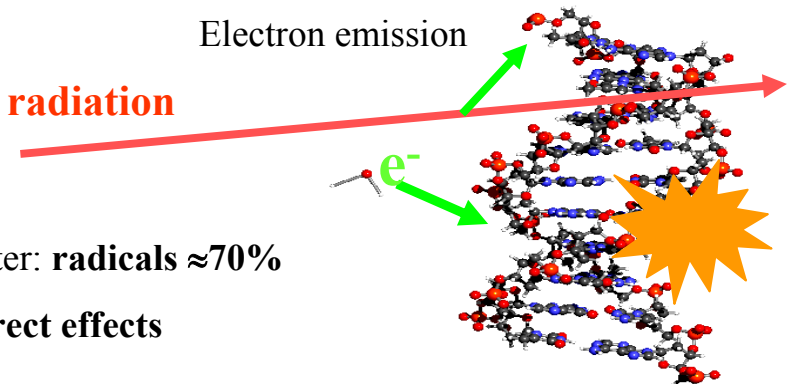
Electron emission and fragmentation of DNA/RNA components induced by proton impact

P.Moretto-Capelle, A.Le Padellec, M.Richard-Viard, J.P.Champeaux and P.Cafarelli

LCAR (UMR5589 CNRS-Univ.Paul Sabatier Toulouse 3) Toulouse, France

Damages induced by ionizing radiation

Target: DNA molecule



Ionization, Base damage

≈30%

> Direct effects

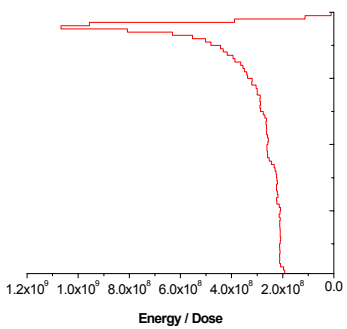
Surroundig water: **radicals ≈70%**

> Indirect effects

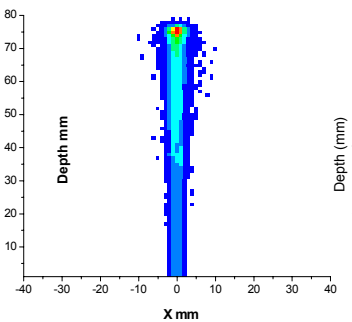
Strand breaks

Interaction of ions with matter: possibility of strong energy deposition in a well defined region around the Bragg peak

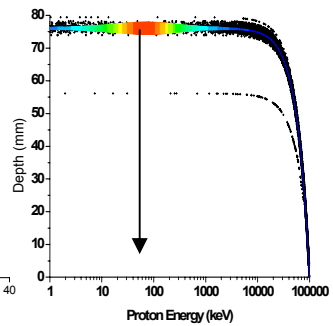
Bragg peak



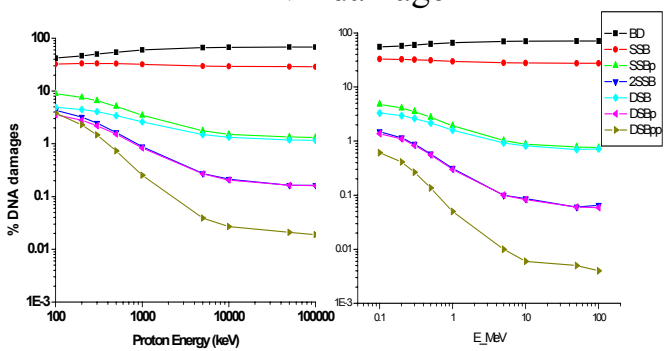
Spatial Dose



Stopping power



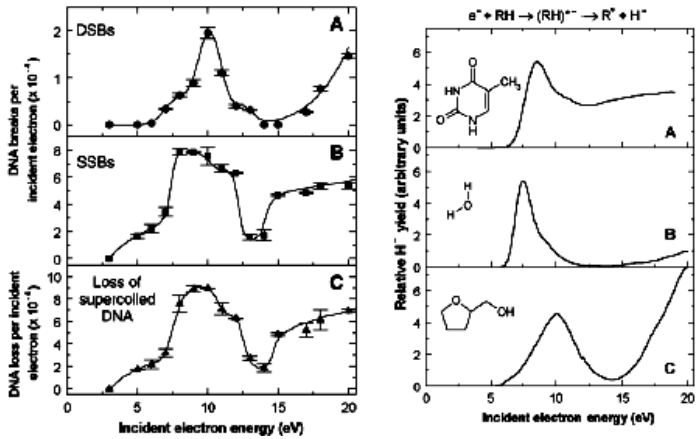
DNA damage



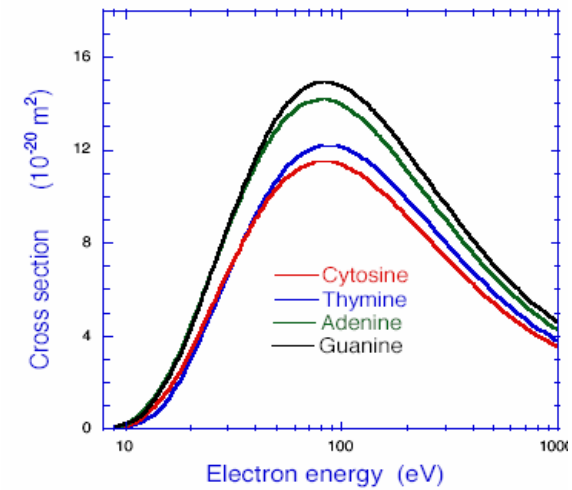
≈ 100keV

Damages induced by electrons ?

E<20eV: Dissociative attachement



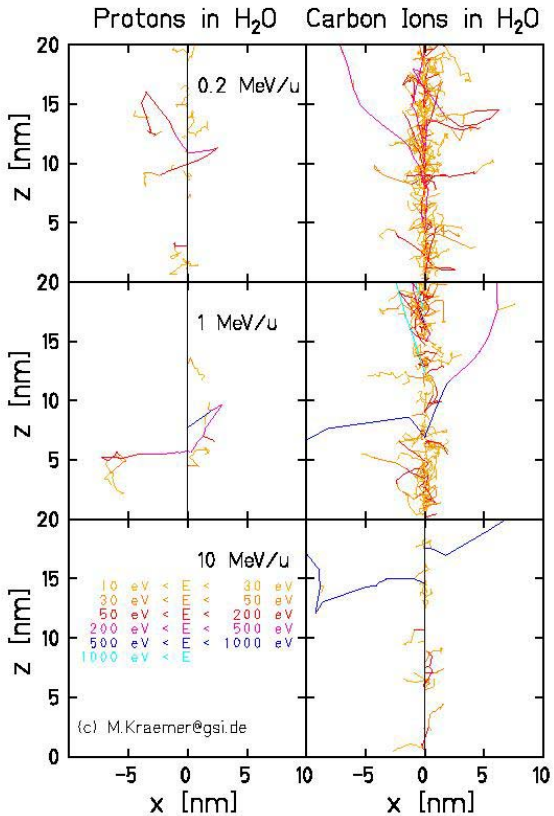
E>20eV: Ionization



Initial electron spectrum??

Tracks:

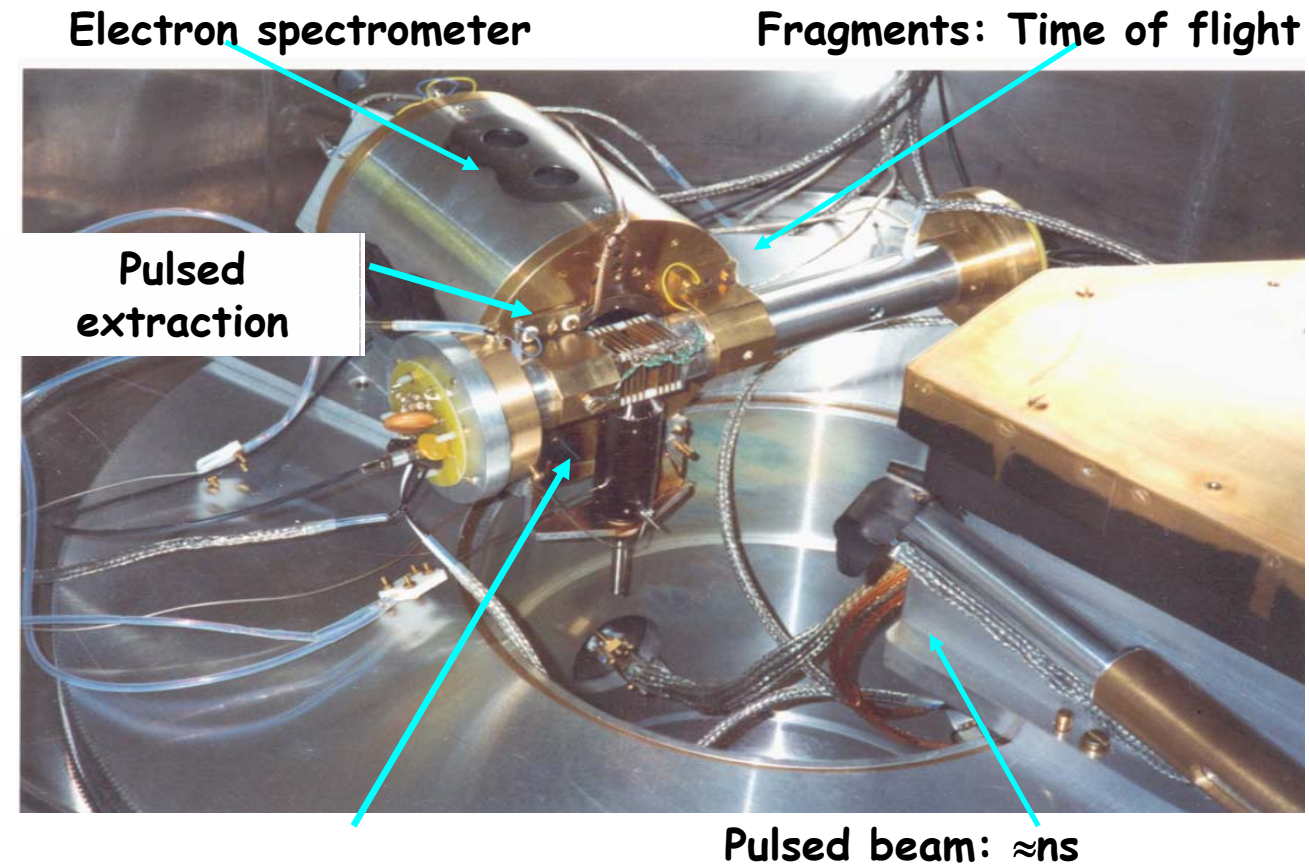
From GSI



Mainly calculation/measurement on water

Direct effects: Component of DNA ?

Experimental method



Electron emission: Tracks calculations needs **D**ouble **D**ifferential **C**ross **S**ection

Absolute value ? Difficulty: density of jet !!

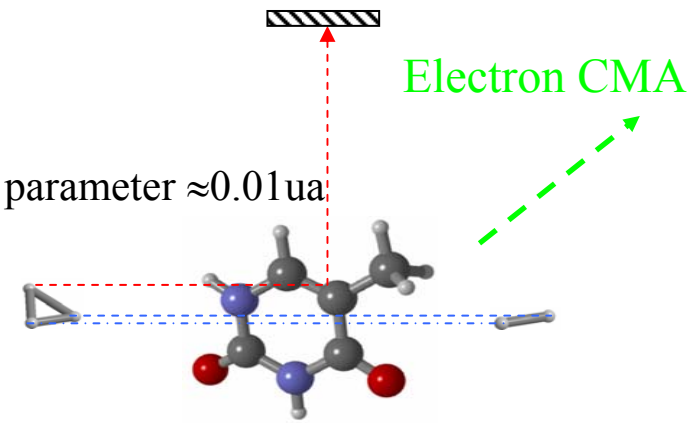
Idea

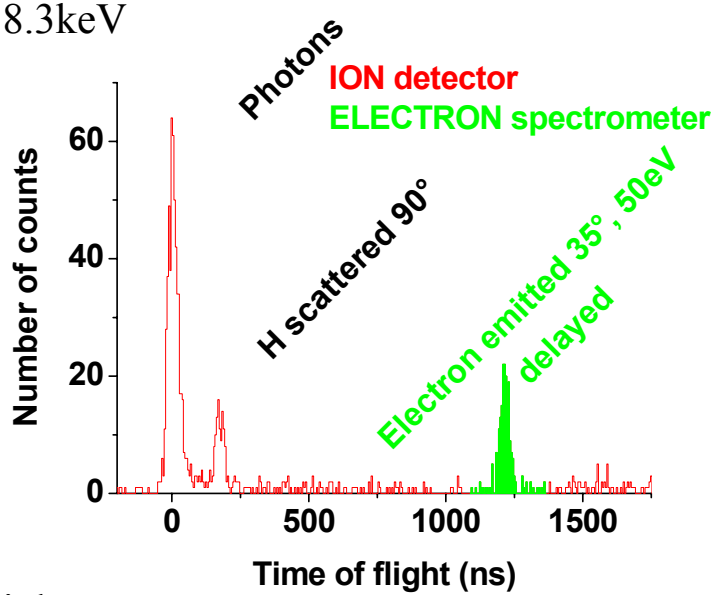
Electron spectroscopy
Given angle and energy (DDCS)

Other 'known' collisionnal process
'Projectile' diffusion DSC

Same experiment

Higher feasility: molecular beam H_3^+_ 25keV≡ 3 H^+_ 8.3keV



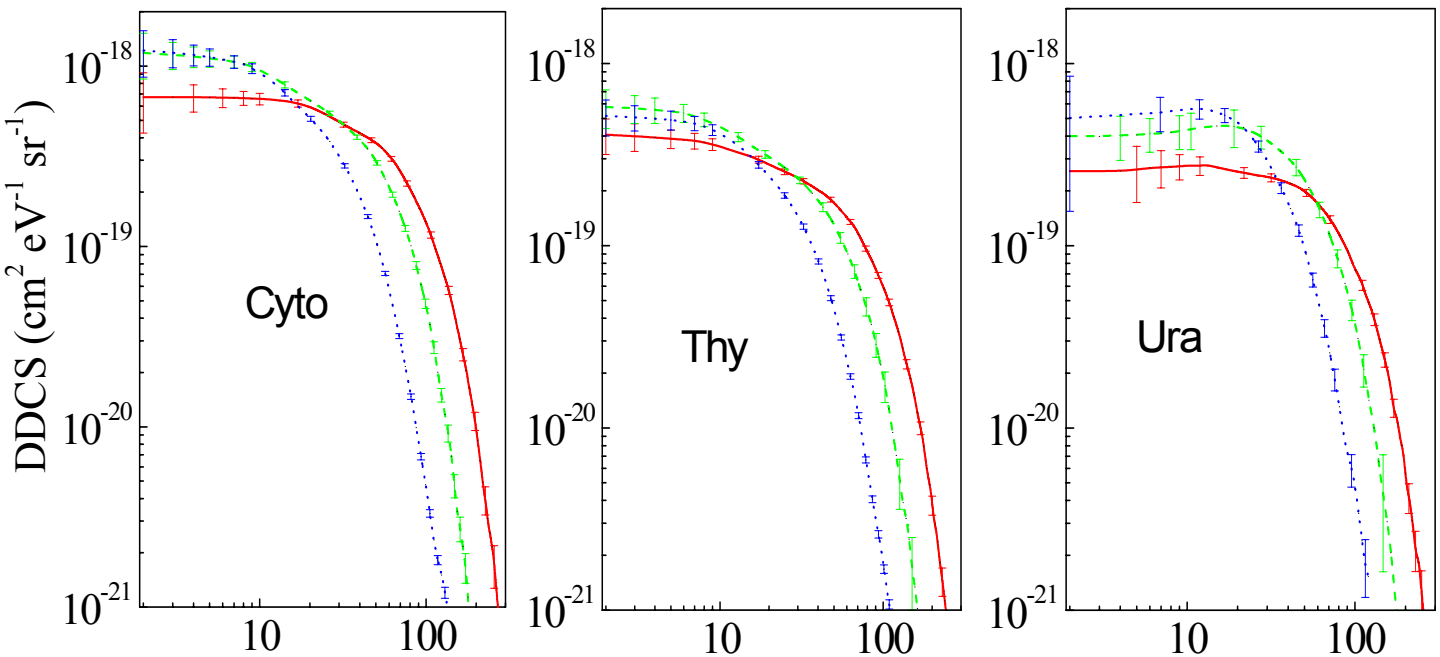


Electron noise reduction: energy and time of flight

Results

Low energy electrons

No K shell ionization



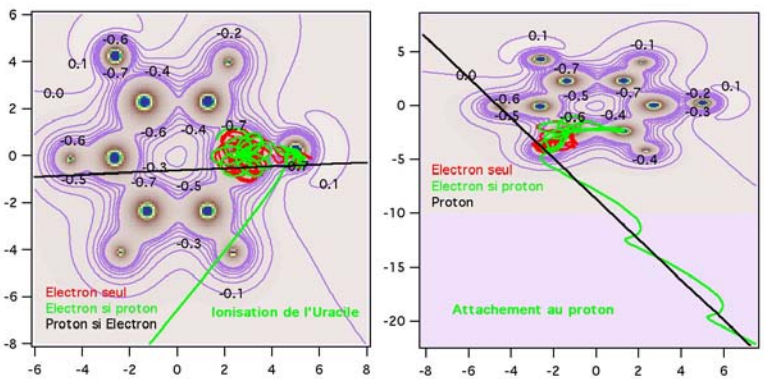
Modelisation: CTMC Calculation

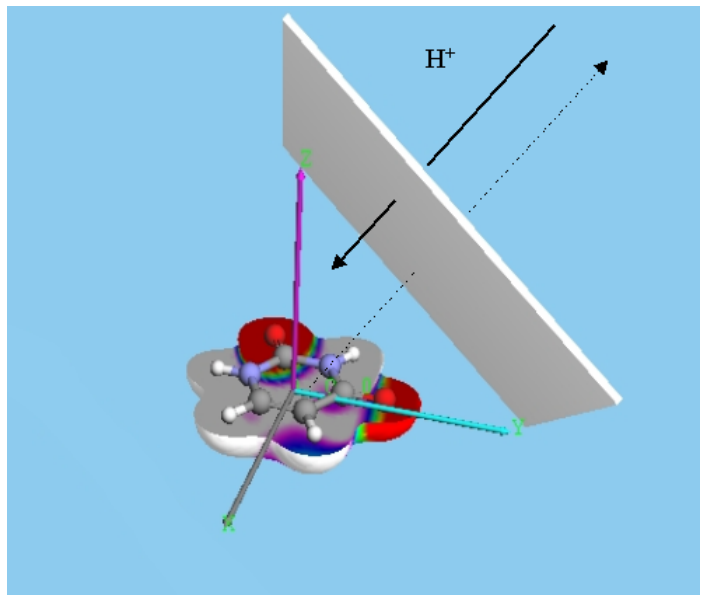
Electron Classical equation of motion

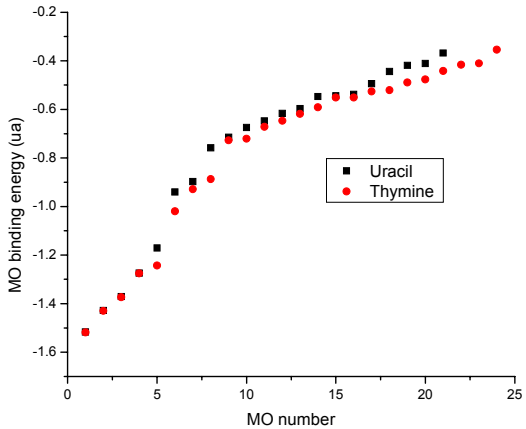
Proton: -1/|Rp-r|

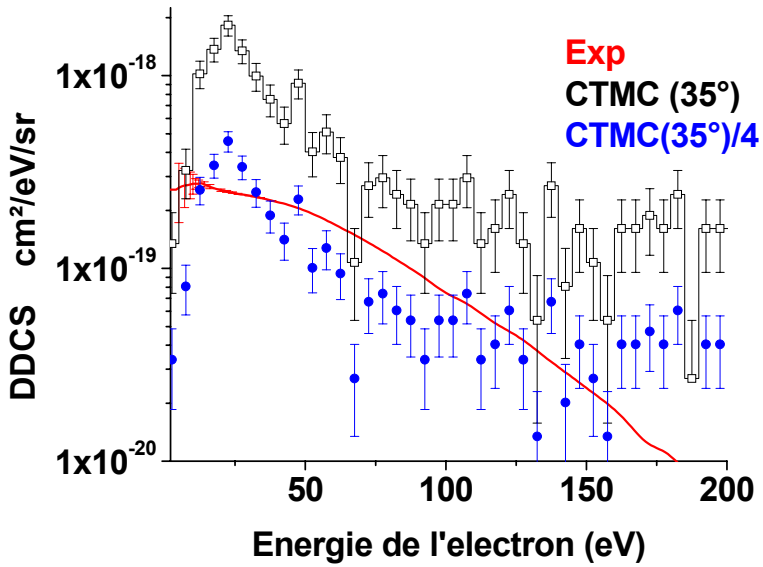
Forces:

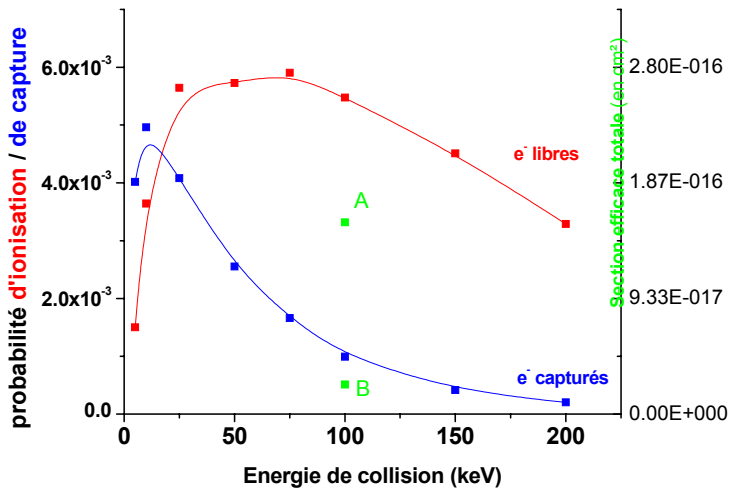
Molecule: $V_e(\vec{r}) = \int \frac{\rho(r)}{|Re - r|} d^3r - \sum_N \frac{Z_N}{|\vec{R}e - R_N|} - \sum_{i=1,n} \Psi_i(\vec{r}) \int \frac{\Psi_i^*(\vec{r}')\Psi(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}'$



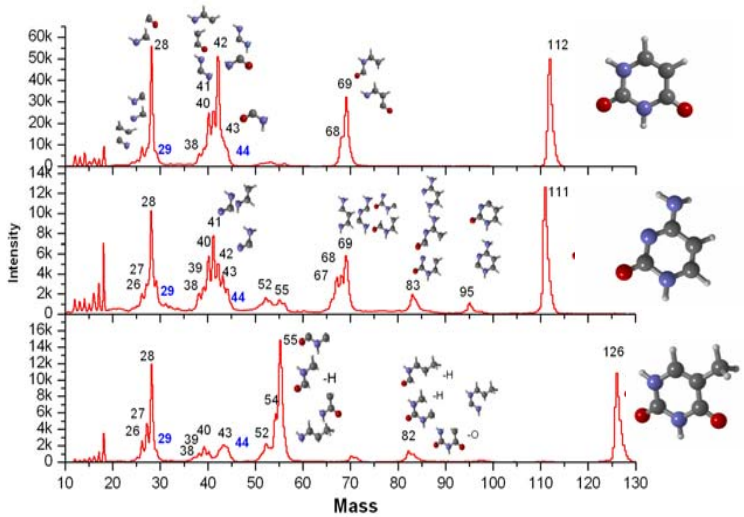


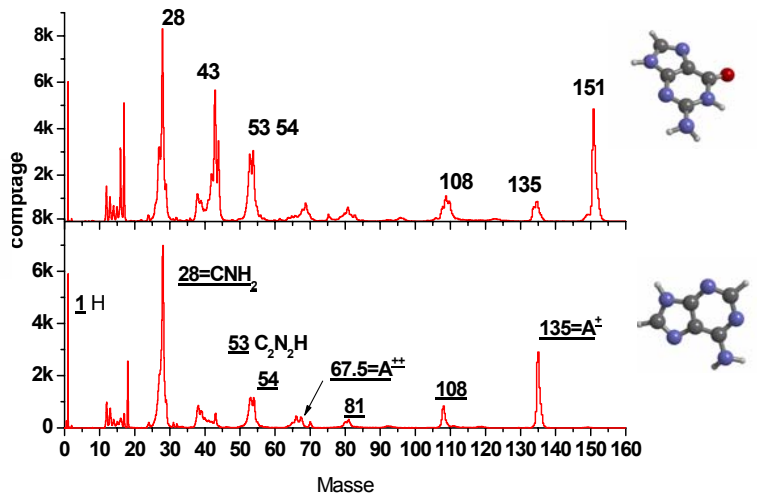

MO binding energy (ua)
MO number
Uracil
Thymine

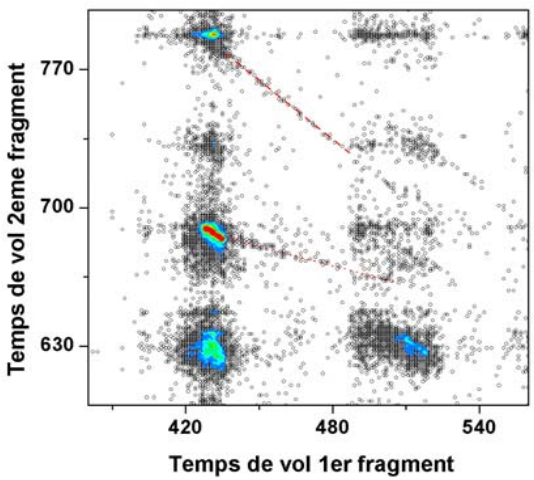

DDCS cm²/eV/sr
Energie de l'electron (eV)
Exp
CTMC (35°)
CTMC(35°)/4

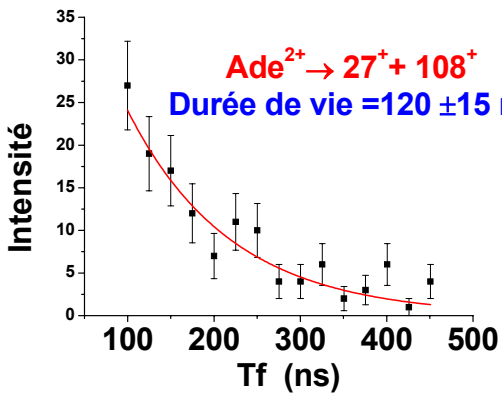

probabilité d'ionisation / de capture
Section efficace totale (en cm²)
Energie de collision (keV)
e⁻ libres
e⁻ capturés
A
B

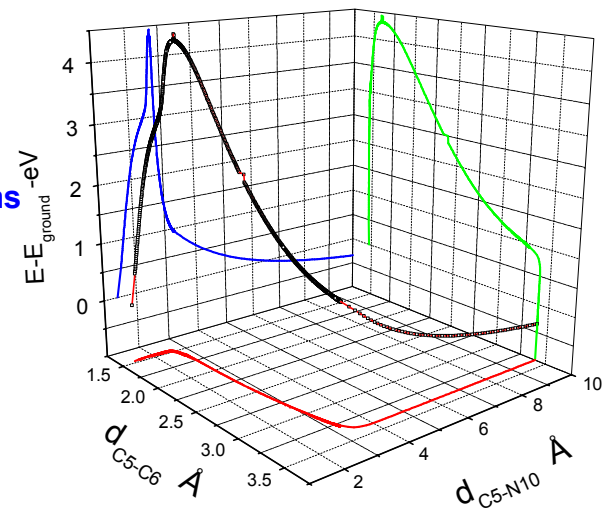
Molecular fragmentation

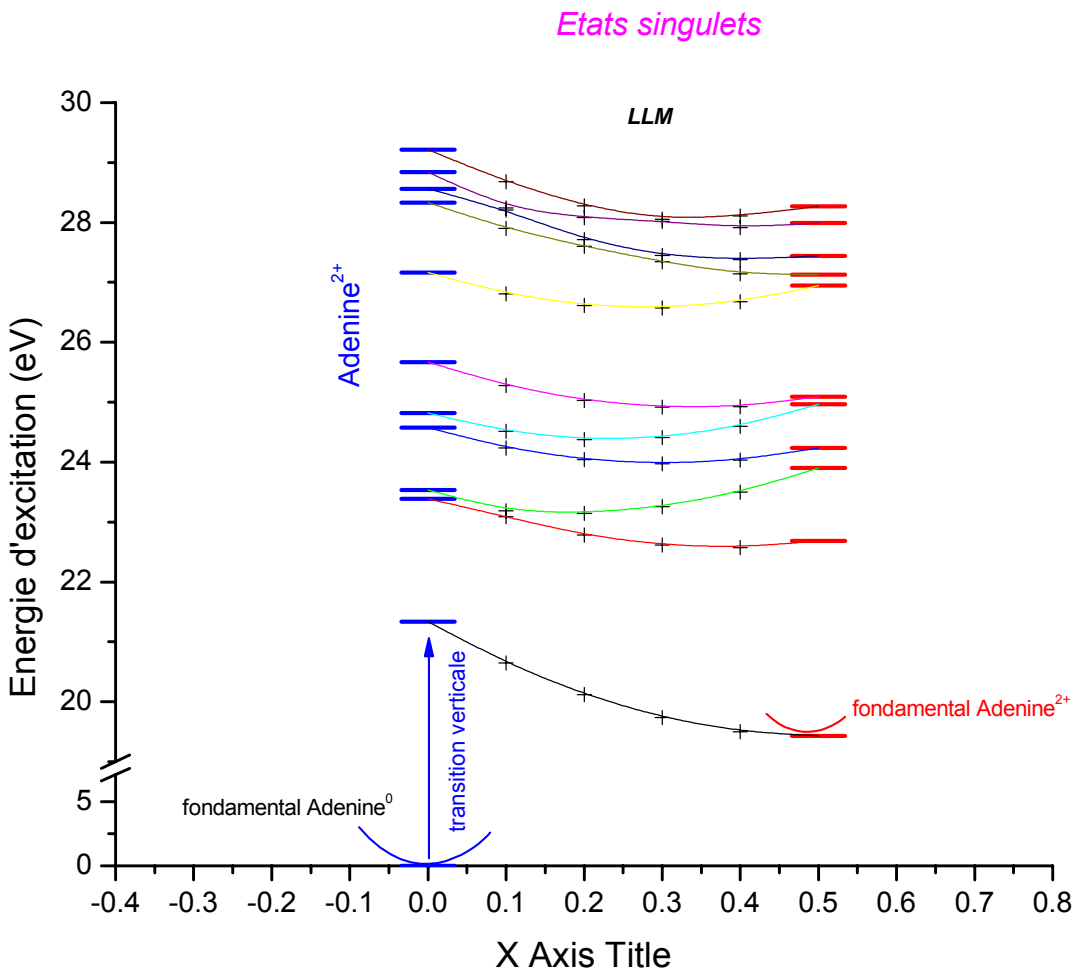











Etats singulets
LLM
Adenine2+
Energie d'excitation (eV)
30
28
26
24
22
20
5
0
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
X Axis Title
fondamental Adenine0
transition verticale
fondamental Adenine2+