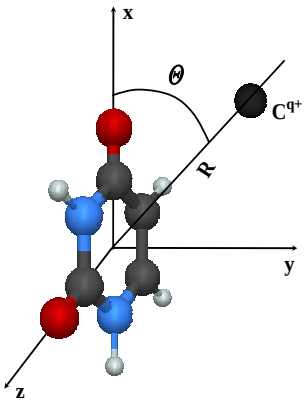
Short visit 07/04/2005-30/04/2005
Scientific report:

We have pursued the work undertaken on interactions between ions and biomolecules. Recent experiments of fragmentation and collision induced excitation have been developed on reactions of C^{q+} ions on Uracil, one of the RNA basis.
We plan to study the different processes involved in this reaction, in particular the charge transfer mechanism, for the different charge and structure of the projectile. Such an approach at the molecular level is essential in the study of radiation effects in biological systems. DNA and RNA involving genetic information may be indeed one of the main possible targets damaged by radiation action in medical treatments, as cancer disease. It is the main underlying mechanism for cancer risk as well as controlled cell killing action in radiotherapy. Action on the DNA and RNA basis is of course a first step and such studies could be extended to the other active parts of the DNA skeleton.

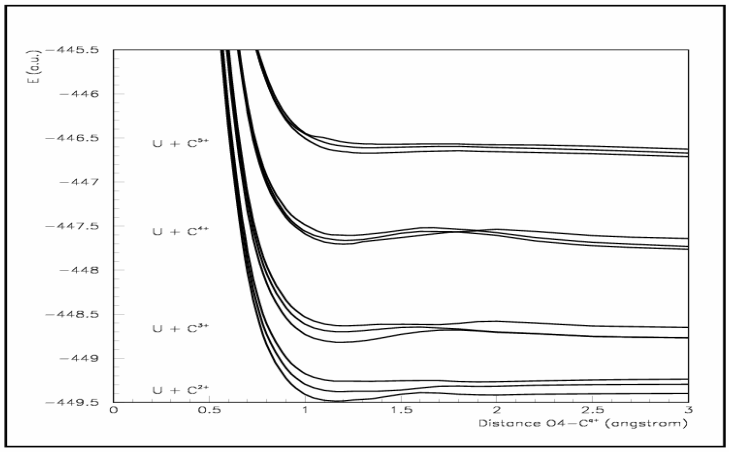
The study of charge transfer mechanism necessitates the calculation of the potential energies of the states involved in the process, as well as the couplings between these states, followed by a collision dynamics in order to reach the cross sections on the different channels which may be compared to experiment (J. de Vries, R. Hoekstra, R. Morgenstern, T. Schlathölter, *J. Phys. B* **35**, 4373 (2002)).



Such calculations have been initiated by two previous short visits in 2004 in the Laboratoire de Spectrométrie Ionique et Moléculaire in Lyon as the Laboratory in Lyon has a well known experience in charge transfer processes. The series of collisional C^{q+} + Uracil, q=2-5, has been investigated in the planar attack corresponding to an angle θ=0°.

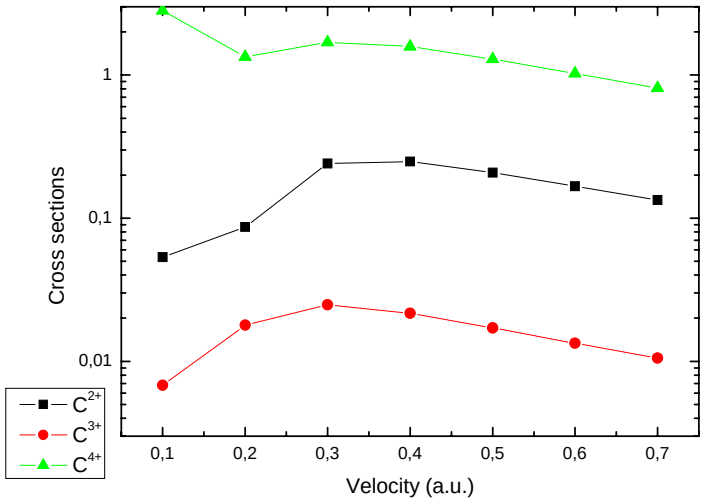
Fig. 1: Σ charge transfer levels of the C^{q+} - Uracil systems.
U + C^{2+} : CT1 $^1\Sigma\ \pi_{CC}\rightarrow 2p_z$*; CT2 $^1\Sigma\ \pi_{C0(2)}\rightarrow 2p_z$*; CT3 $^1\Sigma\ \pi_{C0(4)}\rightarrow 2p_z$*
U + C^{3+} : CT1 and CT2 $^2\Sigma\ \pi_{CC}\rightarrow 2p_z$*; CT3 $^2\Sigma\ \pi_{C0(4)}\rightarrow 2p_z$*
U + C^{4+} : CT1 $^1\Sigma\ p_{02}{}^{a'}\rightarrow p_C{}^{a'}$; CT2 $^1\Sigma\ p_{02}{}^{a'}\rightarrow p_C{}^{a'}$, $\pi_{CO(2)}\rightarrow \pi_{CC}$; CT3 $^1\Sigma\ p_{02}{}^{a'}\rightarrow p_C{}^{a'}$, $\pi_{CO(4)}\rightarrow \pi_{CC}$
U + C^{5+} : CT1 $^2\Sigma\ p_{04}{}^{a'}$; CT2 $^2\Sigma\ p_{04}{}^{a'}$, $\pi_{CO(2)}\rightarrow \pi_{CC}$; CT3 $^2\Sigma\ p_{04}{}^{a'}$, $\pi_{CO(4)}\rightarrow \pi_{CC}$

The molecular calculations have been carried out using the MOLPRO suite of ab-initio programs. Optimized geometries and potential energies have been determined at the CASSCF level of theory using the 6-311** basis set of atomic orbitals. The potential energy curves and radial coupling matrix elements have been calculated for a distance varying from 0.5 to 5 Å, they are displayed in Figure 1.



The charge transfer potentials show clearly avoided crossings in the 1.5-2.0 Å range corresponding to a strong interaction with the entry channel. Such an interaction appears at very short range in the case of the C^{5+} -Uracil system.

A semi-classical collisional approach has then been performed in order to determine the cross sections on the different channels for the same range of collisional velocities as the experimental measurements. In such ion/uracil experiments, three main processes may be considered: the fragmentation of the uracil molecule, the ionization of uracil, and finally the charge transfer between the multicharged ion and the uracil molecule. In the case of the C^{2+} + uracil reaction, it is shown experimentally that the fragmentation process is preponderant at low velocities, then decreases with energy and significant charge transfer can be expected at higher energies. A quite different behaviour is found in the collision of higher charged ions on uracil, where significant charge transfer can take place, even at low energies. Our present results appear to be quite in agreement with such experiments, as we observe an increase of the charge transfer cross sections at low energies for C^{2+} + Uracil, and a general decrease of charge transfer cross sections for the higher charged ions.



Charge transfer cross-sections in the C^{q+} + Uracil process