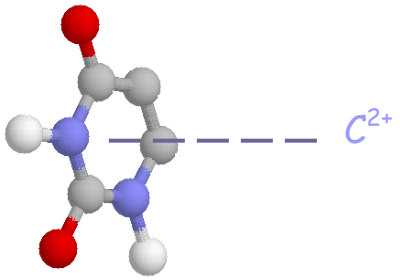
Short visit 01/10/2004-30/10/2004
Scientific report:

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 Uracyl, 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 target 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 a first short visit in august-september in the Laboratoire de Spectrométrie Ionique et Moléculaire in Lyon as the Laboratory in Lyon has a well known experience in charge transfer processes. We have undertaken the study of the C^{2+} + uracyl process. In a first step, we have considered a perpendicular attack of the C^{2+} ion, allowing an equivalent interaction for all the atoms of the uracyl ring.



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. Three main levels have to be considered : the entry channel $C^{2+}(1s^2 2s^2)$ + U, and two exit channels of single electron capture, the $C^{+}(1s^2 2s^2 2p)$ + U^{+} ground state and $C^{+}(1s^2 2s 2p^2)$ + U^{+} channel corresponding to capture and excitation of an electron.

This work has been completed during the present short visit by calculation of the radial coupling matrix elements between the different states involved in the process. 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. Three main processes may be considered in such ion/uracyl experiments : first the fragmentation of the uracyl molecule, secondly the ionization of uracyl, and finally the charge transfer between the multicharged ion, here C^{2+} and the uracyl molecule. Experimentally, it is shown that the fragmentation cross sections appear to decrease with energy in the case of the C^{2+} + uracyl reaction, this lets suppose that significant charge

transfer may thus take place at higher energies. Our present results appear to be quite in agreement with such a hypothesis, as we observe clearly an increase of the charge transfer cross sections with energy which reach a more or less constant value at higher energies.

v(u.a.)	Elab(keV)	$\sigma(10^{-16}$ cm$^2)$
0.1	3.00	4.05
0.15	6.75	5.90
0.2	12.00	6.49
0.25	18.75	9.57
0.3	27.01	8.12
0.35	36.75	9.25
0.4	48.00	8.05
0.45	60.76	8.30
0.5	75.00	9.15

Charge transfer cross-sections in the C^{2+} + Uracyl process

Experimentally, a quite different behaviour is found in the case of the C^{2+} + U process, than in the collision of higher charged ions on uracyl. A compared study is now in progress for a series of C^{q+} ions in order to interpret the different mechanisms involved.