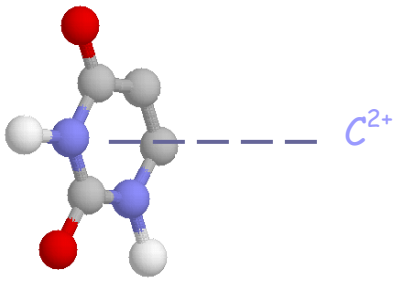
Short visit 15/08/2004-14/09/2004
Scientific report:

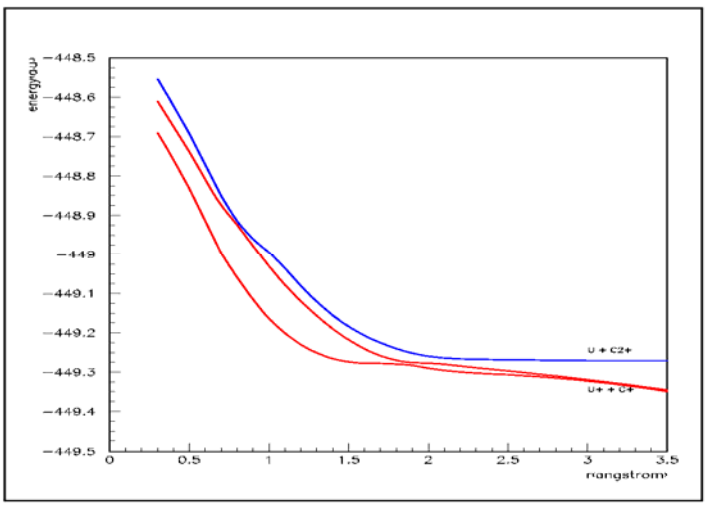
Recent experiments of fragmentation and collision induced excitation have been developed on reactions of C^{q+} ions on Uracyl, one of the RNA basis.
We plan to study the different processes involved in this reaction, in particular the charge transfer mechanism, for the different charge and structure 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 first 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)).

The purpose of the visit in the Laboratoire de Spectrométrie Ionique et Moléculaire in Lyon was to initiate such calculations as the Laboratory in Lyon has a well known experience in charge transfer processes. We have undertaken presently the study of the C^{2+} + uracyl process. 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. The potential energy curves corresponding to the approach of the C^{2+} ion along the perpendicular reaction path show clearly a strong interaction around 2Å between the entry channel C^{2+} + U and the two one-electron capture channel C^{+} + U^{+}.

The present work will be completed by calculation of the radial coupling matrix elements between the different states involved in the process. A semi-classical collisional approach will be then performed in order to determine the cross sections on the different channels.
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 will be undertaken for a series of C^{q+} ions in order to interpret such behaviour.