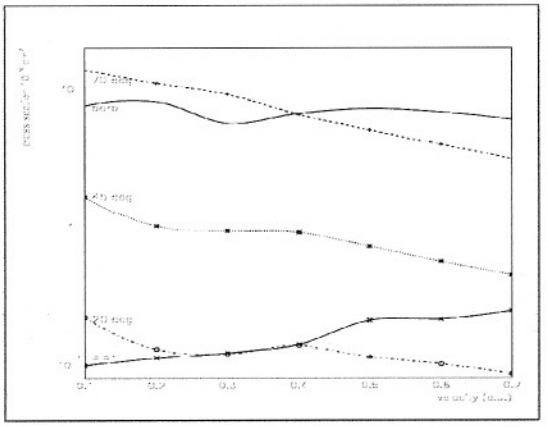
Short visit from 06/09/2006 to 12/09/2006 of Yvette Suzanne Tergiman to the Polytechnical University of Gdansk

Scientific report:

Recent experiments of fragmentation and collision induced excitation have been developed on reactions of C^{q+} ions on uracil, one of the RNA basis [1].
The study of the charge transfer process involved in this reaction for the different charge and structure of the projectile have shown a quite different behaviour in the planar and perpendicular orientations [2]. In order to have a more detailed understanding of the anisotropy of such mechanism, a series of orientation angles of the projectile towards the uracil target have been considered. This necessitates for each orientation, 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 determine the cross sections on the different channels.

The molecular calculations have been carried out using the MOLPRO suite of ab-initio programs and potential energies have been determined at the CASSCF level of theory using the 6-311** basis set of atomic orbitals. A semi-classical collision treatment has then been performed in order to determine the cross sections on the different channels. The results for the C^{4+} + uracil collision system show a strong anisotropic effect. The charge transfer process is clearly favoured in the perpendicular or near-perpendicular attack, the cross-sections are even higher for the angle θ=70°. In this direction, the cross-sections appear to little vary with the collision energy, more or less constant for θ=90°, and slightly decreasing for θ=70°. Outside a solid angle about 20° around the perpendicular direction, the charge transfer process is significantly less efficient, the cross-sections in the θ=45° direction are almost an order of magnitude lower than for θ=70° and decrease slowly with increasing energy. Finally, in the planar or near-planar orientation (θ=20°), the cross-sections are still lower, not higher than 0.2 10^{-16} cm^2 and do not show noticeable variation with energy.



Charge transfer cross-sections for the C^{4+} + uracil system for different attack angles (in 10^{-16} cm^2)

In the case of the C^{2+} + U process, the anisotropic effect is less significant and the charge transfer cross-sections remain low.

[1] J. de Vries, R. Hoekstra, R. Morgenstern, T. Schlathölter, J. Phys. B **35**, 4373 (2002).

[2] M.C. Bacchus-Montabonel, M. Łabuda, Y.S. Tergiman, J.E. Sienkiewicz, Phys. Rev. A **72**, 052706 (2005).

J.E. Sienkiewicz

13 September 2006