Short visit 20/11/2006 – 26/11/2006

Dr. Ágnes Vibók, University of Debrecen
Host's name and Institution: Marie-Christine Bacchus-Montabonel, Laboratoire de Spectrométrie Ionique et Moléculaire, University Lyon I

Reference code: COST-STSM-P9-02449

Research report:

Collisions of multiply and highly charged ions with biological molecules, in particular with DNA bases are very important processes because of their relevance in medical applications. Several experiments have been considered in this field in the last few years. Electron-DNA experiments have shown that collisions of relatively slow electrons (with energy of about 10eV) can lead to the break down of DNA through a mechanism that involves the formation of intermediate resonant states. Therefore, processes that lead to production of electrons are also relevant in the understanding of biological damage. In this respect, electron emission in collisions of ions with water provides the most significant source of electrons in the interaction of ion beams with the cell, as well as OH radical which is highly involved in the damage of biomolecular systems. Although experiments have provided detailed information on such collisions, calculations are not available, mainly because the complexity of the system.

During my short visit, we have chosen a particular system to study in a joined theoretical collaboration with our group (Á. Vibók and G.J. Halász of the University of Debrecen) and the group of M. C. Bacchus-Montabonel in the University of Lyon and also involving Béla Sulik group (Department of Atomic Collisions, Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI)) from experimental side. In the near future, we would like to study the H^+ + OH collisional system which is very important from biological point of view, taking into account the pure charge transfer process as the first step, and then to extend this study to reactive collision processes. Such a study requires very accurate ab-initio potential energy surfaces and non-adiabatic coupling term calculations (obtained by the Debrecen group) followed by appropriate dynamical treatment (treated by the Lyon's group). The theoretical results will be compared to the experimental measurements produced by the group of Béla Sulik.

Debrecen, November, 27. 2006 *Dr. Á. Vibók*