The scientific report of the academic visit by Dr Minaxi Vinodkumar from the Open University, UK to University of Innsbruck, Austria

My visit to Innsbruck with Prof. Michael Probst was very successful and met all the objectives I set for the visit. My main aim was to understand and make use of the Gaussian package for the calculations of ionization cross sections used by Prof. Probst and the Ionenphysik group for the electron scattering from biological molecules a major objective of Working Group 1 of the COST RADAM Action.

One of the goals of radiation biology is to develop a model of how ionizing radiation interacts with living tissues, from the initial energy deposition event at the molecular level, through to the longer term consequences for the whole organism. It is therefore necessary to study the ionisation of biomolecules by both the primary radiation and secondary electrons induced in the initial ionizing events. The study of electron induced ionisation for simple gas phase molecules is a well established field of atomic and molecular physics, with well defined experimental techniques capable of providing accurate cross sections (to within a few percent). However in biology there are many molecular systems that can not be prepared for experiment (e.g short lived radicals of molecules that can not be easily prepared in the gas phase- DNA for example !) for such targets ionisation cross sections must be evaluated using theoretical methods.

Prof. Probst and group at Innsbruck are involved in the study of molecular structure of biomolecules and perform calculations to derive the total ionization cross sections for electron impact on various nucleobases and amino acids. In my short visit I discussed their methods and *how they may be incorporated into my own simulations* of electron interactions with biomolecular targets such that this data may be fed *into track simulation studies.*

Theoretical track structure modelling is used to stimulate the distinctive patterns of ionizations produced by wide range of ionizing radiations. Such methods show us that penetrating radiations produce a significant number of nanometre-sized

clusters of ionization at the low energy track-ends of secondary electrons. Similarly, ions produce an abundance of clustered ionization along the path of the particle track both by the ions themselves and low energy secondary electrons. Such clusters can induce complex strand breaks in DNA, which are less easily repaired than the predominantly simple breaks produced by energetic electrons. The low energy electrons therefore have an important role in determining the overall radiobiological effect of the ionizing radiation and the mechanisms by which it may damage DNA. My research aims to develop methods for probing such electron interactions and therefore my visit to Professor Probst proved to be a key part of my future studies.

I am happy to inform you that during my visit I became familiar with the Gaussian package used to generate the various basis sets, to calculate the orbital energies and to find the population of the electrons in these orbital for the target. These data were then used in Matlab software to generate ionization cross sections. I successfully calculated the ionization cross sections for number of molecules such as BO^-, B_2^-, CH_4, C_2H_6 and H_2CO. In the future development of this collaboration we intend to calculate the total cross sections for more complex biomolecules including amino acids, peptides and nucleotiodes.

Finally I would like to thank the COST Programme (RADAM action) for the opportunity to undertake this visit