STSM Scientific report

COST STSM Reference Number: COST-STSM-P9-1541
Period: 05/06/2007 to 23/06/2007
COST Action: P9

STSM Applicant: Mr Andreas Mauracher, Institut für Ionenphysik und Angewandte Physik, 6020 Innsbruck (AT), andreas.mauracher@uibk.ac.at

STSM Topic: Theoretical and experimental investigations

Host: Thomas Alexander Field, Department of Physics and Astronomy, Belfast (GB), t.field@Queens-Belfast.ac.uk

In this STSM the main goal was to probe electron attachment to amino acids, both experimental and theoretical. Furthermore a task was to exchange knowledge between the two groups about experimental techniques and obtained experimental results, which are going to be published in collective papers. At the end of the visit I attended the RADAM07 conference in Dublin to present some of the results emanated from this collaboration ship.

Experiments: On the first two days Karola Graupner and Prof. Thomas Field finished a test series to inorganic compounds. During this time we spoke about our different experimental setups, which advantages and disadvantages they have and in which way we can combine the different results to optimize future investigations. On the third day there were no experiments carried out, because the closed water cooling system was maintained and therefore the diffusion pumps had to be turned off. Unfortunately there went something wrong, because in the night from the third to fourth day, a water line broke and the whole lab was flooded. Because they were not able to fix the water cooling system until my departure from Belfast, we were not able to carry out our planed experiments on amino acids.

Theory: Because of the failure of the experiments we concentrated totally on quantum chemical calculations. From the experiments obtained in Innsbruck (energy scan for $(Glycine\text{-}H)^-$) we knew that the reaction $Glycine + e^- \rightarrow (Glycine\text{-}H)^- + H$ has two different resonance. The first and strongest resonance is about 1 eV and the second is about 5 eV. In Innsbruck high level G2MP2 *ab initio* calculations were already used to obtain energetic data for two isomers of neutral Glycine which have nearly the same total energy. Also the bond dissociation energies of the five hydrogen atoms were calculated. Additional to these results we finished now the potential energy curves for H-loss from the neutral and negatively charged Glycine. Therefore the B3LYP/aug-cc-pVTZ density functional and basis set were used. In comparison of the theoretical and experimental results, we can conclude that the first resonance in the energy scan can be identified as the loss of a neutral hydrogen from the carboxylic group. For the second resonance at higher electron attachment energies it is not possible to make a clear conclusion with the present results, because the calculated

BDEs of the hydrogen atoms at the other positions are about 2eV too low. A further investigation would be necessary to estimate if any higher exited states are responsible for the second resonance, which is observed in the experiment. Figure 1 shows the potential energy curves for the loss of the hydrogen atom from the carboxylic group.

Other calculations contained the optimized structures, oscillation frequencies and total energies of the neutral and negatively charged D-alanine and L-alanine, but those results are not completed until now.

RADAM07 conference: On the meeting I presented the results obtained from our calculations due to the loss of a neutral hydrogen atom from the negatively charged Glycine within the poster session.

Future collaboration: The experiments concerning the amino acids shall be carried out as soon as the water cooling system is fixed. We are already working on a collective paper concerning electron attachment to nitroaromatic compounds. In fall a stay of Karola Graupner and Prof. Thomas Field in Innsbruck is planed.

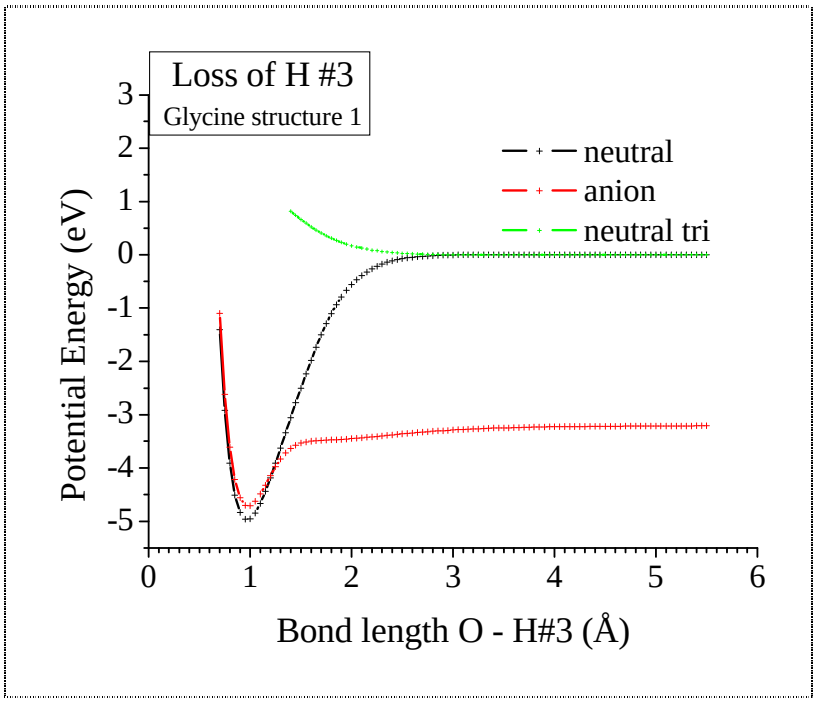

Figure 1