### **SCIENTIFIC REPORT**

#### Title: Investigation of low energy electron interactions with gas phase biomolecules

**REFERENCE:** Short Term Scientific Mission, COST P9

Beneficiary: Dr Janina Kopyra, University of Podlasie Host: Prof. Dr. Eugen Illenberger, Freie Universität Berlin Period: from 21/10/2007 to 20/11/2007 Place: Berlin (DE) Reference code: COST-STSM-P9-03126

#### **Purpose of the visit**

The purpose of the visit was to investigate interaction of the low energy electrons with molecules in the gas phase by means of LIAD technique (laser induced acoustic desorption) as well as a crossed electron-molecular beams technique.

Due to various breakdowns which have had occurred at LIAD machine, requiring lengthy repair time, it was impossible to perform the experiments on biomolecules using this technique. However, this gave me the opportunity to inspect the inside of the equipment that is as important as learning how to use the working LIAD.

### Description of the work carried out

The experiments were performed by means of the crossed electron-molecular beams technique. The experimental setup is housed in a stainless steel high-vacuum chamber and consists of an electron source, an oven, a quadrupole mass analyzer and a detection system. The electron beam of the defined energy is generated by a trochoidal electron monochromator (resolution of 130 meV FWHM) and crossed perpendicularly with the molecular beam under investigation. The generated negative ions are extracted by a weak electric field and accelerated by a series of parallel electrodes onto the entrance hole of quadrupole mass analyzer and detected by a single pulse counting technique as a function of incident electron energy. Calibration of the electron energy scale and estimation of the electron energy was established using the well-known electron attachment process  $SF_6^-/SF_6$ .

#### Description of the main results obtained

During my stay in the laboratory in Berlin I was involved in the study of the trifluoropropene and trifluoropropyne as well as uridine 5'-monophosphate disodium salt compounds by electron attachment.

Indirect, capturing, collisions of electrons with trifluoropropene lead to the formation of the transient anion which decay forming permanent fragment negative ions:

$$CF_{3}CHCH_{2} (96 \text{ amu}) + e^{-} \rightarrow CF_{3}CHCH_{2}^{\#^{-}} \rightarrow CF_{3}CCH^{-} + \text{neutral fragments} \qquad 94 \text{ amu}$$

$$\rightarrow CF_{3}^{-} + \text{neutral fragments} \qquad 69 \text{ amu}$$

$$\rightarrow C_{2}F_{2}^{-} + \text{neutral fragments} \qquad 62 \text{ amu}$$

$$\rightarrow C_{2}H^{-} + \text{neutral fragments} \qquad 25 \text{ amu}$$

$$\rightarrow F^{-} + \text{neutral fragments} \qquad 19 \text{ amu}$$

The most intensive signal was observed at 19 amu and assigned as  $F^{-}$ . The formation of the  $F^{-}$  ion results via a simple bond cleavage and is observed via different resonances between 0 and 11 eV (Fig. 1).

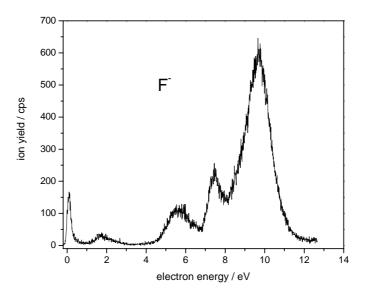


Fig. 1 Anion yield of F<sup>-</sup> following DEA to trifluoropropene.

The remaining anions, i.e.  $(M-2H)^2$ ,  $CF_3^2$ ,  $C_2F_2^2$  and  $C_2H^2$ , are created at the energy range 7-11 eV (Fig. 2) and hence attributed to core excited resonances. All of these are composed of two distinct contributions.

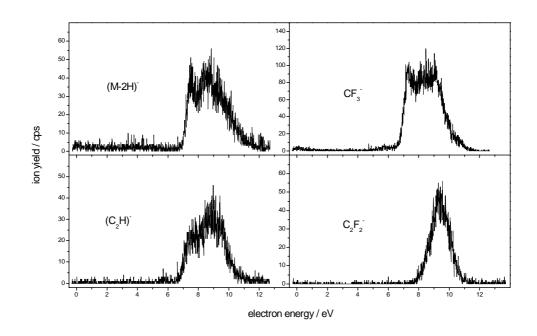


Fig. 2 Anion yields of  $(M-2H)^-$ ,  $CF_3^-$ ,  $C_2F_2^-$  and  $C_2H^-$  following DEA to trifluoropropene.

Trifluoropropyne, similarly as trifluoropropene, is very sensitive towards low energy electrons and an interaction of LEEs with this molecule leads to dissociation into various fragments. The major anionic dissociation products are caused by following reaction pathways:

$$CF_3CCH (94 \text{ amu}) + e^- \rightarrow CF_3CCH^{*-} \rightarrow CF_3CC^- + neutral fragments93 amu $\rightarrow C_2F_3^- + neutral fragments81 amu $\rightarrow CF_2CC^- + neutral fragments74 amu $\rightarrow CF_3^- + neutral fragments69 amu $\rightarrow C_2H^- + neutral fragments25 amu $\rightarrow F^- + neutral fragments19 amu$$$$$$$

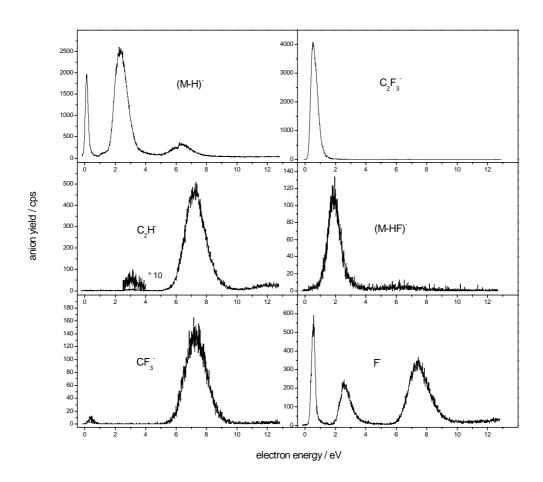


Fig. 3 Anion yields of the products following DEA to trifluoropropyne.

The characteristic ion efficiency curves from trifluoropropyne are shown in Fig.3. It is clearly visible from the spectrum that the most intensive signal appears at mass 81 amu with peak at 0.5 eV. The second dominant feature is a fragment at 93 amu which can be attributed to the molecule after abstraction of the neutral hydrogen atom (M-H<sup>-</sup>) with peaks at 0.1, 2.3 eV and weaker and broader contribution at about 6.3 eV. Next fragment, at 19 amu, arises from the neutral molecule due to the cleavage of the single C-F bond and can be assigned as F<sup>-</sup>. In this ion spectrum three structures are visible - the first, at low energy region, is located at 0.6 eV, the second one at 2.6 eV and the third one at 7.5 eV. The CF<sub>2</sub>CC<sup>-</sup> is formed by the loss of a HF neutral group from the temporary negative ion and is characterized by a low energy resonance at 2 eV followed by a resonance at about 6 eV. For CF<sub>3</sub><sup>-</sup> as well as for C<sub>2</sub>H<sup>-</sup> relatively intensive peaks at about 7.3 eV are

observed. For the later one additionally the weaker structure at low energy region, at 3 eV, was visible.

The preliminary studies of electron attachment to uridine 5'-monophosphate disodium salt were performed as well. The first results are very promising however the measurements have to be continued.

# Future collaboration with host institution

We expect to continue the collaboration in the area of electron attachment spectroscopy.

## Projected publications resulting from the grant

It is planned to publish the results of the trifluoropropene and trifluoropropyne studies as soon as the data analysis has been finished.