ECCL Short-Term Scientific Mission
Scientific report

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Purpose of the visit

The aim of this visit was to continue the collaboration between the two groups in Iceland and Innsbruck in the field of site selective reactions driven by low energy electrons [1, 2]. Open questions concerning the site selectivity of dissociative electron attachment (DEA) to the amino acids proline and dipeptide were planned to be investigated. It was also planned to take these studies further by studying those site-selective bond cleavage reactions in the condensed media of helium droplets.

Furthermore, a new mass-spectrometer is to be constructed at the University of Iceland that consists of an electron monochromator, a very sensitive device. The construction plays a major role in my Ph.D. project. Therefore, it was also the purpose to attain an experience in operating an experimental apparatus consisting of an hemispherical electron monochromator, planned to be used during this visit.

Work carried out

At the start of the visit, the apparatus with the hemispherical electron monochromator was operated and tested with typical calibrants, such as SF_6. Then, measurements were performed with the chemical 1,4-dichlorobenzene that is currently studied with an apparatus consisting of a trochoidal electron monochromator to check for some open questions concerning the shape of Cl^-.

A scheme of the experimental setup is shown in Fig. 1. The collision chamber is attached directly to the hemispherical electron monochromator where the tuned electron beam collides with the neutral molecular beam. Then ions are drawn into a commercial quadrupole mass filter. The substances enter the collision chamber through the bronze capillary of the oven. A solid substance is vaporized when heated inside the oven. Liquid and gaseous substances are introduced into the oven by a flexible Teflon® tube and into the tube via an inlet metal tube system, external to the vacuum chamber (not shown in Fig. 1). A powder of 1,4-dichlorobenzene was used. Due to its high vapour pressure, it could be treated as a liquid.

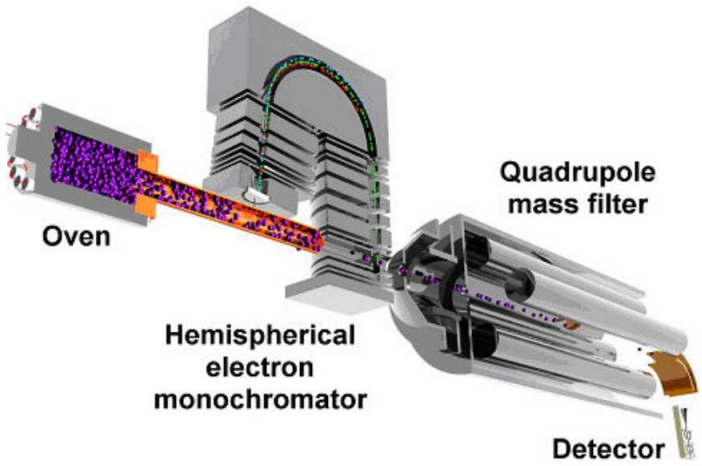

Figure 1: Schematic view of the experimental instrument [3].

Before an energy scan of Cl^- was conducted, an energy scan measurement of SF_6^- was done for zero-point calibration (shown in Fig. 2). Directly thereafter, 1,4-dichlorobenzene was introduced into the system and energy scan of Cl^- was acquired. Fig. 3 shows a plot of three measurements conducted repeatedly within the temperature range of 83 to 84°C and pressure range of 6,0 to $6{,}4\times10^{-6}$ mbar.

From Fig. 2 and 3, the great difference in ion yield is clear. Where SF_6^- peaks at over 35000 counts per second (cps) but Cl^- at less than 1000 cps, indicating the relatively small cross section of Cl^-. It should be noted that the energy scan of Cl^- was conducted in the presence of SF_6^-. So the possible effect of the so called Trojan horse ionization [4] has not been excluded here.

In addition to the energy scans, the mass spectra was measured in the presence of SF_6 and 1,4-dichlorobenzene simultaneously at two different electron energies; 0 eV and 1 eV. The mass spectra is shown in Fig. 4. Two prevalent peaks appear roughly in the mass range 30 to 40 amu and 144 to 150 amu, shown more clearly in Fig. 5. The peaks at 35 and 37 amu are the Cl^- isotopes and the peaks at 146 and 148 amu are the SF_6^- isotopes [1]. It is evident that the signal from SF_6^- is stronger at 0 eV and the signal from Cl^- is stronger at 1 eV as expected.

Main results

Preliminary results from dissociative electron attachment measurements of the shape of the Cl^- anion from 1,4-dichlorobenzene with an apparatus consisting of an hemispherical electron monochromator were obtained.

Furthermore, after this visit, an understanding of the practicalities and the intricacies of electron monochromators has become extensive.

[1] http://winter.group.shef.ac.uk/chemputer/isotopes.html

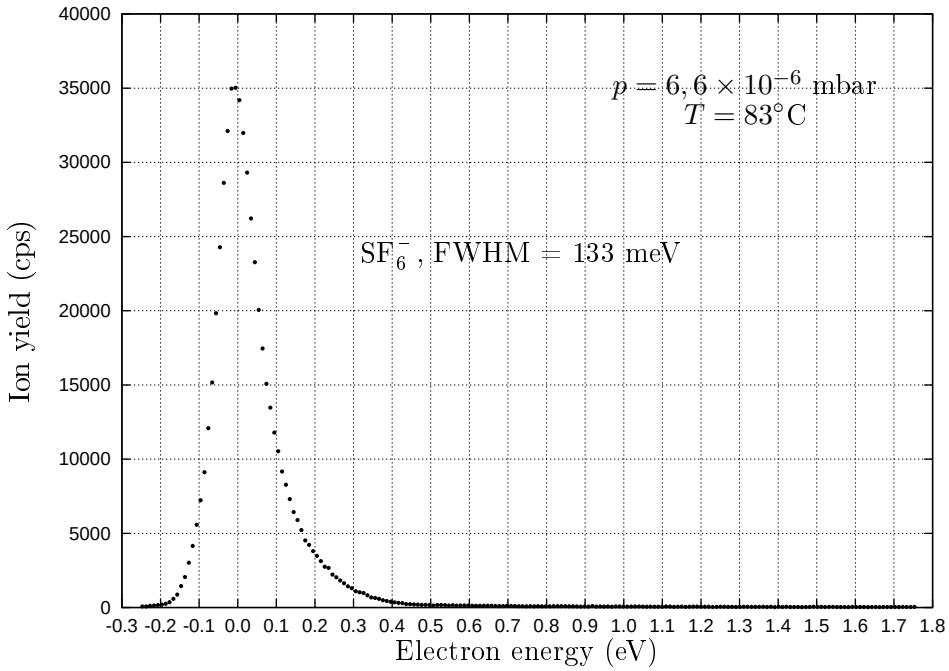

Figure 2: Cross section of SF_6^- for zero point calibration.

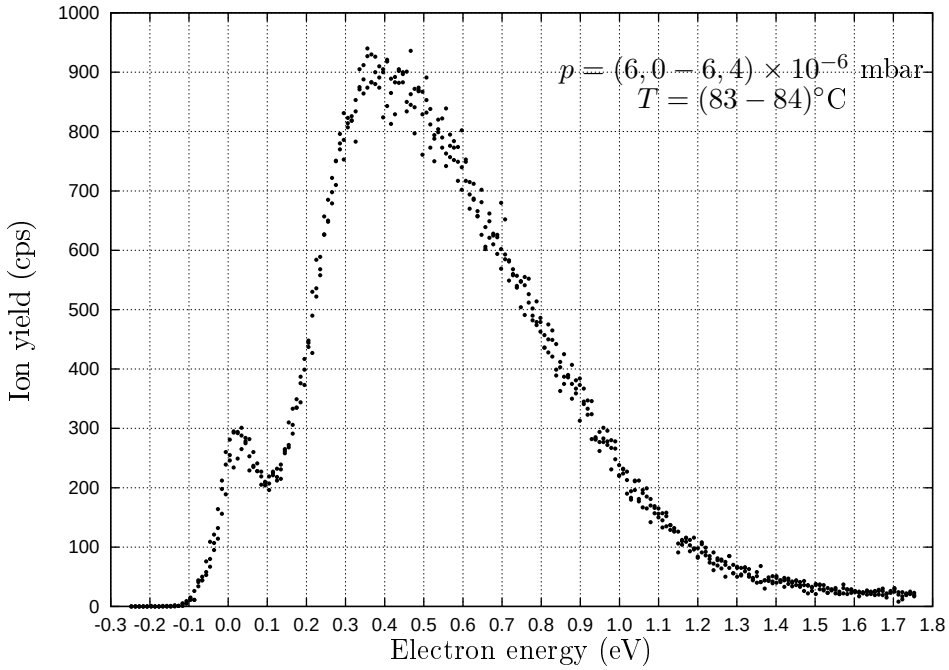

Figure 3: Cross section of Cl^- from 1,4-dichlorobenzene.

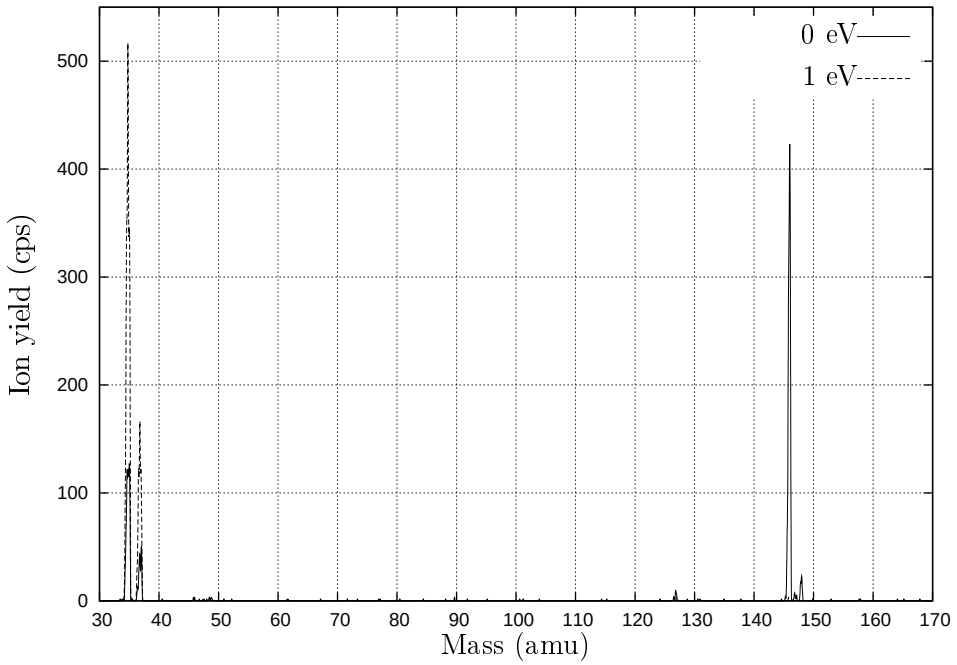

Figure 4: Mass spectra at two different electron energies: 0 eV and at 1 eV.

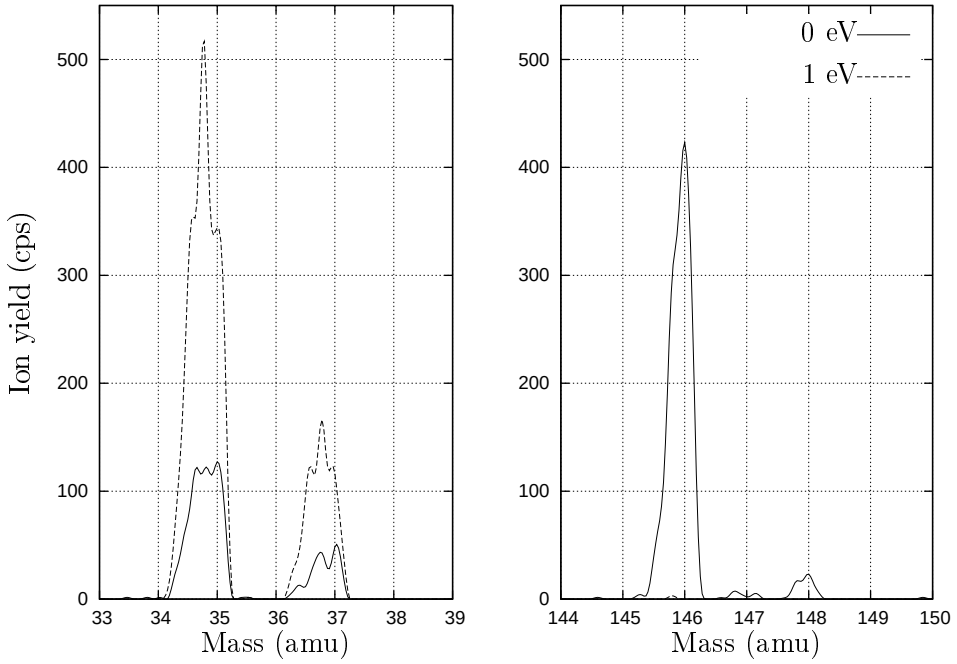

Figure 5: Mass spectra at two different electron energies. Close-up from Fig. 4.

References

[1] Flosadóttir HD, Denifl S, Zappa F, Wendt N, Mauracher A, Bacher A, Jonsson H, Märk TD, Scheier P, Ingólfsson O, *Combined experimental and theoretical study on the nature and metastable decay pathways of the amino acid ion fragment [M-H]*, Angewand Chemie – International edition, 46 (42), 8057 – 8059, 2007

[2] Mauracher A, Denifl S, Aleem A, Wendt N, Zappa F, Cicman P, Probst M, Märk TD, Scheier P, Flosadóttir HD, Ingólfsson O, Illenberger E, *Dissociative electron attachment to gas phase glycine: Exploring the decomposition pathways by mass separation of isobaric fragment anions*, Physical Chemistry Chemical Physics, 9 (42), 5680 – 5685, 2007

[3] P. W. Sulzer, *Dissociative Electron Attachment to Explosives and Biomolecules*, Ph.D. Thesis, University of Innsbruck, Jan 2008

[4] Drexel H, Sailer W, Grill V, Scheier P, Illenberger E, Märk TD, *Electron attachment to C_2Cl_4 and Trojan horse ionization*, J. Chem. Phys. 118 (16), 7394 – 7400, 2003