

## SCIENTIFIC REPORT

**Title:** Low energy electron interaction with halogenated compounds

**REFERENCE:** Short Term Scientific Mission, COST CM0601

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**Host:** Prof. Dr Stefan Matejcik, Department of Experimental Physics, Comenius University Bratislava

**Period:** from 21/06/2009 to 19/07/2009 Place: Bratislava

**Reference code:** COST-STSM-CM0601-04950

### **Purpose of the visit**

During the short visit I have performed experiments using crossed electron-molecular beams apparatus. The purpose of my visit was to investigate interaction of the low energy electrons with molecules in the gas phase. I have studied dissociative electron attachment to series of benzene derivatives (1-nitro-3(1,1,2,2-tetrafluoroethoxy)benzene and 4-fluoro-3-nitrobenzotrifluoride) and 2,2,2-trifluoroethylamine in the energy range from about 0 to 14 eV.

### **Description of the work carried out**

The present studies were carried out with a high-resolution (120 meV FWHM) electron-molecular beam apparatus. The electron beam was formed by a trochoidal electron monochromator and accelerated on desired energy, perpendicularly crossed by a molecular beam formed by effusive molecular beam source. Negative ions produced in the reaction chamber were extracted by a weak electric field from the interaction region and focused into the entrance of quadrupole mass spectrometer. The mass selected negative ions were detected as a function of electron energy in single-ion counting mode using a secondary electron multiplier, ion counting electronic and PC acquisition system. The electron energy scale was calibrated using the SF<sub>6</sub><sup>-</sup> signal yielding a very narrow peak near 0 eV. The measurements were carried out at the gas temperature 371 K.

### **Description of the main results obtained**

The dissociative electron attachment processes to 1-nitro-3(1,1,2,2-tetrafluoroethoxy)benzene and 4-fluoro-3-nitrobenzotrifluoride have shown rich fragmentation patterns. Figure 1 presents the ion yield curves of studied molecules.

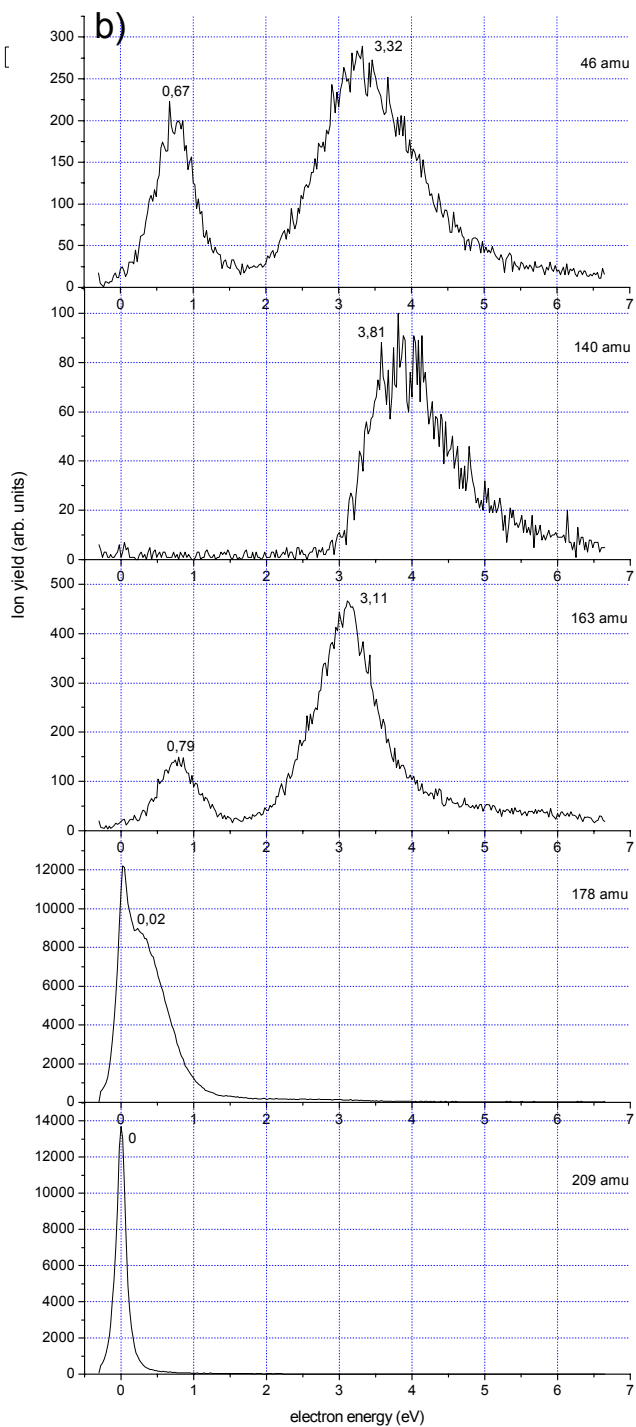
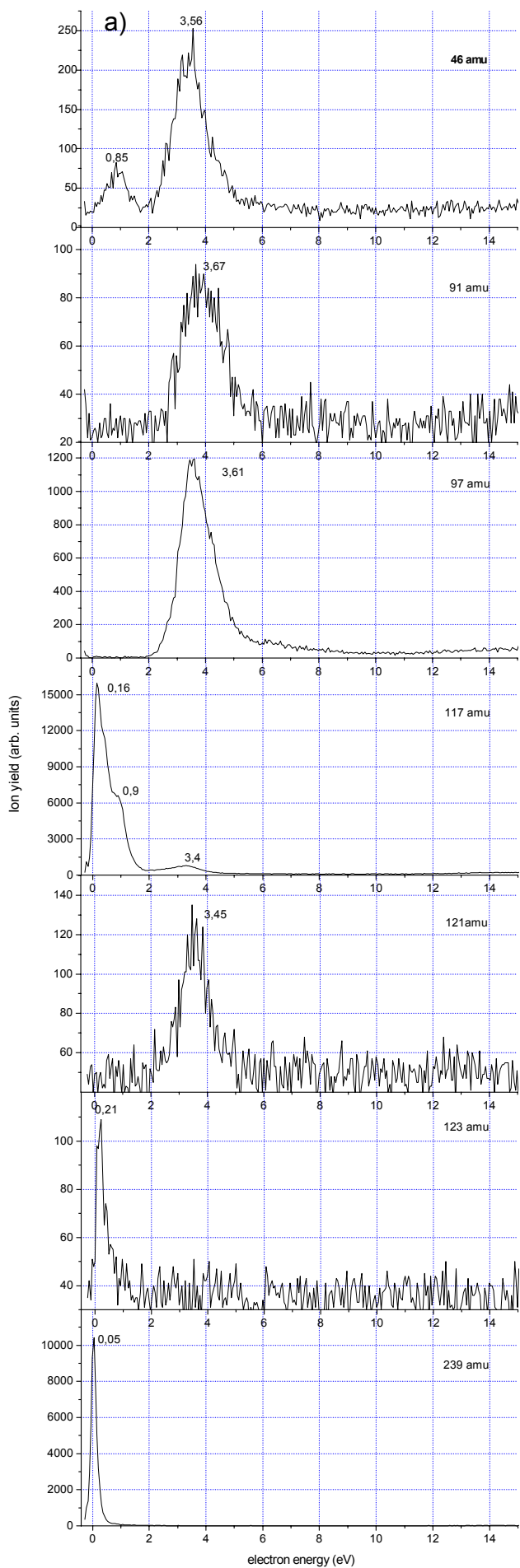
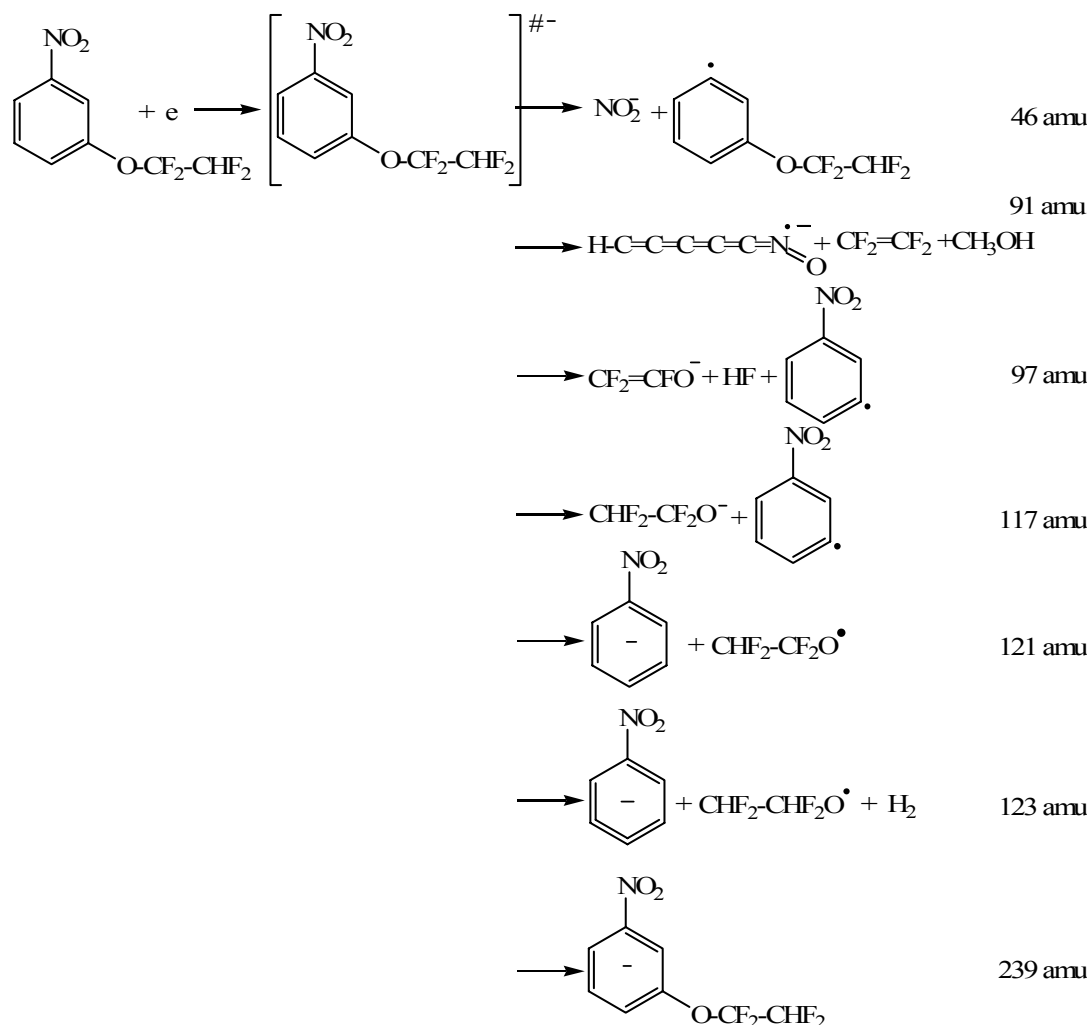


Figure 1. Ion efficiency curves of negatively charged fragments formed by dissociative electron attachment to (a) - 1-nitro-3(1122-tetrafluoroethoxy)benzene and (b) - 4-fluoro-3-nitrobenzotrifluoride.

In these nitrobenzene derivatives we observed deep fragmentation of the parent anion, including rearrangement processes and ring cleavage. Unfortunately in the case of 2,2,2-trifluoroethyloamine we did not observe any electron attachment products (negative ions or parent negative ion). This molecule seems to be not sensitive on low energy electrons.

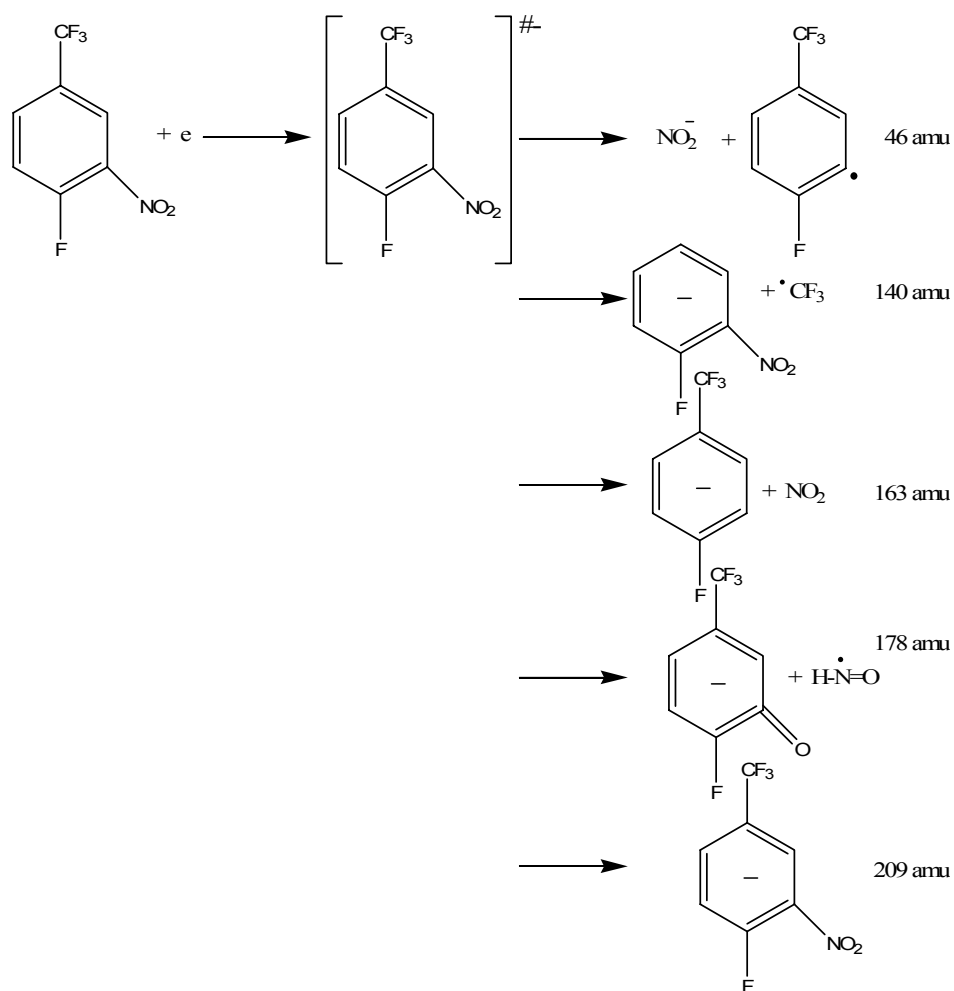
The interaction of low energy electrons with 1-nitro-3-(1,1,1-tetrafluoroethoxy)benzene leads to dissociation into various fragments by following reaction pathways:



The most favorable reaction channel is connected with formation CHF<sub>2</sub>-CF<sub>2</sub>O<sup>-</sup> (117 amu), via the cleavage of the bond between the carbon atom from the benzene ring and the oxide atom. This feature is located near thermal energy. In the same energetic region parent negative ion (239 amu) with the second highest abundance was observed. Ions with the mass of 121 amu and 123 amu are formed via the loss of the radical CF<sub>2</sub>HCF<sub>2</sub>O<sup>•</sup> and in the case of the second mass additionally loss of H<sub>2</sub> molecule. The dissociation channel leading to NO<sub>2</sub><sup>-</sup> formation requires only cleavage of the single bond and exhibited two resonance peaks in the electron energy range below 4 eV, the first one at 0,85 eV and the

second one at 3,56 eV. Almost at the same energetic region (~3,6 eV) were recorded ions with the mass of 91 amu and 97 amu. The first one is most probably formed by cleavage of benzene ring and some rearrangement processes and the second one was created due to multiple bond cleavages, electronic rearrangement and formation of a C=C double bond.

4-fluoro-3-nitrobenzotrifluoride, alike as 1-nitro-3(1122-tetrafluoroethoxy)benzene, is very reactive towards low energy electrons and leads to dissociation into various fragments:



Parent negative ion of this molecule which is the most abundant was observed within a very narrow resonance located at 0 eV. Furthermore, at the thermal electron energy with comparable abundance was observed the ion with the mass of 178 amu. This anion can be formed by abstraction of the radical  $\text{HNO}^\bullet$  and additionally some rearrangement processes. In some of the fragments (46 amu and 163 amu) were observed two peaks located at the energy below 3,5 eV. This anions can be formed by a single bond cleavage as well as the ion with the mass of 140 amu.

All dissociative electron attachment channels for 4-fluoro-3-nitrobenzotrifluoride and 1-nitro-3(1122-tetrafluoroethoxy)benzene molecules were observed at electron energy below 4 eV. In both cases

parent negative ion was the dominant product and ion yield  $\text{NO}_2^-$  exhibits two peaks at almost the same electron energy.

#### **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 1-nitro-3(1,1,2,2-tetrafluoroethoxy)benzene and 4-fluoro-3-nitrobenzotrifluoride studies as soon as the data analysis will be finished.