Chemical reactions induced by slow electrons to 1,3-Diaminebenzene

Report for the Short Term Scientific Mission to Queen's University Belfast
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The aim of this STSM was to investigate electron attachment processes to 1,3-Diaminebenzene. Due to the volcanic ash cloud the chemical supply company was not able to send the substance on time for the measurements. Therefore we had to change our target molecule and investigated Heptacosafluorotributylamine (Figure 1) instead. Heptacosafluorotributylamine is a mass spectrometric standard and is used to calibrate mass scales as well as to tune mass spectrometers. Although studies concerning electron impact ionization to Heptacosafluorotributylamine exist, apparently no electron attachment investigations could be found in the literature.

In Figure 2 one of the 2D scans is shown as an overview. The y-axis displays the electron energy (the energy scale is calibrated by the well known SF_6^-/SF_6 zero eV resonance), the x-axis shows the mass to charge ratio. The ion yield intensity is color coded. One can see many different fragments which occur after electron attachment. We carried out measurements at different ion source pressures and with focus on different regions of electron attachment energies to find also low intensity signals. At the moment we are analyzing the data and assigning the mass to charge ratios to corresponding fragments. Due to the high symmetry there are many different possibilities to form corresponding fragments.

We also started to carry out quantum chemical calculations to derive structures and energetics of Heptacosafluorotributylamine. Due to the high number of electrons (671) wavefunction-based theory is quite expensive also with rather small basis sets. Another problem is a reasonable description of fluorine atoms in the molecule, which demands basis sets with diffuse functions to satisfy the criteria of its large electron density We tested different basis sets and possible Ansätze to safe computational time and still derive accurate results.

In summary this STSM has revealed very interesting results, and we'll continue to work together on the evaluation of the obtained data as well as the quantum chemical calculations.

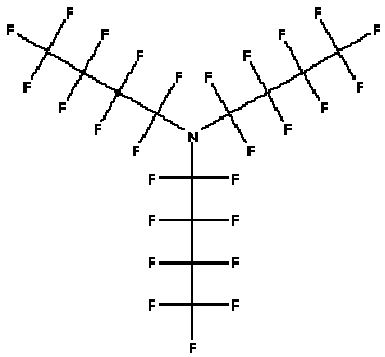

Figure 1 – Fischer projection of Heptacosafluorotributylamine

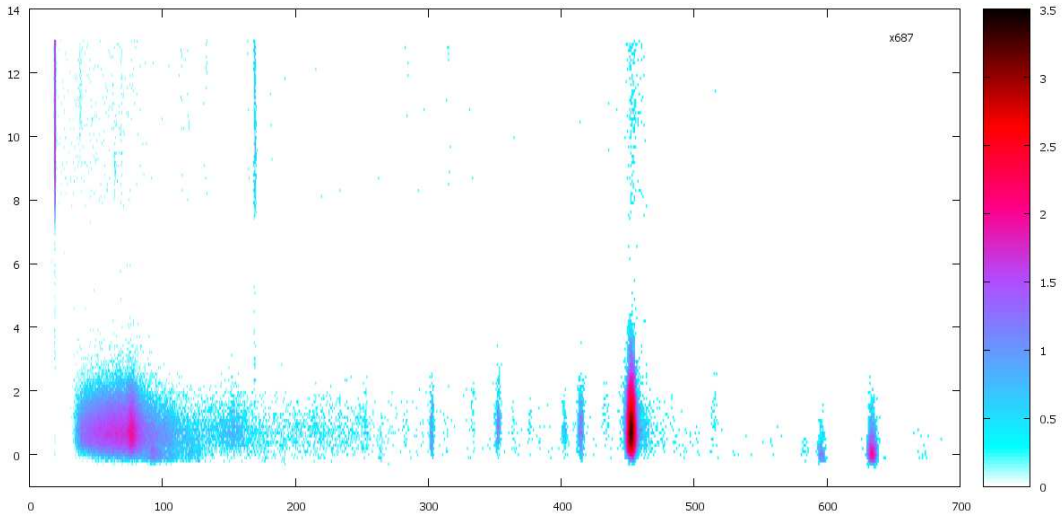

Figure 2 -2D-scan of EA to Heptacosafluorotributylamine