Investigations of chemical reactions induced
by slow electrons to nitro aromatic compounds

Report for the Short Term Scientific Mission to Queen's University Belfast
COST-STSM-CM0601-04497

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During this STSM we investigated dissociative electron attachment (DEA) processes to 2-nito-m-xylene in the gas phase. The experiment was carried out on the ERIC apparatus, which consists of a pulsed trochoidal electron monochromator and a time-of-flight (TOF) mass spectrometer. The ions are formed in the interaction region, where the electrons collide with a diffuse beam of the neutral compound. The produced anions are then accelerated out of the interaction region via the ion repeller and are accelerated a second time afterwards. 1,3-dimethyl-2-nitrobenzene was purchased from Sigma Aldrich with a stated purity of > 99% and used as delivered.

In Figure 1 a two-dimensional map of DEA to 2-nitro-m-xylene is shown. On the y-axis the electron energy is shown, and on the x-axis the time-of-flight, which can be transferred to a m/z-ratio.
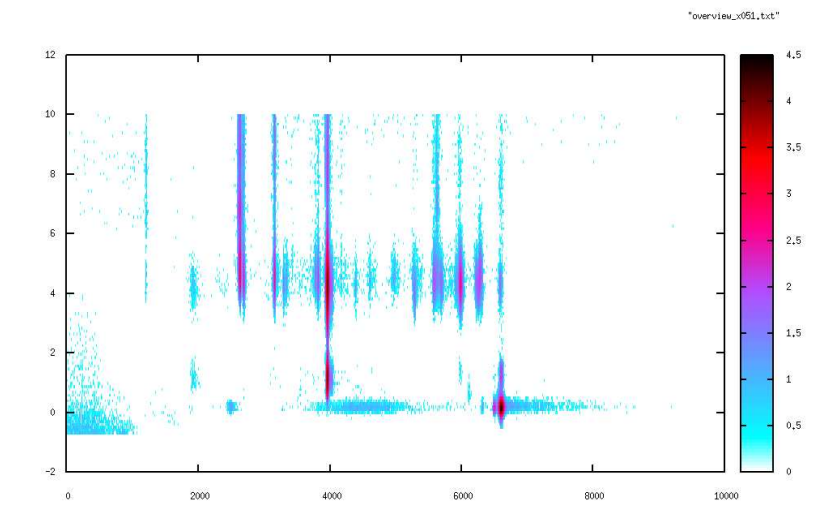

Figure 1 – two-dimensional map of DEA to 2-nitro-m-xylene

One can see that beside the parent anion P^- only $(P-NO)^-$ is formed at electron energies close to zero eV. A further analysis of the data shows, that metastable defragmention occurs only at electron energies around 4.5 eV, indicated by the broad band of ion signal in this region. Due to the fact that the signal for the metastable decay reactions is quite low for an exact assignment of the different metastable decay reactions

experiments on the Innsbruck apparatus VG (a double sector field instrument in reverse geometry) are required.

From the computational point of view we carried out numerous G3(MP2) calculations, to derive bond dissociation energies as well as the electron affinity of fragments. With these energies one can calculate the energetic thresholds of the formation of fragments. In addition Hartree Fock wavefunctions were used to visualize the molecular orbitals and to calculate the dipole moment of the molecule (HF/aug-cc-pVTZ). Figure 2a shows the highest occupied molecular orbital (MO 40) of the neutral molecule, Figure 2b shows the orientation of the dipole moment (3.94 D), Figure 2c shows the electrostatic potential mapped on an isosurface of the total electron density, and Figure 2d shows the singly occupied molecular orbital (MO 41) of the anion.

| Figure 2a | Figure 2b | Figure 2c | Figure 2d |

see text for explanation
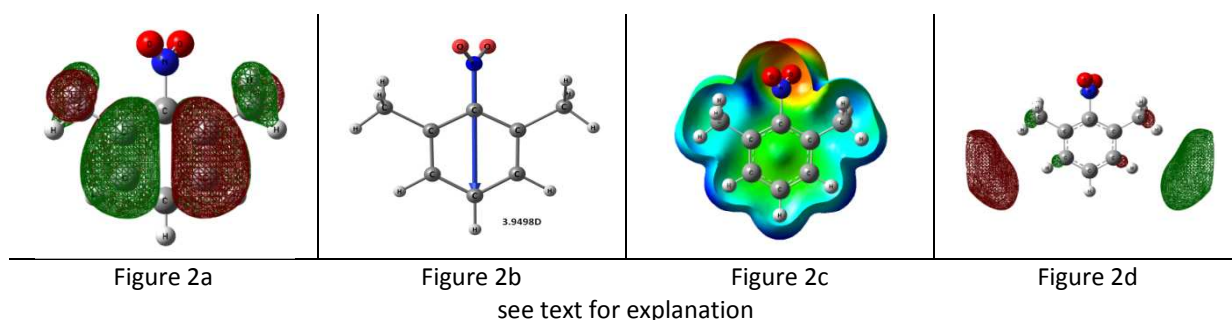
In summary this STSM has been successfully, some of the results of these investigations will be presented in a talk at the ECCL09 conference, as well as a publication in a journal.