

Report on the outcomes of a Short-Term Scientific Mission¹

Action number: CA20129

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Details of the STSM

Title: Temperature dependence of CN anion formation upon DEA to benzonitrile

Start and end date: 09/07/2023 to 22/07/2023

Description of the work carried out during the STSM

In this STSM were carried out ion yield temperature dependence of CN anion formation upon dissociative electron attachment (DEA) to benzonitrile. DEA to benzonitrile leads to CN anion formation via two distinct electronic states, 1st lying at around 2 eV and 2nd having a maximum at 7 eV. Preliminary studies have shown that resonance intensities are temperature dependent. Hence, is needed a detailed study on this particular fragment. The measurements were performed in a crossed molecular beam apparatus, equipped with a trochoidal monochromator and with a Hiden quadrupole mass spectrometer. The first set of measurements were performed at room temperature, 25°C. The benzonitrile molecules in the gas phase were introduced into a high-vacuum (HV) chamber through an effusive gas inlet system, reaching a pressure of 1.5E-4 Pa (base pressure of 1.0E-5 Pa). The molecules crossed a near monoenergetic electron beam, formed in a trochoidal electron monochromator. The formed ions were extracted towards a Hiden EPIC1000 quadrupole mass spectrometer (Hiden Analytical, Warrington UK). The mass spectrometer is equipped with two separate RF generators, which operate within a high (2 – 1000) and low (0.4 – 50) m/z-range. Before performing the measurements, was necessary to guarantee the optimal working conditions. The trochoidal electron monochromator was completely disassembled and cleaned, and a new filament was mounted. Calibration measurements were performed with SF₆. The electron energy resolution was about 200 meV (FWHM) determine by the well-know cross section of SF₆⁻ associative attachment resonance. There were conducted measurements between 25 and 133°C, namely 25, 60, 85 111 and 133°C. From those measurements, the two resonances are evident one at 2eV and another at 7eV. The relative intensities between both against the temperature are described in the figure 1.

Description of the STSM main achievements and planned follow-up activities

Dissociative electron attachment energy dependence studies on benzonitrile have been performed within this STSM. From the present study was possible to conclude that fragmentation channels related with resonances located at 2 eV and 7 eV are not influenced by the temperature. By analysis of figure 1, it is possible to observe

¹ This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

that the ratio of resonances relative intensities is constant for a temperature range between 25°C and 133°C. The small fluctuations are within the statistical error of the measurements. For each measurement a sum of several runs have been recorded to keep the signal to noise ratio as good as we could.

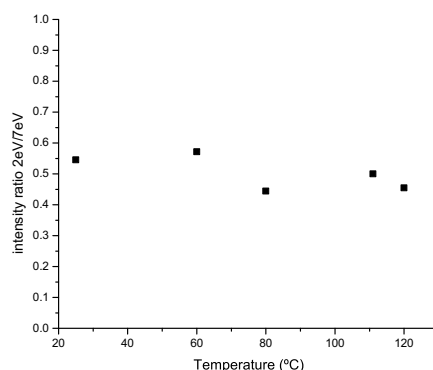


Figure 1 – CN^- formation: temperature dependence for temperature range between 25°C to 133°C. Ratio between the maximum intensity of 2eV resonance and 7 eV resonance.

The obtained results will complement a publication in preparation on DEA to benzonitrile. The results will help on understanding molecular fragmentation pathways and temperature dependence upon low energy electron irradiation of benzonitrile. Moreover, during the visit to prof. Oddur Ingólfsson laboratory, was possible to discuss results on electron ionization of propylene oxide and start drafting a join publication. It is expected to submit by the end of the year. For the two studies, benzonitrile and propylene oxide, the collaboration between the two groups, have shown to be important not only for the complementary of experimental results, but also for the better understanding and strong connection between the two laboratories. Both studies are in line with the objectives MultiChem COST action, namely in electron interactions with organic molecules in the gas phase.

Furthermore, there is planned to performed measurements on PAH, namely 2-cyanonaphtalene. This compound has also astrochemical relevance. Additionally, there is a set of experimental improvements on the set-up that we plan to develop in collaboration. It is planned a design for a new acquisition program, more reliable, actualized and more efficient in the data acquisition and data treatment. This software should be developed by the Lisbon group, that has expertise and have recently updated its own software. Monochromator electronic circuits and power supplies should also be renewed. A new inlet system, end a deep maintenance of the vacuum system should also take place.