

## Report on the outcomes of a Short-Term Scientific Mission<sup>1</sup>

**Action number: CA20129**

**Grantee name: Daniel Bou Debes**

### **Details of the STSM**

Title: Exploring CN- Formation from Benzonitrile: Unravelling Dynamics via Velocity Map Imaging and Electron Energy Loss Spectroscopy

Start and end date: 01/09/2024 to 19/09/2024.

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

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

*(max. 500 words)*

During the STSM, we conducted detailed experiments on the scattering of electrons from benzonitrile, using two-dimensional electron energy loss spectroscopy (EELS) as the primary investigative tool. During these experiments, electrons with a range of different incident energies are directed at benzonitrile molecular gas phase targets. As these electrons scatter off the molecules, we record the energy of the scattered electrons. This process allows us to determine the probability of energy loss for the electrons, as a function of the incident electron energy. By analysing the EELS data, we are able to gain valuable insights into the vibrational excitations of the benzonitrile molecule. These excitations can occur through two different mechanisms: either via direct, non-resonant scattering, or indirectly through resonances that temporarily trap the electron before releasing it. This comprehensive approach helps us understand both the direct and resonance-driven pathways of electron interaction with benzonitrile. We recorded the two-dimensional EELS spectrum for both incident and scattered energies in the range of 0 to 1.2 eV, with steps of 10 meV. Additionally, EELS spectra were measured at constant incident energies of 0.75 eV and 2.6 eV, providing further insights into the energy-dependent behaviour of electron scattering from benzonitrile.

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

<sup>1</sup> 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.

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

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words)

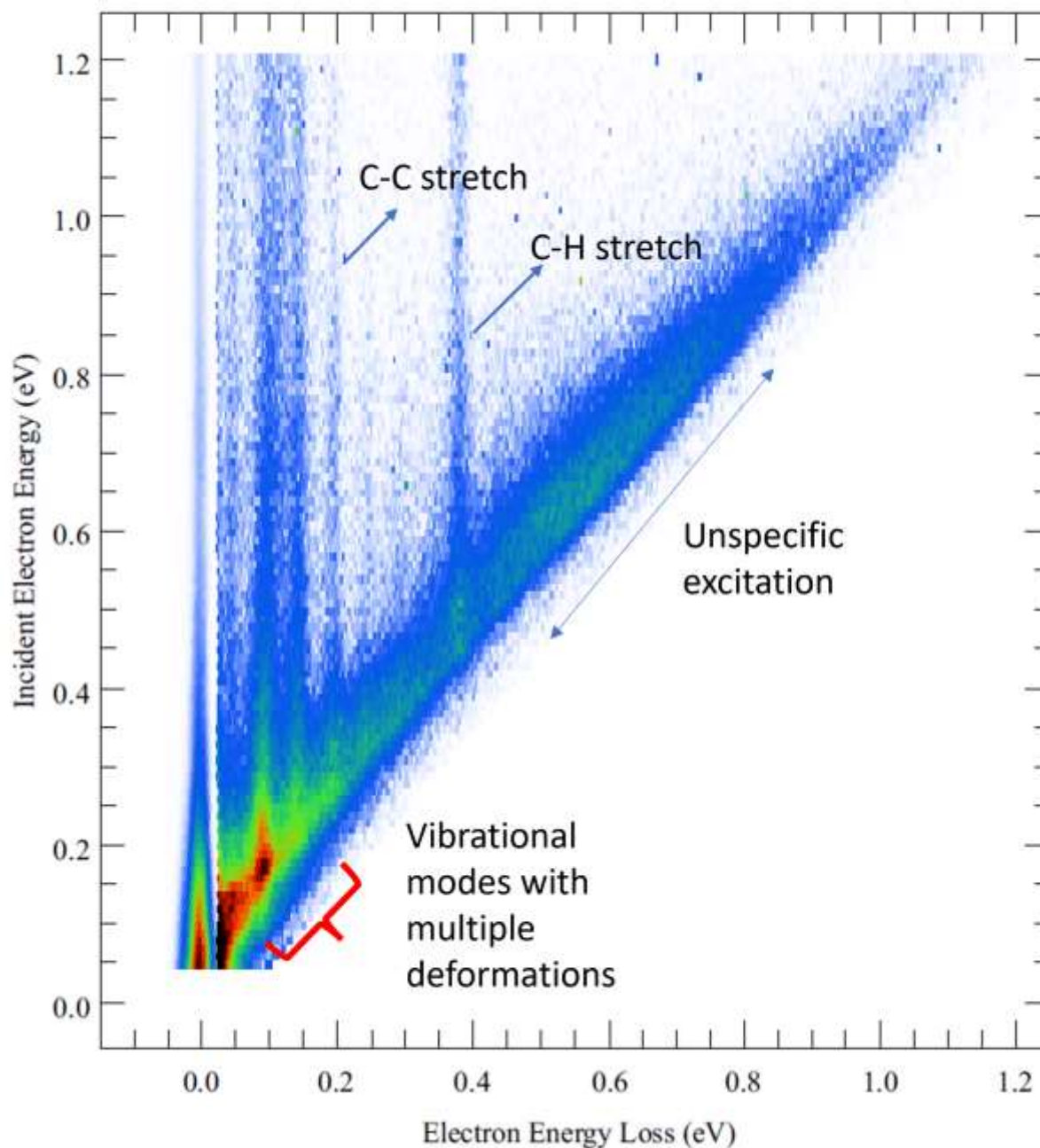


Figure 1: Two-dimensional electron energy loss spectrum (EELS) of Benzonitrile.

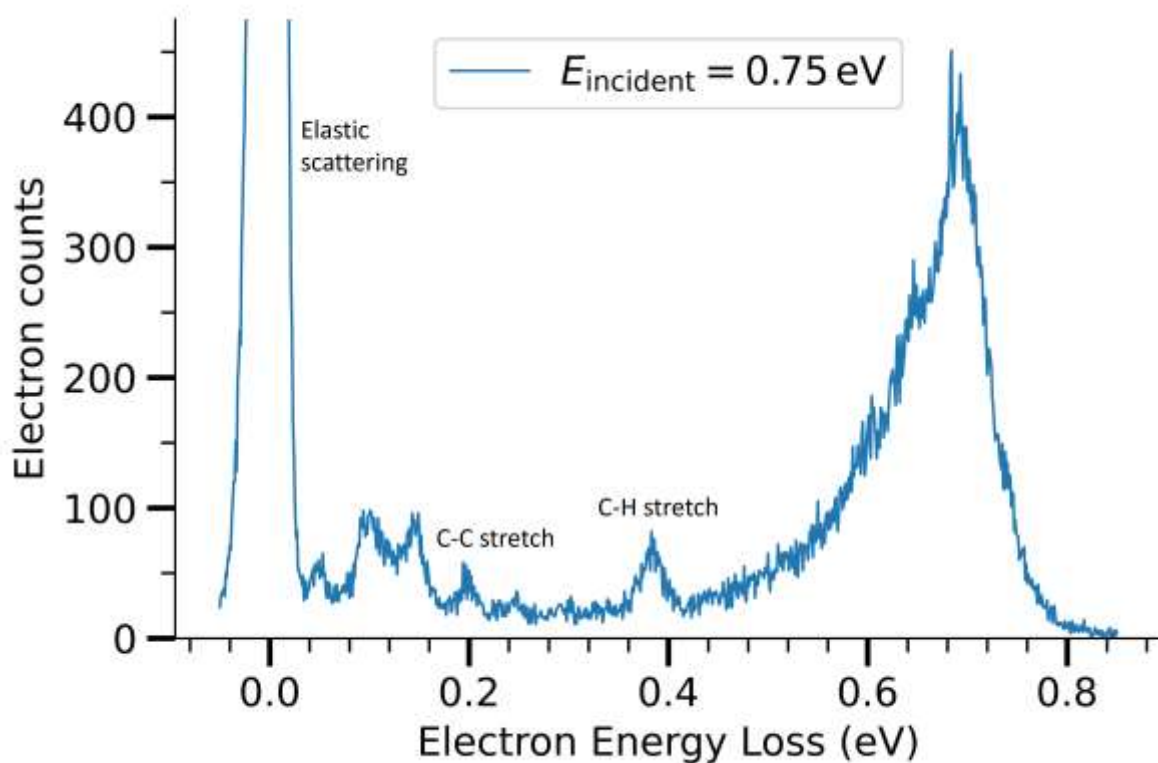


Figure 2: EELS spectrum at 0.75 eV incident electron energy.

Several vibrational excitations are visible in the 2D EELS spectrum shown in Fig. 1, as well as in the EELS spectrum recorded at an incident electron energy of 0.75 eV. The excitations observed between 0.05 and 0.15 eV are attributed to vibrational modes involving multiple deformations of the molecule. The excitation at 0.2 eV is associated with the C-C stretching between carbon atoms on the phenyl ring, while the excitation at 0.4 eV corresponds to a C-H stretching mode between carbon and hydrogen atoms on the phenyl ring.

The most intriguing feature is observed at energies between 0.45 and 0.8 eV, where a resonant temporary non-dissociative electron attachment occurs. This attachment is followed by the detachment of the electron on a microsecond timescale, revealing the dynamics of the interaction.

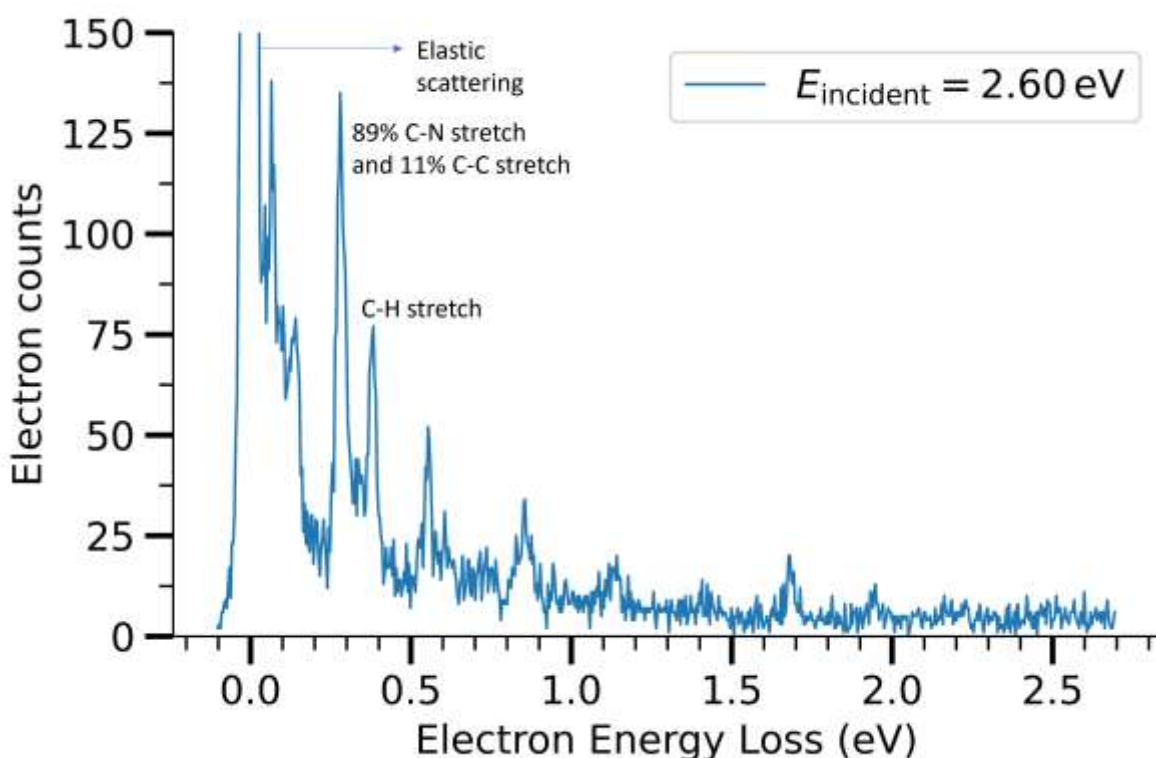


Figure 3: EELS spectrum at 2.6 eV incident electron energy.

The formation of  $\text{CN}^-$  due to dissociative electron attachment (DEA) has been previously studied by Illenburger et al.<sup>1</sup>, with the first resonance responsible for this dissociation occurring between 1.75 and 4 eV, reaching peak intensity around 2.6 eV. As a part of the STSM plan, we wanted to measure velocity-map images of the  $\text{CN}^-$  anions, however, this was not possible due to technical problems of the DEA-VMI spectrometer. Instead, we measured an EELS spectrum at a constant incident electron energy of 2.6 eV. This spectrum reveals the appearance of an intense peak at 280 meV, which corresponds to a combination of C-N stretching and C-C stretching between the carbon atom on the phenyl ring and the carbon attached to the nitrogen atom. This provides valuable insight into the specific vibrational modes that contribute to  $\text{CN}^-$  anion formation through DEA.

The results are currently being prepared for publication.