Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA20219

Grantee name: Kevin Li

Details of the STSM

Title: Ion Formation by Irradiation of Ternary Clusters and Nanoparticles

Start and end date: 22/05/2023 to 02/06/2023

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)

In the first week, we investigated clusters produced by the coexpansion of HCOOH/H2O with increasing water content. These clusters were subsequently probed by mass spectrometry, employing both positive ionization (electron impact at 70 eV) and negative ionization (electron attachment 0-15 eV) techniques, with a specific emphasis on investigating the influence of water on the underlying processes (e.g. intracluster ion molecule reactions, electron induced chemistry, etc.). Experiments involving the coexpansion of HCOOH and HNO3 (nitric acid) were not carried out due to the chemical reaction between the acids, resulting in their decomposition into CO2 and NO2.

During the second week, we carried out pickup experiments. Firstly, we explored the pickup of formic acid on hydrated HNO3 clusters. We conducted measurements with multiple pickup pressures in order to investigate the influence of the number of doped molecules on cluster chemistry. We also performed the experiments in the opposite manner, i.e., we investigated the pickup of nitric acid onto hydrated formic acid clusters to explore changes in the resulting cluster chemistry. Subsequently, we conducted experiments involving the pickup of dimethylamine (DMA) on nitric acid clusters, using a similar approach to the HCOOH pickup experiments. The aim was to investigate the influence of the number of doped DMA molecules on the resulting cluster chemistry. Lastly, we conducted a double pickup of DMA and HCOOH on hydrated nitric acid clusters, testing different pickup conditions to ensure the successful uptake of both precursors onto the clusters.

[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.

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

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.

(max. 500 words)

During the STSM, we successfully achieved the initial characterizations of molecular clusters containing organic acids. We began by investigating the coexpansion of formic acid and water, focusing on the basic behaviour of cluster generation and comparing it to the behaviour of inorganic acid counterparts. By varying the water ratio in the source solution, we observed corresponding changes in the clusters. Higher water content resulted in higher hydrated clusters. For clusters with 30% acid content, we found clusters with up to 25 water molecules. Interestingly, even in the case of a 98% formic acid solution, the clusters exhibited a significant water content, the origin of which remains unclear. The 2% water present in the solution could be sufficient to supply the necessary molecules, or it could originate from the formic acid itself through dissociation.

In our analysis of the negative ionization electron scans conducted via electron attachment, we observed the behaviour of hydrated formic acid clusters. The initial maximum intensity was observed in the region between 2 eV and 3 eV, with another small maximum found around 8.5 eV. Further analysis of the spectra revealed differences in the ion species depending on the mass-to-charge ratios. Lower electron energies and lower mass-to-charge ratios favoured deprotonated ions, while higher masses and higher electron energies predominantly showed protonated species.

Furthermore, we investigated the addition of ternary components through pickup experiments. Although the pickup of nitric acid on formic acid was unsuccessful, we achieved successful pickup of formic acid on hydrated HNO3 clusters. We discovered cluster series containing hydrated nitric acid and formic acid, with the measured clusters containing a maximum of only one formic acid molecule.

Measurements with double pickup of DMA and formic acid resulted in signals for both single pickups. While depending on the pressure in the pickup chambers the exact ratio between the intensities of different pickup changes, the signals of the DMA pickup is generally more intense. Clear double pickup signals were not found. As the used molecules have similar masses, mass coincidences make the evaluation of the mass spectra more difficult and time consuming. Especially, the coincidences between nitric acid and DMA propose a challenge. Therefore, additional evaluation of the gathered data is needed.

The results gathered so far give us a first insights into the clustering behaviour of formic acid. Using nitric acid further information about its interactions with different molecules and their inner dynamics are obtained. As mentioned above further analysis is needed to uncover more information of the formic acid clusters.