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

Action number: CA 21126

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Details of the STSM

Title: Interstellar ethers: IR action spectroscopy of intermediates and products in the reaction of protonated ethanol and neutral ethanol (C_2H_5OH)

Start and end date: 14/07/2024 to 19/07/2024 (effective departure date changed from 12/07 to 14/07 due to logistic issues)

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)

Experiments have been performed in the cryogenic 22-pole ion trap instrument, FELion, coupled with the widely tunable free electron lasers at FELIX, at the Radboud University in Nijmegen (NL). We used a storage ion source (SIS) as chemical reactor to generate both intermediate clusters and product ions of the proposed ion-molecule reaction between protonated ethanol and neutral ethanol, to give before the proton-bound complex ($C_4H_{13}O_2^+$) at m/z 93, as an intermediate, and then protonated diethylether as a product. For the reaction studies, precursor ions have been produced by electron impact ionization of C_2H_5OH vapor in the SIS source, where intermediate and product ions have been formed via successive reactions, namely self-protonation of the alcohol and alkyl transfer reaction. Vibrational spectra have been recorded by infrared predissociation (IRPD) spectroscopy of rare-gas tagged ions with Ne (with a short and intense gas pulse) using FEL-2 in the energy range 300 - 1000 cm^{-1} and 600 - 1600 cm^{-1}. Spectra have been recorded by monitoring the dissociation of the weakly bound rare gas-ion clusters as a function of laser wavelength. Saturation depletion measurements have been used to quantify the isomeric abundances and to exclude the presence of any isobaric impurities. All target ions exhibit characteristic vibrational modes in the spectral fingerprint region. The use of FELIX was essential because there is practically no other source type providing widely tuneable radiation with sufficient intensity for the experiments in the required range.

[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)

The mainly investigated ions were the protonated dietyhlether ($DEEH^+$), at m/z 75, and the product at m/z 73 ($DEEH^+$, H_2 loss). They were efficiently produced via dissociative ionization of pure ethanol in the SIS. The formation of the m/z 93 ion (proton-bound ethanol dimer) was optimized after all the measurements done for the m/z 73 and 75 ions, due to major differences required for the optimization. Both the ions were successfully tagged with Ne, to give the m/z 93 and 95 ions ($DEEH^+$, H_2 loss-Ne tagged, and $DEEH^+$-Ne tagged). No tag with Ne was possible for the proton-bound dimer (m/z 93), but it was successfully tagged with H_2.
During the first shift, the IR-PD scan of both the m/z 73 and 75 Ne-tagged ions were performed in the 600 to 1600 cm^{-1} energy range by using FEL-2. For the m/z 95 (75-Ne tagged), in Figure 1, ion we observe strong features around 600, 820, 840, 970 cm^{-1}, with weaker bands around 1370 and 1500 cm^{-1}. In the case of the m/z 93 (73-Ne tagged) ions, in Figure 2, the most intense features in the investigated range were at 770, 960, 1340 cm^{-1}, with weaker bands at 1180 and 1420 cm^{-1}. The assignation of the signals, by comparing the experimental and synthetic spectra, are still under discussion. In the second shift, the IR-PD spectra for the same ions were recorded in the lower energy range, from 300 to 1000 cm^{-1}. The acquired data is still under analysis. We also managed to retrieve depletion scans on the investigated ions to assess the presence of one or more isomers. In the case of the m/z 95 (75-Ne tagged) ions, Figure 3, the depletion measured on three different bands was close to 100% in all the cases, confirming the presence of only one isomer. Regarding the m/z 93 (73-Ne tagged) ion, the depletion was measured on two distinct bands, with an outcome of about 80%, suggesting the presence of several isomers being present at the same time. However, this last dataset is still under detailed analysis.
The higher energy range (up to 3500 cm^{-1}) was chosen not to be investigated both because of lack of time, and because of the (most likely) presence of a single intense feature in the synthetic spectra of both the isomers, ascribable to the asymmetric C-O stretching. This could be anyway investigated during a following beamtime.

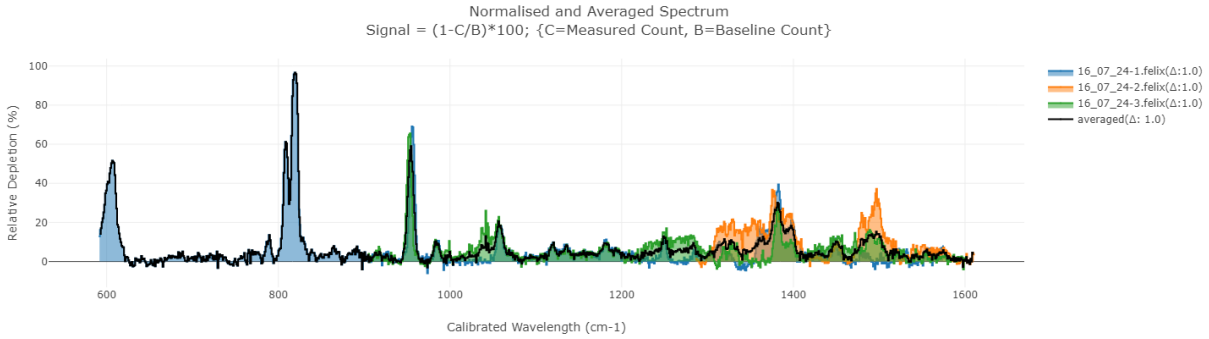


Figure 1: Spectrum of the m/z 95 (75-Ne tagged) ion acquired during the first shift. The features from 300 to 1000 cm-1 have been better explored during the second shift.

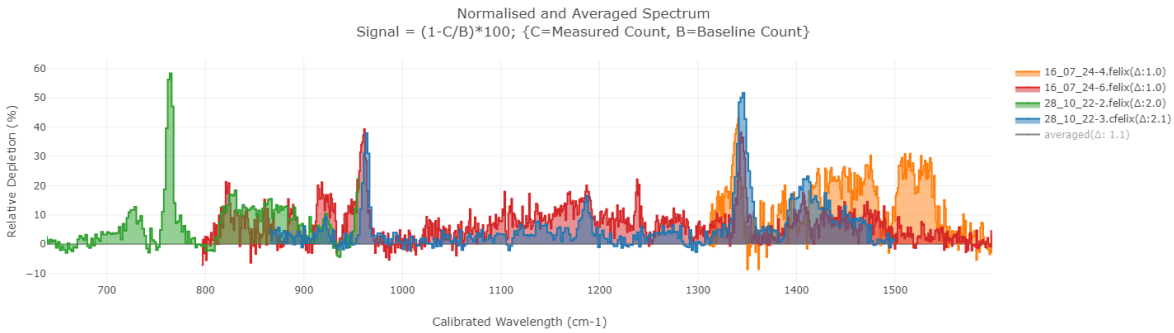


Figure 2: Spectrum of the m/z 93 (73-Ne tagged) ion acquired during the first shift. The features from 300 to 1000 cm-1 have been better explored during the second shift. The orange trace in the figure has been discarded due to instabilities during the acquisition.

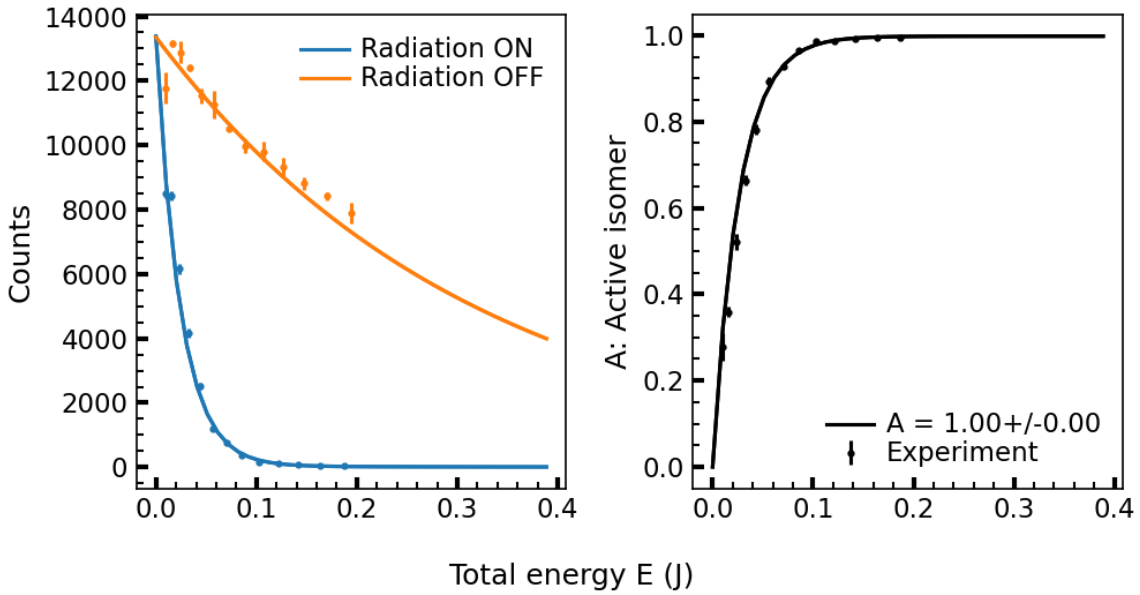


Figure 3: Depletion scan for the transition at 820 cm-1 (blue trace), investigated for the m/z 95 (75-Ne tagged) ion. The off-resonance depletion (orange trace) has been investigated at 840 cm-1. The blue trace shows a 100% depletion, revealing the presence of a single isomer (together with the other depletion scans) contributing to the absorption of the IR-photons.

As a conclusion and based on the results obtained so far, these investigations promisingly allow for boosting the knowledge of C-based, O-bearing molecular species in space (in this specific case, interstellar ethers). Even if still under analysis, the spectroscopic data collected will then give room to the study of the reactivity of such species in space, that could result in different channels also giving carbonaceous materials as products. With the participation of several people from different institution, this STSM contributed to promote the creation of an interdisciplinary research team to develop future laboratory experiments that will probe the formation, spectroscopy and reactivity of nC.