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

Action number: CA20129

Grantee name: Eva Muchova

Details of the STSM

Title: **First time observation of KLM Auger-Meitner process in organic chloro-compounds**

Start and end date: 10/10/2023 to 16/10/2023

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)

We followed the working plan during the beamtime, e.g. we concentrated on the near-threshold KLM Auger-Meitner 2D map spectra for chlorinated organic compound. We selected three samples CH_2Cl_2, $C_2H_4Cl_2$ and trans-CHCl=CHCl that had suitable vapor pressure for the experiment. All samples were successfully characterised. Besides the 2D KLM maps, we measured a complex X-ray characteristic of the samples such as XPS at both K-edges (Cl and C edges), KLL Auger 2D maps and we have also tested and performed the acquisition of the KMM maps.

The employed energies were in the range 3100-3500 eV for the X-ray characterisation and ~3200 eV for the 2D maps. The 2D KLM map example for dichloromethane CH_2Cl_2 is provided in Figure 1.

[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.

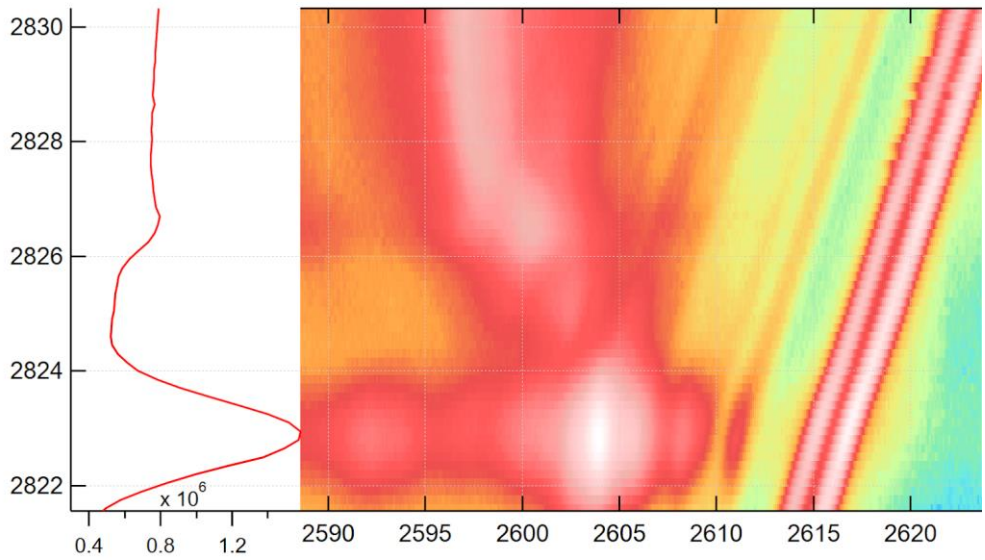

Figure 1: KLM 2D map of the CH_2Cl_2 with logarithmic z scaling. The XAS spectrum is on the left side, resonance maximum is at 2823 eV.

We have observed varying peaks in the sample set showing molecular-like characteristics of the KLM decay which is due to differences in the valence band of the molecules (the M-shells are different).

Besides, we have also recorded the KMM maps because the signal was high enough also for less probable events. The KMM maps, however, exhibit a significant overlap with the valence band direct photoionization peaks and the signal subtraction may not be trivial. An example of the KMM 2D map for the CH_2Cl_2 is presented in Figure 2.

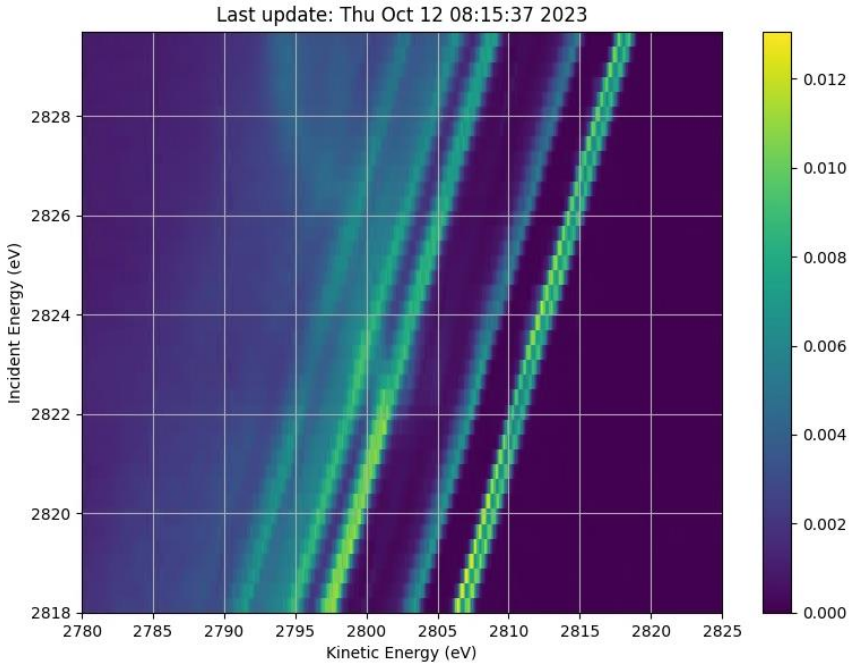

Figure 2: The KMM 2D map of the CH_2Cl_2.

The obtained data require theoretical interpretation which will be performed by the applicant. Modelling of the KLM processes is challenging from different perspectives and will certainly require method some method development because the theoretical tools for core/excited and decaying states are still limited compared to the UV-Vis domain and in this project the decay involving both L and M-shells must be addressed. The theoretical activities performed by the applicant will involve X-ray absorption

calculations, analysis and interpretation of the core-excited transitions, assessment of individual peaks in the KLM spectra. The measured spectra show additional complexities related to post collision interaction or possible induced ultrafast dynamics. During the beamtime, we also discussed the results within the team and planed for the interpretation of the results.

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 main aims of the STSM were achieved, during the beamtime the full X-ray spectral characterization and KLM 2D maps have been recorded for the first time. The experiments were successfully conducted and we managed to measure 3 samples (instead of anticipated 2). The experiments were performed with resolution achievable at Galaxies at SOLEIL. We have obtained spectroscopic fingerprints of valence-band in the KLM. The resonances formed during the experiment will be furthermore theoretically modelled in terms of the Fano-Feschbach theory, the decay widths will be modelled most probably via on one-centre atomic radial Auger integrals using the multistate restricted-active-space perturbation theory.

The aims of the STSM fully comply with the action aims to acquire a fundamental-level understanding of Irradiation-Driven Chemistry (IDC). The full X-ray characterization and mainly information encoded in resonant Auger spectra now recorded at unprecedented Cl 1s edge (otherwise hardly accessible) can be used to understand how the molecular chemical environment changes atomic-like. Next, the STSM helped to promote the collaboration between theoreticians and experimentalists and to extend the network. The on-site discussions helped to make functional decisions about measured data which can speed up the experiment.

The follow-up activities will involve post-processing of the obtained spectral data and their experimental characterization. The applicant will perform *ab initio* modelling and interpretation of the spectra using the theoretical toolbox, a further development is also anticipated. The KLM maps have proven to contain an the “chemical aspect and can be useful for further development of the method for spectroscopic characterization of dynamics in the excited or ionized states.