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

Action number: CA20129

Grantee name: Lassi Pihlava

Details of the STSM

Title: Effect of solvation on the response of cancer radiosensitizer to ionising radiation

Start and end date: 01/10/2024 to 07/10/2024

Description of the work carried out during the STSM

The STSM mission went largely according to the initial working plan. The first day of the mission was spent on travelling. Our local contacts at the beamline had already prepared the aerosol delivery system and the experimental setup by the grantee's time of arrival. Therefore, no additional preparatory work during the first day was needed. The beamtime started at 8 am on the second day of the STSM and ended at 8 am on the final day. We (the grantee and the rest of the experimental team) ran the experiments 24 hours per day in three overlapping 12-hour shifts (3am-3pm, 9am-9pm, 3pm-3am).

When we received the first light of the beamtime, we started testing the aerosol setup with NaCl (aq) solution. We started setting up the hemispherical electron spectrometer and linear Wiley-McLaren ion time-of-flight (TOF) spectrometer. The latter turned out to be more problematic than usually as the beamline staff had changed the old MCP detector of the ion TOF spectrometer to a new one a few days prior to our beamtime. The signal from the ion TOF was initially very noisy but over the course of the beamtime we managed to reduce the noise by optimising various settings, allowing us to carry out measurements. Considerable effort was also spent aligning the photon beam and the aerosol jet with respect to each other.

One of the goals of the STSM was to measure high resolution electron spectroscopy measurements on nanosolvated radiosensitizers. Here, the sample molecule was 2-bromo-5-iodo-4-nitroimidazole. From testing prior to STSM, we knew that electron spectra can be obtained from water-sample aerosols. The measurements were conducted successfully also now and we measured various electron spectra in different conditions: i) wet condition where the aerosols are directed through a separator that removes only the largest droplets and ii) dry conditions where the aerosols travelled through a two-stage drier setup that removes more water than the separator. We also used two different carrier gases over the course of beamtime: He and N2. We measured spectra upon valence, N1s, Br3d, I3d, and I4d ionisation. Most of the spectra we of photoelectrons, but we also low kinetic energy electrons in search of ICD (inter-

[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.

molecular Coulombic decay) electrons: However, their potential presence in the spectra can be only be seen later on after applying careful analysis on the data.

Despite the initial technical problems, we eventually managed to get the ion TOF spectrometer running reliably. Yet, we mostly the carrier gas and some water in our spectra. The measurements were carried upon the above ionisations. Unfortunately, the experimental conditions were not deemed good enough for time-consuming electron-ion coincidence spectroscopy measurements and we decided to focus the remaining beamtime on electron spectra.

During the last night, we measured ICD electrons from nimorazole (aq) and pure water aerosols in the same conditions as with the primary sample. This was an addition to the initial plan. Nimorazole is a radiosensitizer drug used in cancer treatments. Comparison may offer insight into radiosensitization.

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

The goal of the STSM was to study solvated 2-bromo-5-iodo-4-nitroimidazole molecules in water aerosols at the Finnish-Estonian beamline (FinEstBeAMS) of the MAX IV synchrotron radiation facility. The same molecule has been studied earlier in the gas-phase and the experiment here was carried out to study the effect of the water environment on the dissociation dynamics. The results offer further insight into the molecular level radiosensitization mechanisms that are still not fully understood. The primary goal was to measure electron spectra and this goal was successfully accomplished. We measured various spectra that we had planned (different photoelectrons and ICD electrons). We also extended the measurements to a proven radiosensitizer drug nimorazole, which was our back-up sample. The inclusion allows us to carry out further comparisons during the analysis. The secondary goal was test whether the used setup could be utilised for i) measuring ion TOF spectra of the fragment ions from the aerosol surface and ii) carrying ion-electron coincidence spectroscopy experiments. The secondary goals were known to be extremely challenging, yet full of potential for future experiments if successfully implemented. Ion TOF signal from the aerosol jet was measured, but the experimental conditions at the time were not considered suitable for coincidence spectroscopy experiment. This result is important as we plan future studies on photodissociation dynamics of radiosensitizers in aqueous environment in contrast to studies on gas-phase molecules.

The data analysis on the measured data is planned to commence shortly in continued collaboration of the international experimental team present at the beamtime. The collaboration will likely include also people who could not attend the experiment. The experimental team comprised of researchers from the University of Uppsala (Sweden), MAX IV laboratory (Sweden), the University of Kassel (Germany), and the University of Turku (Finland, the grantee's home institution). We aim to present the results of our experiments in a preferably open-access journal for better visibility. The collaboration between the participating research groups will continue after this project.