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Second update report

Laboratory Astrophysics: Athena Spectral Features

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AHEAD2020

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Foreword

This second update report covers activities of WP13 Laboratory Astrophysics Task 13.1 Athena spectral features from December 1st 2021 until November 30th 2022.

WP13.1A Collisional excitation rates

Liyi Gu (SRON), Task leader: Jelle Kaastra, SRON

Motivation

As the launch of XRISM is approaching (expected May 2023), the SPEX team is accelerating our activities implementing the updates on atomic data, including the calculation carried out using the AHEAD funding on the L-shell collisional excitation for cosmic abundant elements. The atomic data have been tested in single temperature calculations before imported to SPEX, however, a more extensive verification is required to ensure the data match well with the observations in all conditions. The errors on the theoretical rates can also be obtained by comparing with the observations.

Method and results

We suggest that the atomic data uncertainties can be inferred by a statistical sampling of discrepancies between the models and well-calibrated, well-understood spectra, which can be treated as the absolute true values within their quoted uncertainties. This approach is valid when (1) the sampling size of spectral feature measurements is statistical significant, and (2) the observed discrepancies are not driven by other types of uncertainties, such as statistical uncertainty and systematic uncertainties from astrophysics and instrumental calibration.

We perform comparison on the following data: for the collision excitation forming Fe-L, we choose the Chandra high energy transmission grating (HETG) data of Capella and HR 1099; the Chandra low energy transmission grating (LETG) data of Capella are used to calibrate the L-shell data of Mg, Si, S, and Ca, as well as lowly-ionized Fe. Both targets are well-studied X-ray bright stellar corona mostly in quiescent.

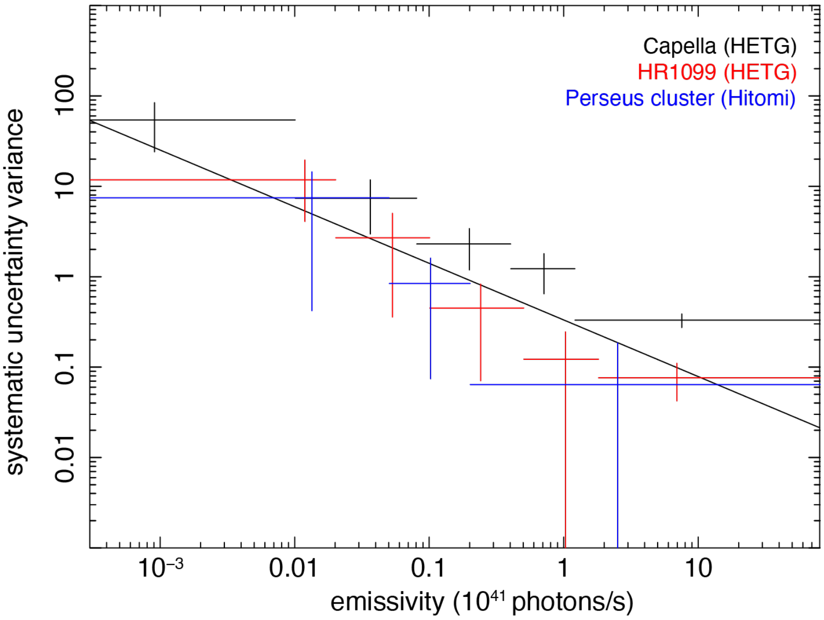


Figure 1 Variances of the systematic uncertainties in line intensities for Capella (black), HR 1099 (red), and the Perseus cluster (blue) as a function of emissivity. The solid line shows the analytic fit to the combined data with a power-law.

Although the HETG and LETG are well-calibrated stable instruments, we perform a set of improved instrumental modeling and fine-tuning, aiming to correct any possible energy-dependent calibration residuals and remaining biases throughout the wavelength range.

The obtained discrepancies in the emissivities of the Fe-L lines are shown in Figure 1. For strong transitions, the fractional uncertainties are found to be around 10%, while for the weak lines, the uncertainties increase to unity or larger. To describe the observed uncertainty-emissivity relation, we divide the emissivity range into a number of bins, and assume for each bin that the distribution of uncertainties follows a Gaussian function with zero mean value. The derived variances of the systematic uncertainties, as plotted in Figure 1, can be approximated by a simple power-law function,

$$\sigma = a \times (\frac{I}{10^{41}})^b$$

Where σ is the variance, I is the line emissivity in unit of photons per second, a and b are the free parameters. This relation holds for both Capella and HR 1099.

The comparison between LETG data and the L-shell emission at longer wavelength are performed in a similar manner with a master research project of a student from Leiden observatory, under the guidance of L. Gu.

Conclusion

The collision excitation calculation by L. Gu on L-shell lines should be considered valid in general as the discrepancies between model and data are ~10% for strong lines. The line diagnostics using weak lines, on the other hands, would be caveated as the uncertainties increase, which is not surprising given the complexity in atomic physics concerning the weak transitions. The routine for error calculation has been implemented in SPEX. This will improve the interpretation of the data from upcoming XRISM and Athena missions.

Publications

Gu, L., Shah, C., Mao, J. et al. 2022, A&A, 664, 62

WP13.1B Spectral features, inner-shell measurements

Task leader: F. Nicastro. WP's scientists: M. Coreno, J. Crespo, M. De Simone, A. Mohammed, F. Nicastro

Summary

Main goal of WP13.1B within the project is to measure energies and cross sections of electronic transitions of astrophysical abundant metals. During the reported period we exploited the synchrotron facilities at Elettra together with an Electron Beam Ion Trapper (EBIT) and an, in-house, octupole-quadrupole mass-spectrometer (Octomass) to measure: (a) energies of the main electronic transitions of the Be-like ion of oxygen (OV, or O4+), (b) the isotopic shift of electronic transitions from ^{16}OV and ^{18}OV, and (c) the mass-spectra of low-ionization, high mass/charge ions of Ar and Kr (a preparatory test for lower mass/charge ions of O, Fe and possibly N).

Background Information

As already reported in our previous report, the milestone 53 (MS53) of the project was partly modified because of the difficultly in hiring a PhD student to assemble and test the in-house (Elettra) Octomass setting to measure high mass/charge ions, due to the two years of pandemic. We instead developed a collaboration with Dr. J. Crespo at MP-Heidelberg to transfer one of his mini-EBIT to the synchrotron facility of Elettra (in Trieste, Italy) where we were awarded a long-program (total of 2 months distributed over 2-3 years) to measure, instead, low mass/charge ion's energy and cross sections. This has been done towards the end of 2021 and the first half of 2022 (see below) and the measurements have been presented by the collaboration in May 2022 at the workshop "The 1st Mondragone Frontiers of Astronomy Workshop" (https://astrodragon.web.roma2.infn.it/).

About a year later (fall-winter 2022) we had a second run scheduled at Elettra, but we had to postpone it because of unavailability of the EBIT machine. This second run, was initially scheduled for the first semester of 2023, but it has already been canceled because of the global energy-crisis, which imposes the shut-down of the Elettra facility for all the first semester of 2023. It has now been rescheduled to the fall 2023. Very recently, however, we managed to successfully hire a PhD student (fall 2022) and decided to go back to our original program and use the last months of 2022 and the upcoming period without beam of 2023 to measure energies and cross sections of high mass/charge ions of oxygen, iron and (possibly) nitrogen. This requires an accurate set-up and testing of an octupole-quadrupole mass spectrometer (octomass) at Elettra. A first setting has already been performed in October 2022 and tests have been run to measure mass spectra of Ar+,++,+++ and Kr+,++ (see below).

Min-EBIT First-Light at Elettra

In 2021 we proposed for and were awarded a long-program to use Electra synchrotron light with a mini-EBIT made available to us from the MPI-K (Heidelberg) side of the collaborations. The first two weeks of the program were dedicated to the transportation of the EBIT from the MPI-K to Elettra (Trieste, Italy; Fig. 1), its installation on the Gas-Phase line at Elettra and its first light. The mini-EBIT was installed in the GasPhase line at Elettra on 18 November (Fig. 2, left). After performing a standard energy calibration of the beam-line in the region of K-edges, the initial part of the beamtime was devoted to alignment of the EBIT with the synchrotron beam. A preliminary test was then run on 6-time ionized ions of oxygen on 1 December 2021 (Fig. 3). We observed the fluorescence of He-like oxygen ions after initial photoexcitation to verify the successful overlap of the photon beam with the highly charged ions produced by and stored in the EBIT (Fig. 2, right, top panel). We optimized in several shifts the spectral line shape of the signal (Fig. 2, right, bottom panel).

Figure 2 The mini-EBIT in the VAN at the MPI-K in Heidelberg (Germany), ready to be transferred to the Elettra synchrotron facility at Basovizza (Trieste, Italy).

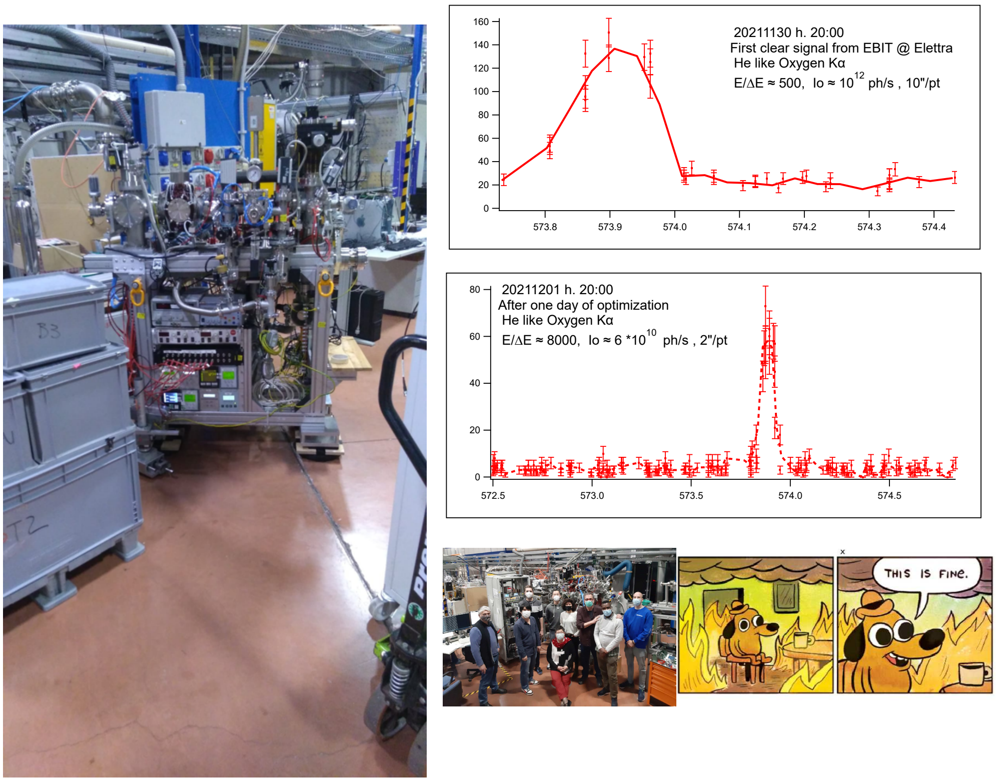


Figure 3Left: the EBIT installed at the GasPhase at Elettra. Right: First clear signal of the EBIT at Elettra, showing the resonant $K\alpha$ transition from He-like ions of oxygen. The top panel shows the first-light, at low-resolution (R=E/ΔE=500), while the bottom panel show the same line after one day of optimization: the resolving power is now R=8000.

The Kα, inner-shell, transition from 4-time ionized oxygen

The second two weeks of the beamtime program, in February 2022, were dedicated to the investigation of the, astrophysically relevant, Kα transition of Be-like oxygen at 553 eV. We precisely determined its energy by successively exciting neighboring lines of He-like nitrogen, which are theoretically well known and therefore suitable for calibration, and explored isotopic shifts. More precisely, we measured the transition energy of the "$1s^22s^2 \rightarrow 1s2s^22p_{3/2}$" Kα transition of Be-like O. The ions were produced and trapped in an electron beam ion trap and excited with synchrotron radiation from the Elettra synchrotron. With the EBIT, both radiative decay channels and autoionizing decay channels can be measured in parallel. The charge state distribution is determined via a time-of-flight measurement, so that ions with different charges and masses can be resolved separately. This makes it possible to search for the O_{16}/O_{18} isotope shift. We did this by using two methods. Method-1 used the histograms from all measured resonance energy values of O_{16} and O_{18} (left and middle panel of Fig. 3). The centroid of the normal distribution was obtained by a least square fit of a gaussian profile, which yielded: $E(0_{16})$= 553.4677(13) eV and $E(0_{18})$ = 553.4705(12) eV, respectively. By then subtracting the two centroid values an isotope shift of ΔE_{Shift} = 3.9 ± 1.8 meV (EO18 − EO16) is obtained. Method-2 used the histogram produced from all energy difference values of O_{16} and O_{18} (right panel of Fig. 3). The centroid of the normal distribution is again obtained by a least square fit of a gaussian profile. This yielded ΔE_{Shift} = 2.6 ± 1.8 meV.

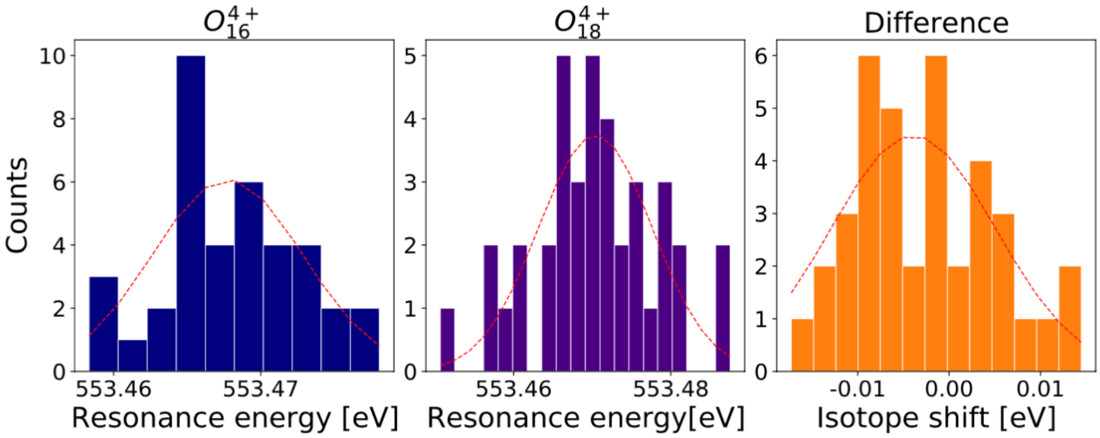


Figure 4 O16/O18 isotopic shift for the OVI K transition. See text for details.

The first two runs at Elettra and their main scientific results are summarized in a bachelor thesis in Physics by J.W. Danisch, at the department of Physics and Astronomy of the University of Heidelberg (Germany), were first presented at the international conference "The 1st Mondragone Frontiers of Astronomy Workshop" by our PhD student A. Mohammed, and are currently being drafted in a paper, which will be submitted soon to the ApJ.

Hiring of a PhD student and testing of the octupole-quadrupole mass spectrometer at Elettra

In fall-winter 2022 we had a second run scheduled at Elettra, but we had to postpone initially to the end of the first semester of 2023 (because of unavailability of the EBIT machine) and then to the fall of 2023 because of the global energy-crisis that imposes the shut-down of the Elettra facility for all the first semester of 2023. Because of these unforeseen and forced delays, and thanks to our recent successful hiring of the PhD student A. Mohammed (fall 2022), we decided to use the second half of 2022 (and, in the near future, the upcoming period without beam of 2023) to measure energies and cross sections of high mass/charge ions of oxygen, iron and (possibly) nitrogen. This requires an accurate set-up and testing of an octupole-quadrupole mass spectrometer (octomass) at Elettra. A first setting has already been performed in October 2022 and tests have been run to measure mass spectra of Ar+,++,+++ and Kr+,++. In the following we describe these first tests and measurements.

The Ar-Kr Experiment at Elettra

The experiment performed at Elettra, at the CiPo beamline, used the set-up shown in fig.4 with the radiation produced from electromagnetic elliptical wiggler (EEW).

In this experiment we used grazing incidence monochromator (SGM) of the beam line, gratings G3 and G4 which cover the photon energy 30-100 eV.
The atomic gas sample was inserted through a needle valve with pressure up to 1.1x10^{-5} mbar with base pressure of 2.7x10^{-7} mbar. The photons ionized the target atoms, then the produced ions were guided through electrostatic lenses to the octupole.
The absorption of the photons by the atomic gas samples (Ar and Kr) produces significant ionic fragmentation; then, the quadrupole can filter the produced ions and select the m/z of our interest as a function of the photon energy.

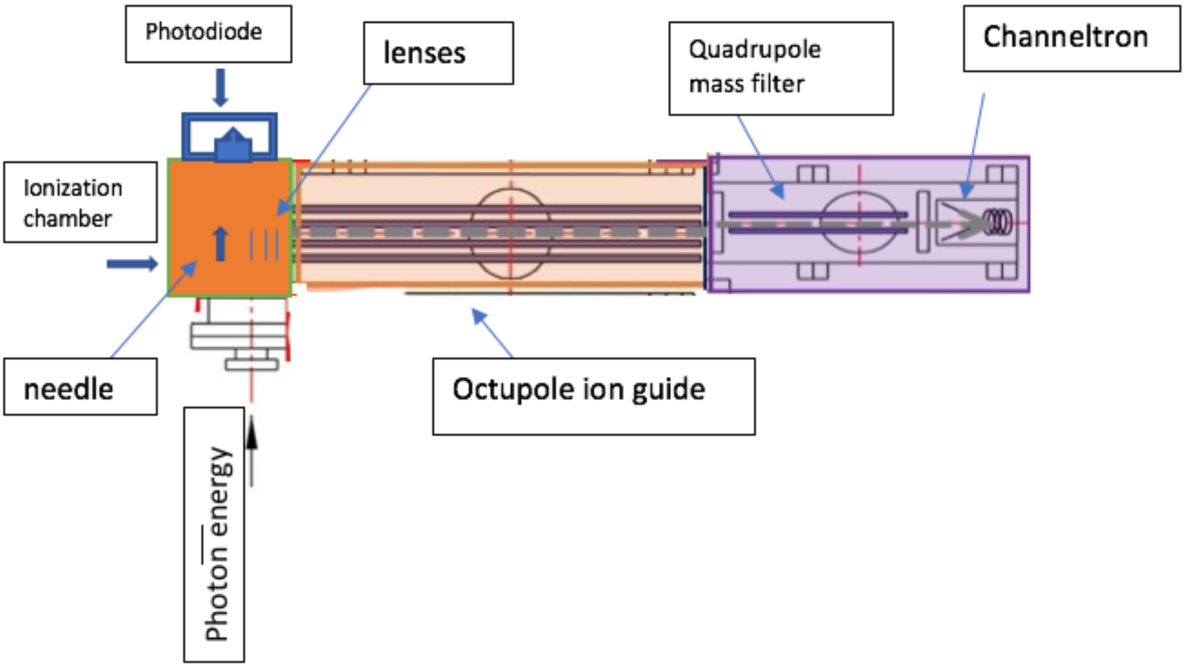


Fig 4 Shows the set-up has been used for the Ar-Kr experiment. The size of the octupole is of the length 40 cm and 1 cm in diameter. The ions guided to a quadrupole mass filter (10-4000 amu). The octupole is operating as an ion guide with a RF at 6 MHz and 175 V peak-to-peak amplitude.

Results and discussion

Fig. 5 shows a mass spectrum of Ar at two different energies in the mass range (8 - 45) amu. The spectrum at hν = 50 eV shows that the main contribution comes from the ion yield of Ar^+ (with observation of Ar^{2+} and Ar^{3+}) ions produced by multiple photoionization. At hν = 266 eV the main contribution comes from of Ar^{2+} , with observation of Ar^+ and Ar^{3+} ions.

Fig. 6 shows the ion yield spectra of Ar^+, Ar^{2+}, and Ar^{3+}, which are recorded by fixing the masses at 39.7 amu, 19.7 amu, and 12.8 amu respectively, and scanning the photon energy in the range (243 - 255) eV , with a 50 meV energy step.

Fig. 5 Mass spectrum obtained at hv=50 eV which contain main contribution of Ar^+ and hv=266 eV with main contribution of Ar^{2+}.

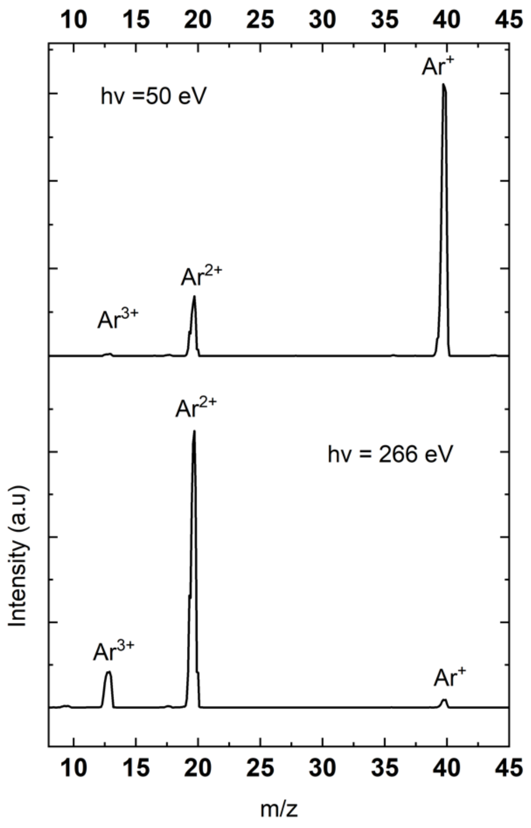
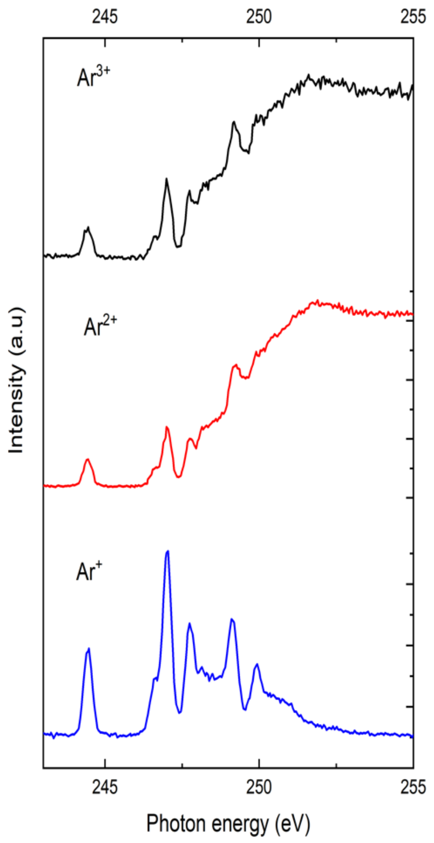


Fig. 6 Ion yield spectrum of Ar^+, Ar^{2+}, and Ar^{3+}.



In fig.7 we show the scanning of the photon energy within a smaller range (243.5 – 247.5) eV but with higher resolution to better resolve the spectra and clearly see that the second band consists of two separate lines.

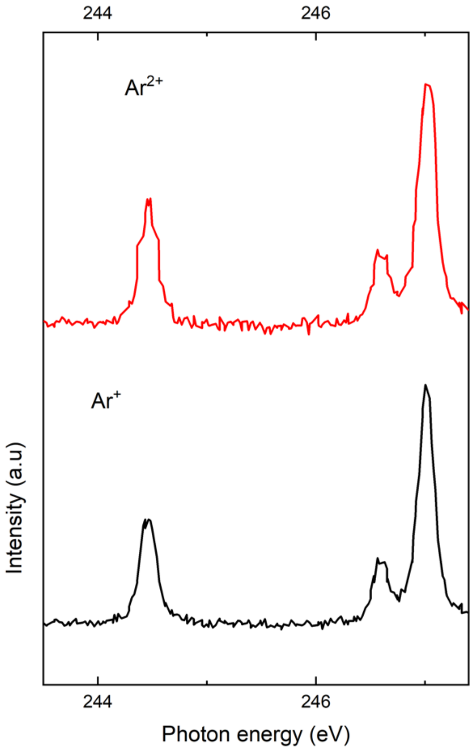


Figure 7 High resolution spectra of Ar^{+} and Ar^{2+} ion yield

In Fig. 8 we show the mass spectrum of Kr excited at the photon energy of hv = 88.35 eV and we can appreciate that Kr^{2+} is 10 times more intense than Kr^{+}.

Finally, Fig. 9 shows the atomic Kr 3d XAS spectra based on Kr^{+} and Kr^{2+} ion yields.

The tests performed on Ar and Kr ions, served as preparatory tests and feasibility studies for the more astrophysically motivated experiments on lower mass/charge ions of O, Fe and possibly N. These experiments will be set up during the first semester of 2023, and performed with synchrotron light during the second half of 2023.

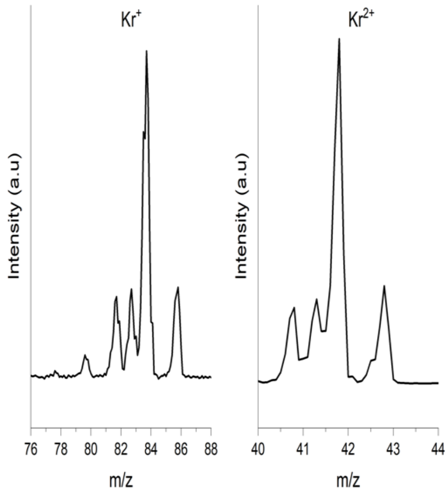


Fig. 8 Mass spectrum of Kr ion yield at hv = 88.35 eV with main contribution of Kr^{+} in mass range (76 - 88) amu and Kr^{2+} in mass range (40 -44) amu

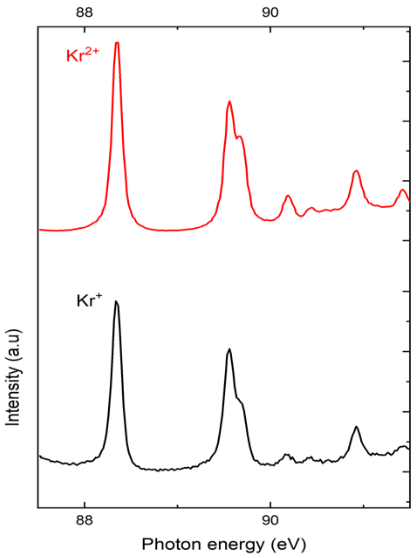


Fig. 9 Kr atom spectra measured by Kr^{+} and Kr^{2+} ion yield

WP13.1C Experimental CX activities

Task leaders: François Pajot, IRAP/CNRS and José Crespo López-Urrutia, MPIK

Motivation

Charge Exchange (CX) is a process that describes a close interaction between a highly charged ion and a neutral atom or molecule; the ion captures one or more electrons from the neutral into an excited state and subsequently radiatively de-excites, thus emitting line emission, often in the X-ray energy band. X-rays emitted from CX have been observed frequently in the solar system, for example from comets, the Earth's exosphere, and Jupiter, and has been suggested to occur in, for example, supernova remnants, galaxy clusters, and galactic winds. Future high-resolution observations of CX from objects such as these with the *Athena* X-IFU will provide a new window into learning about the properties of the emitting sources. However, many discrepancies still exist between theoretical models of CX and experimental benchmarks

One challenge of accurately benchmarking CX theory with experiments is utilizing atomic hydrogen as the neutral partner. Atomic H is the most abundant species in space, and is the default neutral partner in most theoretical CX models. However, atomic H is not easy to produce and maintain in the laboratory; it quickly recombines to produce molecular hydrogen (H_2), which has different properties that influence the CX interaction and resulting X-ray spectrum.

In order to overcome this challenge, collaborators at MPIK and IRAP have designed an experiment to more efficiently produce and maintain atomic H for long enough for the atoms to undergo CX with a beam of highly charged ions produced from an Electron Beam Ion Trap (EBIT).

Planned to be measured with high-resolution microcalorimeter detectors which are current-generation versions of what will fly on *Athena*, measurements will first rely on standard CCD X-ray detectors in order to validate the experimental setup and get preliminary results on CX. In the long term we will obtain high-resolution experimental spectra of astrophysical CX to benchmark the most recent models and improve them in advance of the launch of *Athena*.

Overall Progress

The conjunction of the departure of the task leader and of the sanitary crisis did not allow the hiring of a skilled student to carry on the measurements campaign as planned. The last MS in this task "*CX measurement campaign and preliminary data analysis completed*" is yet to be done. As reported in the First update report, the H source is ready for use, first using conventional detectors for the validation of the complete EBIT and H source setup and the determination of the first CX data, then using high-resolution spectrometers.

Way forward

Hiring a student is now the top priority for the continuation of the activities. This will likely have an impact of about one year on this task, which is not seen as critical : the overall duration of the AHEAD program will give enough time to achieve the preliminary measurements as planned in the last MS. Target date for this MS is now postponed to 01/12/2023.