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First update report

Laboratory Astrophysics: Athena Spectral Features

Project acronym:
AHEAD2020

Project Title:
Integrated Activities for the High Energy Astrophysics Domain

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Foreword

This first update report covers activities of WP13 Laboratory Astrophysics Task 13.1 Athena spectral features up to November 30th 2021. Initially planned for March 1st, it was delayed by 9 months due to the pandemic situation.

After leaving the project on October 21st 2021, Gabriele Betancourt-Martinez (IRAP) WP13 leadership was transferred to François Pajot (IRAP)

WP13.1A Collisional excitation rates

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

Results

The Hitomi results on the Perseus cluster led to improvements in the atomic data, including both wavelengths and collisional excitation rates, for precise diagnostics of the 4 keV collisional plasma. However, model uncertainties remain, both within but especially beyond the Hitomi's spectral window. For the time being, a major challenge is to model the L-shell lines, which is an assembly of principle quantum number n=3 to n=2 transitions with Na-like to Li-like ions, affected by direct collisional excitation but also by secondary processes, including resonant excitation, dielectronic recombination, radiative recombination, and innershell ionization. These processes was not fully modeled in the SPEX code before the AHEAD work. To prepare the SPEX code for the coming X-ray missions (XRISM 2023 and Athena 2030s), we urgently need to improve the atomic data of the L-shell excitation especially on the secondary processes mentioned above, for the relevant cosmic abundant elements (Mg, Si, S, Ar, Ca, Cr, Mn, Fe, and Ni).

A large-scale theoretical calculation was carried out for Fe on collisional processes in particular for excitation through resonances and dielectronic recombination. We ran the FAC code (Gu, M. F. 2008, Canadian Journal of Physics, 86, 675) taking into account the relativistic electron interaction and full configuration mixing for singly and doubly excited states with n up to 15. Based on the complete atomic structure, we calculated the individual cross sections through each possible resonant channel, and formulated the total rates taking into account all primary and secondary processes, as well as the necessary corrections such as the radiative branching ratios. A comparison of these rates with the recent results obtained with a different theoretical code (R-matrix) showed that two calculations agree within 20% while our new data cover more levels than R-matrix. We implemented the new Fe calculation in SPEX version 3.06.

We have then applied the same recipe to the calculation of Mg, Si, S, Ar, Ca, Cr, Mn, and Ni L-shell excitations. The atomic structures, excitation cross sections, and transition matrices are all available, and we are now working on the rates. We expect to incorporate these new atomic data in the next SPEX version hopefully early next year, after they are fully tested and validated. This will fulfill all the milestones in the AHEAD proposal.

The quality of the theoretical calculation can only be assessed by comparison with laboratory benchmark measurements and real observation data. In Gu et al. (2020), we tested our Fe L-shell

calculation using a new measurement at Max-Planck Institute for Nuclear Physics at Heidelberg with the Electron Beam Ion Trap (EBIT) device. The excitation rates are calibrated with the measurement values, and further verified using the Chandra grating spectrum of the quiescent corona of Capella. In a later paper (Gu et al. Submitted), we evaluated the systematic uncertainties of the Fe-L modeling and atomic data based on a quantitative comparison with the Capella spectrum.

List of publications

Gu, L., Shah, C., Mao, J. et al. 2020, A&A, 641, 93
Gu, L., Shah, C., Mao, J. et al. Submitted to A&A

WP13.1B Spectral features, inner-shell measurements

Task leader: Fabrizio Nicastro, INAF

Wavelengths and cross-sections of inner-shell transitions of elements from C to Ni are generally poorly known and mostly based on theoretical computations. Laboratory measurements have only become available recently, and only for the lightest of these elements at energies <0.8 keV (e.g. McLaughlin et al. 2017, MNRAS, 465, 4690 Within AHEAD2020 our main task is the build a new experimental setup will perform new measurements at the Gas Phase beamline of the Elettra Synchrotron Laboratory with the twofold aim: develop a prototype set-up for a dedicated end-station for laboratory astrophysics for the upgrade of the Gas Phase beamline, which has been funded within the Elettra 2.0 project (i.e. the general upgrade of the Elettra synchrotron radiation ring expected after 2025); and improve accuracy and complete existing data-sets in this photon energy range.

Our initial strategy foresaw modification and optimization of an existing OCTOMASS ion trap owned by the CNR-ISM. This instrument would have allowed us to produce and store atomic ions with a charge of +1 to +3 (possibly +4), in order to analyze them with synchrotron radiation between 100 and 900 eV. The modification of this instrument could be accomplished by the local CNR staff of the GasPhase beamline at Elettra, in collaboration with the CNR-ISM personnel of the ISM headquarters in Rome that developed the OCTOMASS, and that regularly comes to Elettra for experiments, with the assistance of a senior technician specialized in ultra-high vacuum and precision mechanics to be hired.

Unfortunately, it has been immediately clear that the outbreak of the pandemic would make it impossible to follow such an initial plan. In the months from March to May 2020, CNR personnel not involved in COVID or essential research activities were put to work from home, whereas the almost normal experimental activity resumed only after October 2020.

But the interruption of the experimental activities prompted us to look for an alternative. To this purpose INAF and CNR have formed a new collaboration to undertake the experimental project with José Crespo López-Urrutia, and his group at MPIK (Heidelberg, D), who are already involved in a different task of WP13.

The plan was to move a mini-EBIT, currently in Heidelberg, to Elettra, Trieste, to have highly charged ions (HCI) as a calibration source with which to measure absolute energies, cross-sections and widths of inner-shell resonant and metastable transitions of all ions of carbon, nitrogen, oxygen and neon.

In addition to having already demonstrated its versatility, EBIT by working both on synchrotron light lines of energy comparable to that available at Elettra (at Bessy II) and on X-ray lines (at Petra III) will allow us to broaden the study to atomic species ionized up to the hydrogen-like state. So, despite a considerable delay on the roadmap, the use of a mini-EBIT in place of the originally planned OCTOMASS will significantly improve the project.

Another planned activity for the first semester of the AHEAD2020 project was the recruitment of a Ph.D. to be trained in Laboratory Astrophysics with synchrotron radiation. Due to the pandemic, this step encountered major problems, too. A PhD candidate from University of Khartoum (Sudan), Ms. Amel Al

Alhalassan was in fact selected among the most promising post-graduate students performing training at Elettra within the educational programs of the International Centre for Theorethical Physics (ICTP, Trieste). She could qualify for a PhD in Laboratory Astrophysics, co-funded by ISM-CNR at University of Camerino; but unfortunately, the enrollment in Camerino could not be finalized before the start of the academic year. Nonetheless in July 2021 a new post-graduate student joined our group at Elettra, Mr. Awad Mohamed from University of Khartoum, after a successful application to the Training in Italian Laboratories (TRIL) of ICTP, with a specific training program in Laboratory Astrophysics. After his TRIL program, the student is expected to qualify for a PhD in the academic year 2022-2023.

In the first semester of the AHEAD2020 project (March – September 2020) , our team (MPIK, CNR, INAF) discussed and prepared a Long Term Project (LTP) on spectroscopy of highly charged ions (HCI) with synchrotron radiation. The proposal contains a detailed schedule for installation of the EBIT set-up at Elettra, measurements and analysis of spectroscopic results from HCI In order to improve signal and detection sensitivity. The LTP was submitted in September 2020 to the Elettra review panel; it was later approved (Dec 2020) for 4 semesters of beamtime at the Gas Phase beamline (2021-2022).

The EBIT should have received first light in June 2021, after its transfer from Heidelberg to Elettra; but again our experimental plan experienced significant delays due to Covid-19 and travel restrictions. Thus, the start of the measurements had to be postponed to the beginning of December 2021. This prevented the implementation of the preliminary measures envisaged by the project.

Training of CNR personnel with the EBIT is foreseen in Germany, and it is actually being carried (September-November 2021). The EBIT set-up has been transferred to Elettra in November 2021 (Figure B1 and B2). CNR staff at Elettra has meanwhile started an instrumentation upgrade to adapt the high vacuum environment of the beamline to the UHV conditions necessary to run experiments with highly charged ions with the EBIT, as well as adaptation of laboratory space to host the set-up from Heidelberg.

First light at Elettra is foreseen at the beginning of December and experiments will be run immediately after in the first semester 2022, too. We plan to start our experimental measures of energies and cross-sections of inner- and outer-shell transitions (including metastable transitions), on the ions of nitrogen and oxygen. Depending on the results of the first two semesters of operation at Elettra, we will discuss specific and detailed experimental plans for the 3rd and 4th semesters of LTP, to be performed in winter 2022-2023.

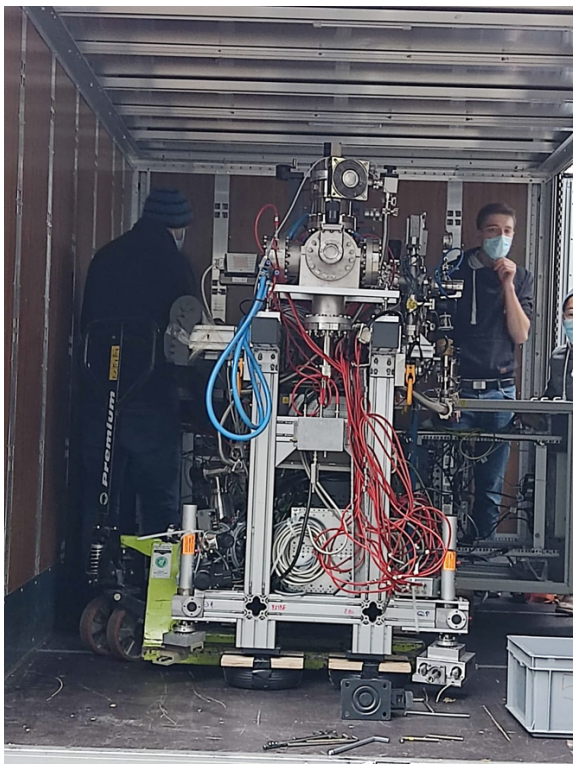

Figure B1: The mini-EBIT Leaving the Max-Plank-Institute for Nuclear Physics (Heidelberg) to the GasPhase @ Elettra (Bassovizza, Trieste). The Italian-German WP13 Collaboration:

Max-Plank-Heidelberg (Crespo J. et al.)
CNR-IOM, ELETTRA (Coreno, De Simone et al.)
INAF-OAR (Nicastro et al.)
INAF-OATs (Fiore et al.)

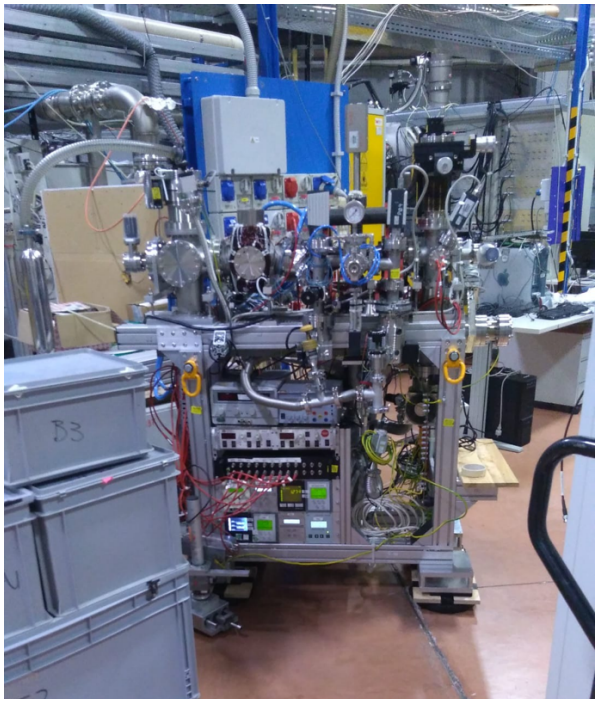

Figure B2: The mini-EBIT on the "line" @ Elettra (Trieste). First vacuum-test after moving and pre-alignment in line. First light expected November 30th 2021.

WP13.1C Experimental CX activities

Task leaders: Gabriele Betancourt-Martinez, 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 (e.g. Beiersdorfer et al. 2000; Betancourt-Martinez et al. 2014; Leutenegger et al. 2010; Otranto et al. 2007)

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 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). This will be measured with high-resolution microcalorimeter detectors which are current-generation versions of what will fly on *Athena*. We will thus have 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 milestones for this reporting period include:

MS 51: Preliminary version of atomic H source complete
MS 54: Construction and characterization of atomic H source complete.

Overall progress towards our milestones and deliverables is on track, taking into account the delays induced by COVID-related machine shop closures and facility access restrictions. However, there was one major deviation from our proposal due to mission-level changes in the *Athena* baseline. Because of the change of the *Athena* detector readout system from Frequency-Domain Multiplexing to Time-Domain Multiplexing, the hardware installation for the IRAP test bench, including the high-resolution microcalorimeter spectrometer that was to be used for the final CX experiments for this project, is severely delayed. Experiments using this detector are no longer feasible with the AHEAD2020 project funding timeline. We are thus falling back onto our contingency plan of using a solid-state detector, already located at MPIK, to measure the spectra during the final experiments. This will lead to lower resolution spectra, but the resolution should still be high enough to distinguish spectral features that result from CX with H compared to H_2. We will thus still provide much-needed experimental

benchmarks, while also completing a feasibility study for the H source so that it is ready for use with high resolution spectrometers in the future.

Technical Progress and Results

Following a literature study, a rough concept was generated for a compact atomic-hydrogen source and a charge exchange cell, in which a beam of highly charged ions from an EBIT can interact with hydrogen atoms from the source. Next, specifications and a detailed design of all elements was produced, and the final design was transferred to the manufacturing mechanical workshop for production for the parts. An ion-transfer beamline was also designed based on a combination of existing elements, and its feasibility was assessed. Figure C1 shows a schematic of the total assembly.

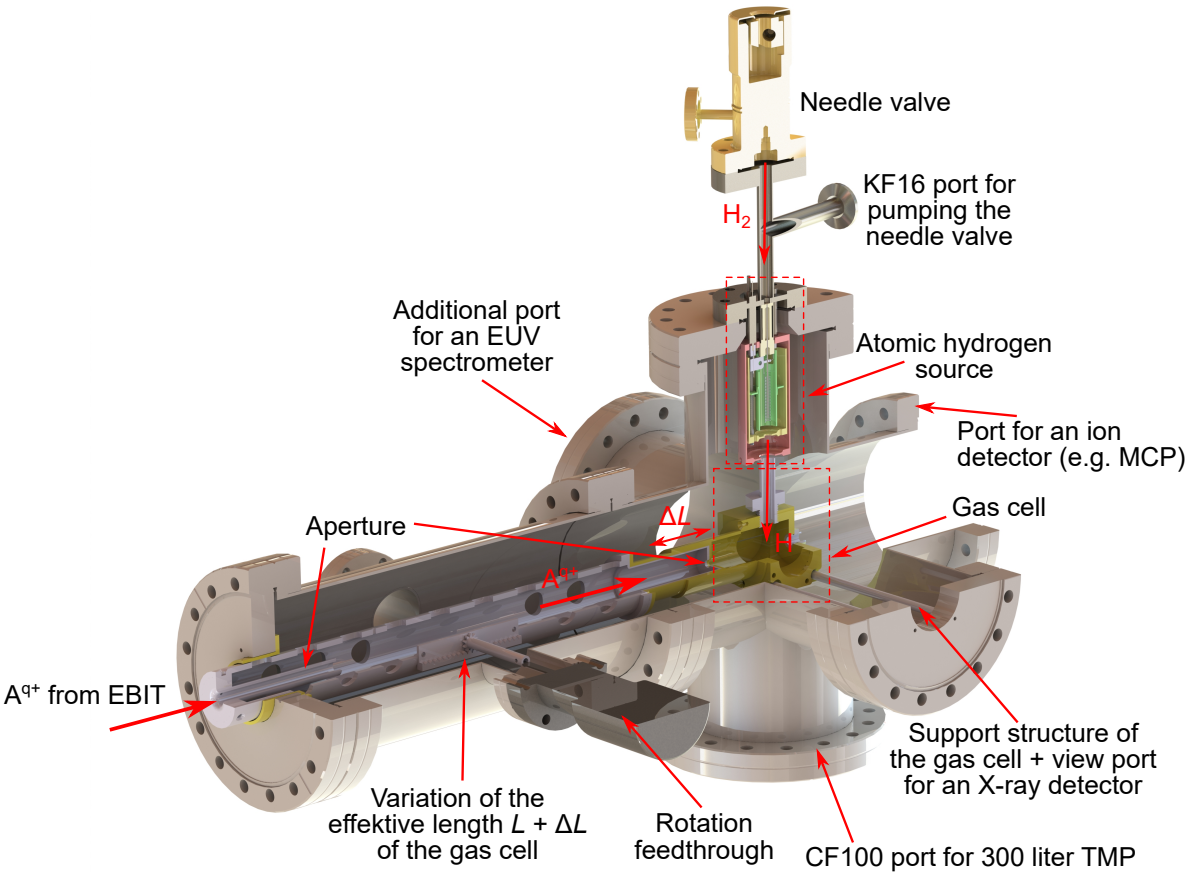

Figure C2: A schematic of the experimental setup including the atomic hydrogen source, gas cell, and the vacuum feedthroughs connecting the H source and gas cell to the EBIT ion beam and ports for X-ray spectrometers.

The main components of the H source include a Tungsten capillary which is heated to >2000 K by radiative heating and electron bombardment from a Tungsten filament. A controlled amount of molecular H_2 is passed through this hot capillary. The H_2 is thermally cracked apart into atomic H atoms. The dissociation fraction of H_2 to H is a function of the capillary temperature and the pressure in the capillary (Leutenegger et al. 2016). The H capillary and filament are surrounded by several Tantalum heat shields to protect the rest of the vacuum setup from the high temperatures. Figure C2 shows a schematic of the H source.

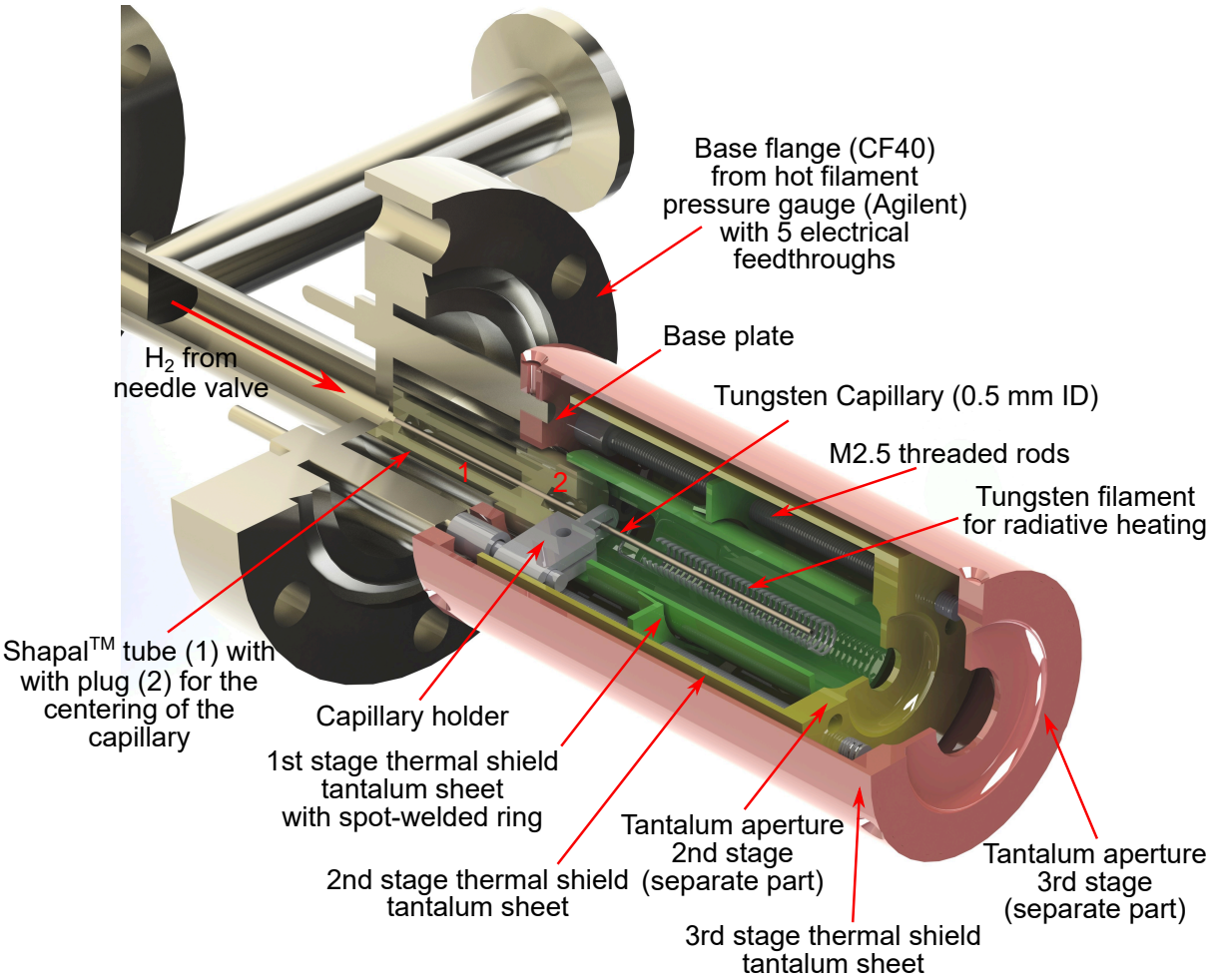

Figure C3: A schematic of the atomic H source, including a feedthrough for the molecular H_2 supply, a capillary, a Tungsten filament to heat the capillary, and several heat shields.

One of the challenges of designing an H source CX setup is making the path between the creation of the H atoms to the CX interaction region as short and collisionless as possible, in order to prevent the H from recombining into H_2. However, the length must not be so short that heat is easily conducted into the interaction region. In order to minimize recombinations on the walls of the gas cell, it was made with Teflon. Figure C3 depicts a schematic of this design and Figure C4 shows the gas cell parts (as well as some of the thermal shields) after machining.

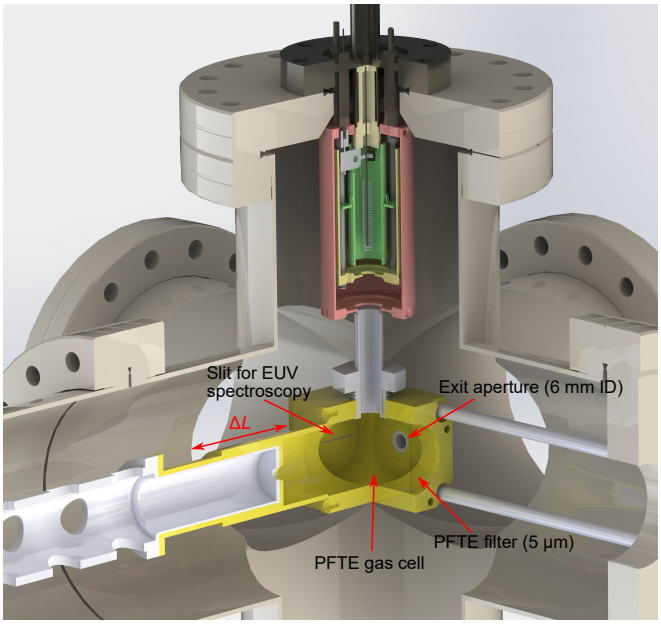

Figure C4: The gas cell, or CX interaction region.

Figure C5: H source parts after machining.

The H source and gas cell are mounted at the end of a beam line, shown in Figure C5. Highly charged ions generated in the EBIT are passed through a Wein filter and are led into the gas cell. Here, these ions interact with the H/H_2 mix generated by the H source and undergo CX. The resulting X-rays are measured by X-ray and/or EUV spectrometers that are mounted onto the beamline.

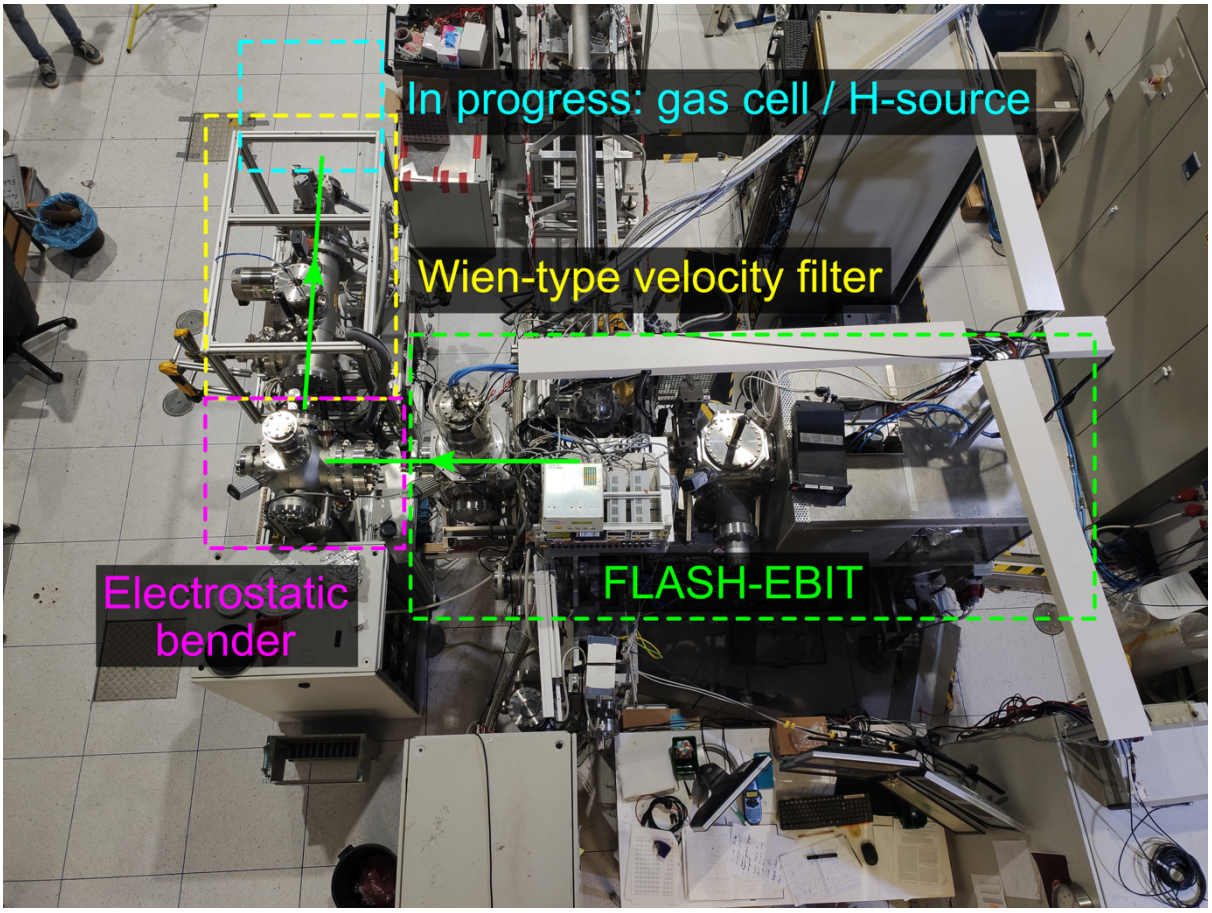

Figure C6: H source beamline. The H source is mounted at the end of the line, after the Wien filter.

After initial design, machining of parts, and setup, we had thus completed Milestone 51 and began characterizing the H source. In order to do this, we first used a pyrometer to estimate the temperature of the capillary. We calibrated the temperature measurements to a standard halogen bulb. Figures C6 and C7 show the pyrometer setup and the view into the H source chamber with the hot filament. We used the temperature measurements to determine the emission current necessary to reach our desired dissociation fraction.

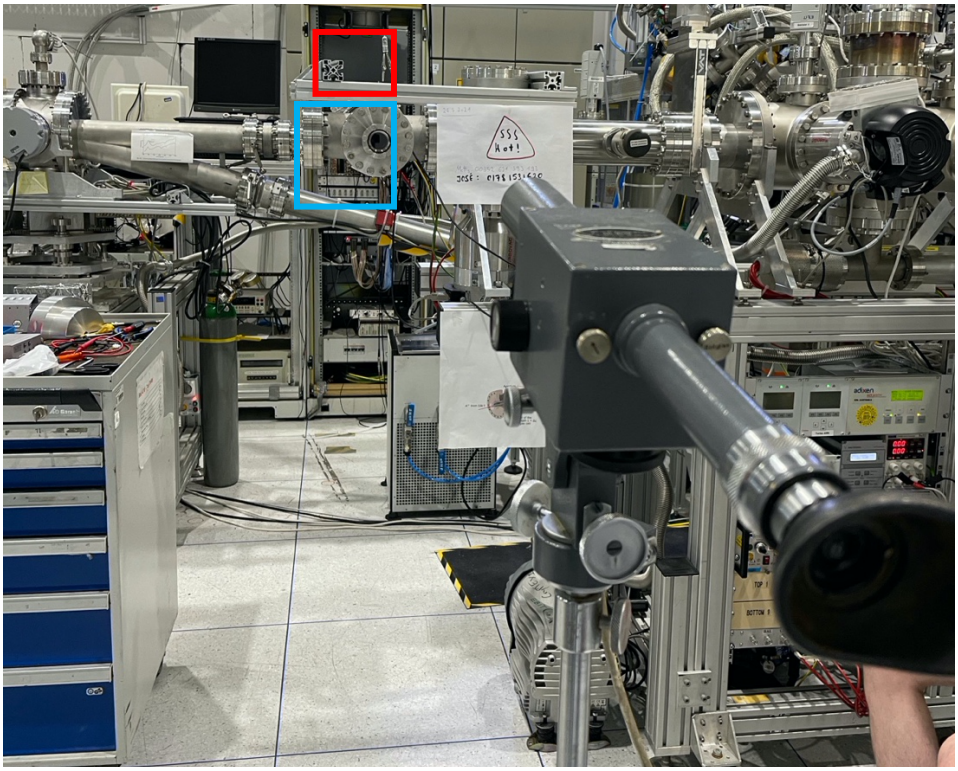

Figure C7: The pyrometer set up to observe the H source chamber (blue box) and a halogen bulb for calibration (red box).

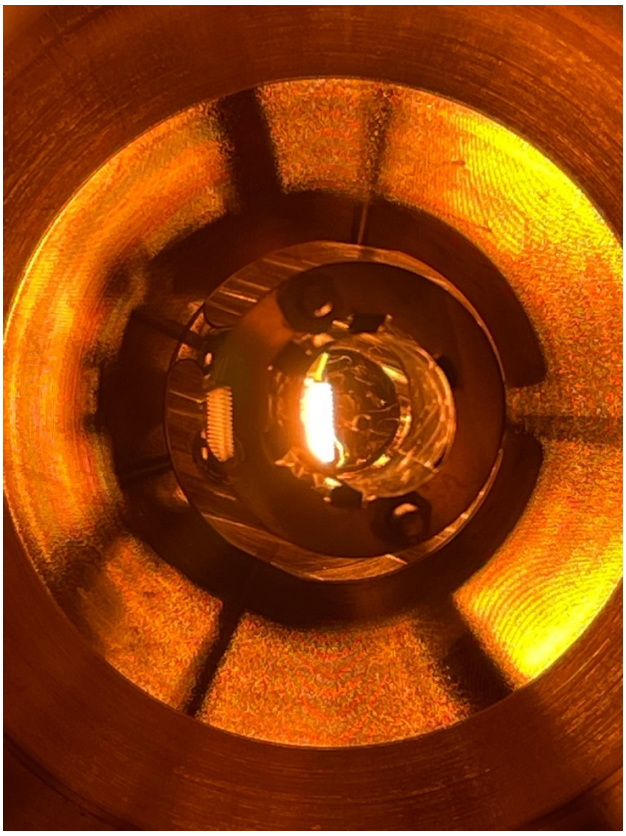

Figure C8: The inside of the H source chamber, showing the glowing Tungsten filament.

Next, we mounted a LEYSPEC residual gas analyzer (View 200s) onto the source chamber to determine the cracking fraction of our source as a function of capillary emission current (thus temperature). Figure C8 shows this setup.

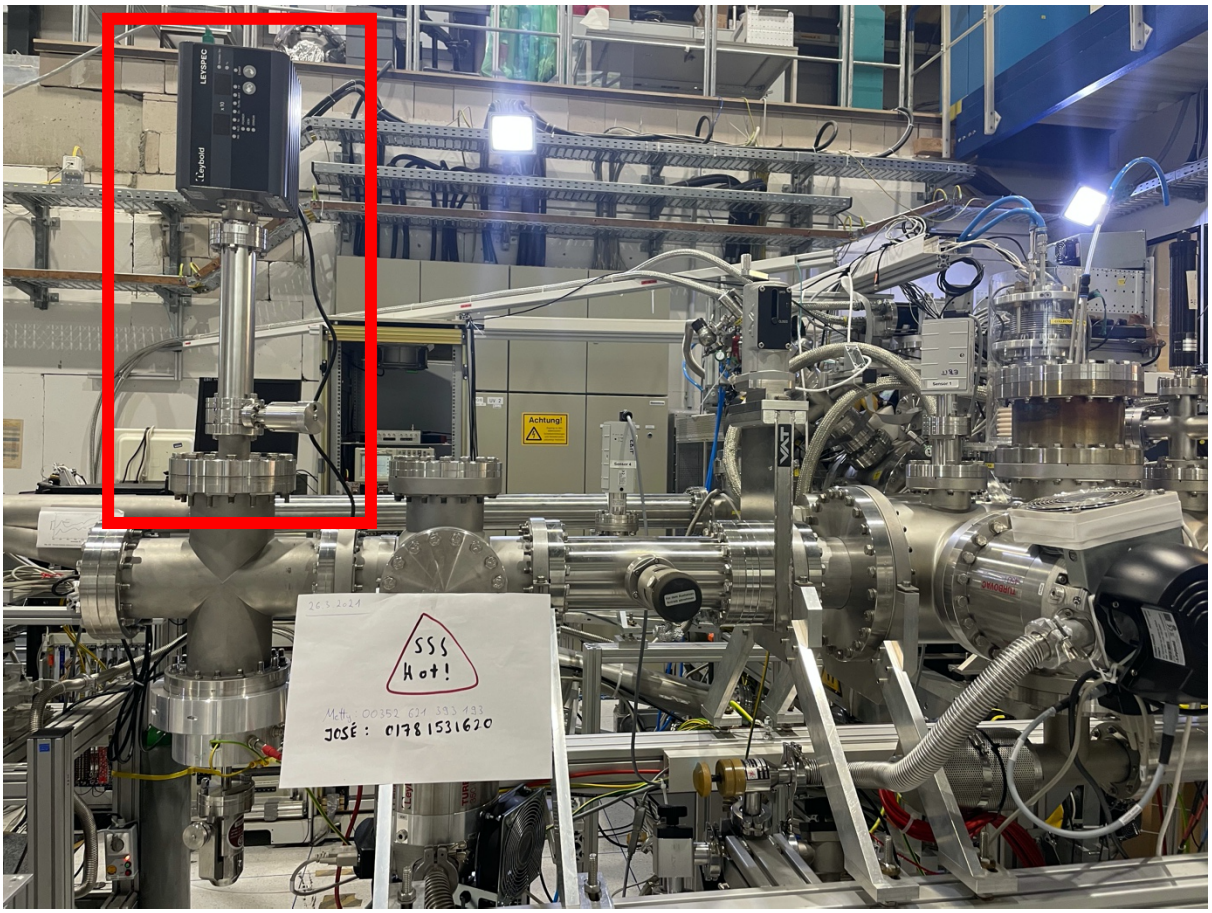

Figure 9: Residual gas analyzer (top left, red box) mounted onto H source chamber (rotated with respect to Figure 6) with a shutter to block the ballistic flow of gas.

Although we baked out the new components to remove contaminants and had good vacuum before beginning tests with the gas analyzer, we did not get clear results. There was no way to disentangle the amount of H and H_2 as a function of chamber pressure or emission current on the filament. It is possible that the gas analyzer was situated too far away from the H source, and any atomic H produced recombined on the chamber or gas analyzer walls. We will, however, close Milestone 54 because we have indeed performed characterization tests on the setup, unfortunately with inconclusive results. This is reminiscent of the results obtained by Leutenegger et al. (2016) showing that full characterization of the H source with a similar setup is complex due to the unstable nature of atomic H.

While modifications to the H source characterization setup will continue in the coming months, the most accurate way of determining the cracking fraction of our H source may be through spectroscopic

analysis of CX experiments. Leutenegger et al. (2016) showed that specific differences in spectral line ratios arising from CX with H_2 versus H. We thus expect to have complementary characterization measurements to the ones described here once CX experiments begin.

References

1. P. Beiersdorfer, R. E. Olson, G. V. Brown, H. Chen, C. L. Harris, P. A. Neill, L. Schweikhard, S. B. Utter, and K. Widmann, Phys. Rev. Lett. **85**, 5090 (2000).
2. G. L. Betancourt-Martinez, P. Beiersdorfer, G. V. Brown, R. L. Kelley, C. A. Kilbourne, D. Koutroumpa, M. A. Leutenegger, and F. S. Porter, Phys. Rev. A **90**, 052723 (2014)
3. M. A. Leutenegger, P. Beiersdorfer, G. V. Brown, R. L. Kelley, C. A. Kilbourne, and F. S. Porter, Phys. Rev. Lett. **105**, 063201 (2010).
4. M. A. Leutenegger, P. Beiersdorfer, G. L. Betancourt-Martinez, G. V. Brown, N. Hell, R. L. Kelley, C. A. Kilbourne, E. W. Magee, and F. S. Porter, Rev. Sci. Inst. **87**, 11E516 (2016)
5. S. Otranto, R. E. Olson, and P. Beiersdorfer, J. Phys.: Conf. Ser. **58**, 165 (2007).