# *From Molecular to Highly-Charged Ions: Expansion of Laboratory Astrophysics Through Use of the Electrostatic Storage Ring and Electron Beam Ion Trap*

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## ABSTRACT

Described herein is the use of an electrostatic storage ring (ESR) coupled to a variety of ion sources to generate and store positive and negative molecular ions, as well as highly-charged positive ions. Studies of collision phenomena within each class of ion targets provide information on plasma properties of astrophysical objects. These objects range from cool molecular clouds – detected through their infrared absorption and emission spectra – to stellar mass ejections and quasars with highly-charged ion (HCI) emissions – detected by their X-ray emission spectra. A summary is given of the capabilities attained by combining an ESR with molecular-ion sources, or an electron beam ion trap for HCIs. This work anticipates the continued rich return of space observations from, for example, Spitzer, SOFIA, Herschel, and ALMA in the infrared region; to SOHO, Chandra, XMM-Newton, Constellation X and NEXT in the EUV and X-ray regions. The ESR would enable one to make measurements of phenomena such as (for molecular systems) direct and dissociative ionization, direct and dissociative recombination, and lifetimes of negative ions. For HCIs, one may study direct and indirect ionization, direct and dielectronic recombination, excitation, and lifetimes of levels in the $10^{-9}$ to $10^{-3}$ second range. Since the ESR is completely electrostatic, its trapping depends only on the target energy, and hence a broad range of masses (diatomic molecules to DNA!) can be trapped. Because there is no magnetic field, Zeeman mixing of excited levels is obviated and since the ions circulate for ≈10-100 seconds, the targets will be in their ground vibrational-electronic state. There are three ESRs in the world: two in Japan, and the original ring at the University of Aarhus, Denmark. The system described herein would be the first ESR in the United States. It would both sharpen and continue the JPL focus on understanding astrophysical processes in the laboratory. The research team represents renowned colleagues in experimental molecular chemistry, theoretical and computational quantum chemistry, charged-particle optics design, ion traps, and ultrahigh vacuum; together with ESR experts at the DESIREE ring in Stockholm (Schmidt *et al*. 2008).

## INTRODUCTION

The astounding advances in astrophysics through ground-based spectrometer observations, and through NASA's and ESA's flight spectrometers, have extended our view of the Universe from the far infrared to the X-ray region of the electromagnetic spectrum. Rich molecular absorption and emission spectra are observed by the National Radio Astronomy Observatory, ISO, NICMOS, and Spitzer; with measurements to be expanded by the upcoming SOFIA and Herschel missions. Spectra of highly-charged ions (HCIs) are observed in our Sun, stars, and quasars by EUVE, Lyman/FUSE, Suzaku, SOHO, Chandra, and XMM-Newton; and measurements are to be expanded by the upcoming Constellation X and NEXT missions. Examples of molecular infrared spectra observed by Spitzer are shown in Fig. 1 (Noriega-Crespo et al. 2004, Boogert et al. 2004), and the rich, HCI emissions from Capella observed by Chandra and XMM-Newton are given in Fig. 2 (Gu et al. 2006).

Underlying these measurements is the need for a broad understanding of the plasma properties of the various astrophysics objects. Such understanding is intimately connected to the underlying atomic and molecular collision physics. For molecular-ion targets, there is an ongoing need for accurate cross sections and rate constants for direct and dissociative ionization,

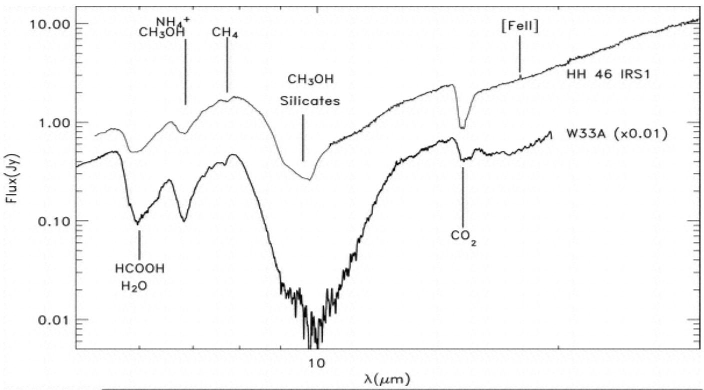


**Figure 1a:** ***Spitzer*** **IRS ionic and molecular spectrum of the HH 46 IRS 1 source (*upper line*) compared with that of W33A (*lower line*), a high-mass protostar, scaled down by a factor of 100 (from Noriega-Crespo *et al*. 2004).**

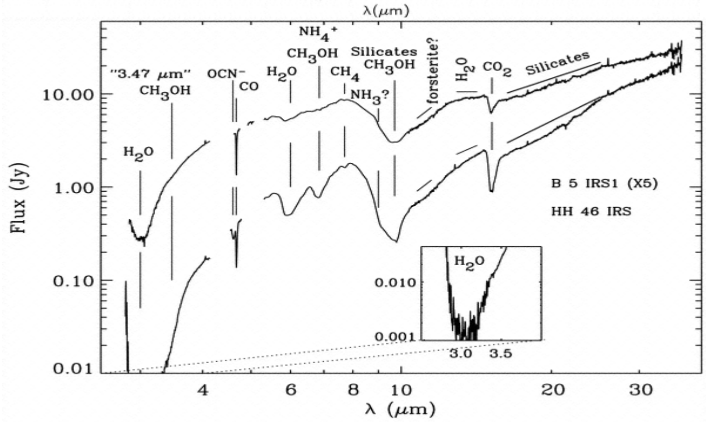


**Figure 1b: Combined *Spitzer* and ground-based *L*- and *M*-band spectroscopy of B5 IRS 1 (*top*; multiplied by factor of 5 for clarity) and HH 46 IRS (*bottom*).**

direct and dissociative recombination, and electron detachment. For HCIs one requires cross sections for excitation, direct and dielectronic recombination, single- and multiple-charge exchange (in HCI-neutral collisions), HCI level lifetimes (nanosecond to millisecond range), and *f*-values. A review of these processes and needs may be found in Chutjian (2004) and Greenwood et al (2004).

Since one cannot measure every required cross section or lifetime, benchmarking of theoretical results is a critical and important aspect of laboratory astrophysics. As an example, recent JPL results of absolute e-$Fe^{13+}$ excitation cross sections have helped resolve the so-called "Iron Conundrum," in which the under-abundance of the Fe density (relative to Mg, Si, Ca, *etc*.) in Seyfert Galaxies compared to its density in our Sun was successfully explained by a too-large collision strength for the $Fe^{13+}$ $^2P^o_{1/2} \rightarrow ^2P^o_{3/2}$ fine-structure transition calculated in an 18-State R-Matrix theory, relative to that of the more accurate 135-State Breit-Pauli R-Matrix theory (Hossain *et al*. 2007). While the topic is not addressed herein, the development of accurate (10% level) theoretical approaches to the calculation of astrophysical phenomena is also essential to meeting NASAs and ESAs ongoing and future, high-quality space observations.

## EXPANDING THE CAPABILITIES FOR LABORATORY ASTROPHYSICS

The profound extension of space observations into the infrared and X-ray regions of the spectrum has revealed a rich population of new molecules and highly-charged ions! In order to address the current and anticipated rich return of space data, one now requires a concomitant expansion of experimental methods and facilities for measuring (in *molecules*) ionization and recombination cross sections; and (in HCIs) collision strengths, lifetimes, charge-exchange cross sections, ionization cross sections, direct and dielectronic recombination cross sections, and

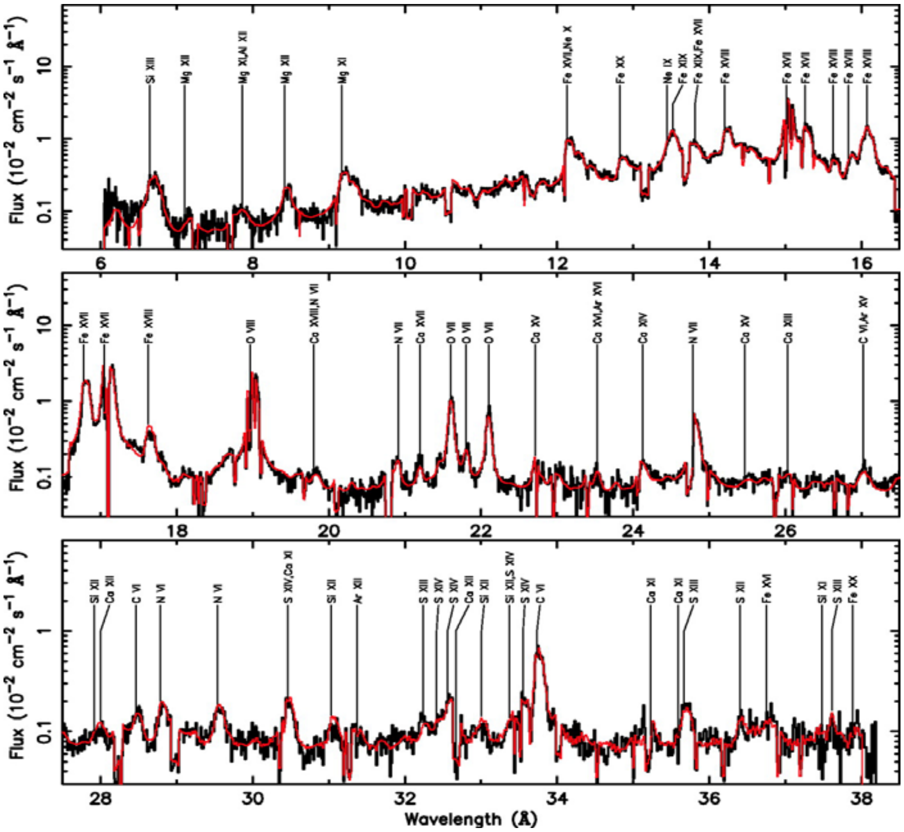


**Figure 2: X-ray spectra of the rich HCI emission features at the Capella corona observed by the *Chandra* and *Newton* spectrometers.**

Comparison is given of the measured (black) and simulated (red) emission features (Gu *et al.* 2006). Excitation of the HCI emissions results from hot electrons in the stellar corona.

lifetimes. Many of these phenomena (cross sections and lifetimes) are already being measured. Use is made of the electron energy-loss method (developed at JPL) with merged beams of electrons and HCIs (Hossain *et al.* 2007). Single and multiple charge-exchange cross sections are measured using a collision gas cell and retarding potential difference analysis of the charge-exchanged HCI ions (Djurić, *et al*. 2008); and metastable lifetimes are measured using a Kingdon ion trap (Smith *et al*. 2005). Three separate beam lines are involved. A photograph of the JPL facility is shown in Fig. 3, and a close-up of the charge-exchange beam line is shown in Fig. 4.

There are distinct enhancements to the present JPL approach. For example, **(1)** the *Caprice*-type electron cyclotron resonance ion source can produce charge states in Fe only to about $Fe^{15+}$, whereas one requires beams of $Fe^{18+}$-$Fe^{25+}$ ions for measuring cross sections applicable to energetic solar-flare emissions and coronal mass ejections. **(2)** In some cases, one requires a better measure of the metastable content of an HCI beam; or better yet, one would like to have a *cool* beam where all metastable levels have decayed. A translational energy spectrometer is being designed to quantify the metastable content in the JPL beams, but this is a somewhat unwieldy subsystem requiring beam line changes and additional power modules. **(3)** One would like to have a means of measuring lifetimes in the $10^{-9}$-$10^{-3}$ range in just a single experimental apparatus. **(4)** To measure collision phenomena in molecular ions, one requires a means of changing ion sources to generate negative ions (use a hollow-cathode glow discharge), positive ions (use a Nielsen-type source), or large clusters and biomolecules (use electrospray ionization). **(5)** The experimental system should have a straightforward means of studying

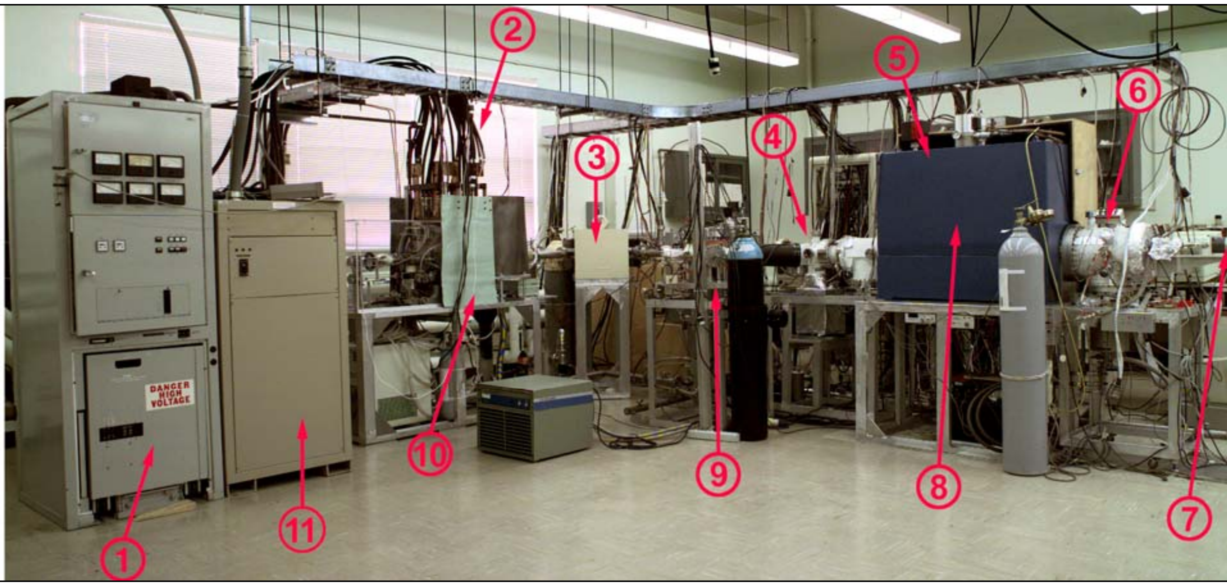


**Figure 3: The JPL Highly-Charged Ion Facility.** The numbered sections are, ① high-power Ku band amplifier, ② cooling lines for the *Caprice* HCI source solenoidal magnets, ③ HCI charge/mass selection magnet, ④ Y-switcher for directing the HCI beam into one of three beam lines, ⑤ solenoidal magnet for merging electron and HCI beams, ⑥ vacuum manifold for electrical feedthroughs, ⑦ stepper motor for measuring beams profiles, ⑧ merged-beams chamber for measuring absolute excitation cross sections, ⑨ Kingdon ion trap for measuring HCI lifetimes, ⑩ *Caprice*-type HCI source with lead shielding, **(11)** 1000-A supply for the *Caprice* solenoidal magnets.

direct and indirect electron ionization and dissociation phenomena for both molecular and HCI targets.

A holistic approach to the issues in (1)-(5) above is to design and build an electrostatic storage ring (ESR), coupled to an electron beam ion trap. A photograph of a tabletop ESR is shown in Fig. 5. The ELISA (**E**lectrostatic **I**on **S**torage **R**ing, **A**arhus) was originally built at Aarhus University in Denmark, and served as the model for rings at the Tokyo Metropolitan University, and at the KEK, Tsukuba. Coupling the ESR to a variety of ion sources would allow one to access an extremely broad range of molecular and HCI targets. Molecular ions of

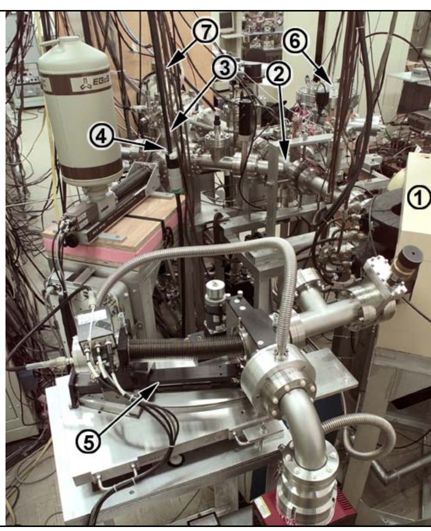


**Figure 4: Close-up of the JPL Charge-Exchange Beam Line.** The numbered sections are, ① HCI charge/mass selection magnet, ② Y-switcher for direction the HCI beam into one of three beam lines, ③ charge-exchange gas cell, ④ HPGe X-ray spectrometer, ⑤ U. Connecticut X-ray grating spectrometer (not attached), ⑥ Kingdon ion trap for measuring lifetimes, and ⑦ merged-beams chamber for measuring excitation cross sections.

astrophysical interest include $CH^+$, $H_3^+$, $H_3O^+$, $CO^-$, and $C_4H^-$; and HCIs include $Mg^{8-11+}$, $Si^{5-13+}$, $Ca^{10-19+}$, and $Fe^{15-23+}$. Large molecules, clusters, and biomolecules can also be injected into the ESR using electrospray ionization methods (Andersen *et al*. 2004).

Generation of HCIs is considered a critical part of understanding solar and stellar spectra, including solar and stellar winds interacting with neutral clouds and comet atmospheres to generate X-rays (see, for example, Djuri□ et al. 2008 and reference therein). As such, an integral part of the future infrastructure to laboratory astrophysics will be the addition of a state-of-the-art HCI source. The Refrigerated Electron Beam Ion Trap (REBIT) can generate practically any charge state of any ion, and will provide coverage for the vast majority of HCIs encountered in astrophysics. A schematic diagram of the REBIT is shown in Fig. 6a, together with a mass spectrum of xenon charge states up to $Xe^{45+}$ displayed in Fig. 6b. The source is commercially available, and would be procured as part of the build (McDonald & Schneider 2005).

**Figure 5a: Photograph of the ELISA electrostatic storage ring at the University of Arhus.** In addition, a double (merged) ESR ring system is in the final phases of construction at Stockholm University (Schmidt *et al.* 2008).

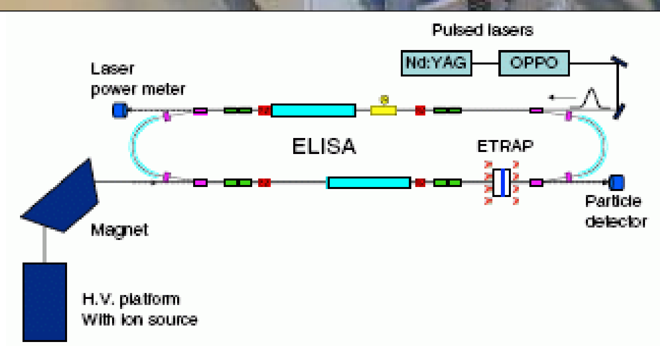


**Figure 5b: Schematic Diagram of the Aarhus ESR.** System is shown with an Nd:YAG laser, pumped tunable optical parametric oscillator (OPPO), and electron- gun target (ETRAP). It is configured to measure dissociation of the target molecular ions using the array particle detector. The dimensions of the ring are 2m (length) H 1m (width).

## NEEDED LABORATORY DATA AND RECOMMENDATIONS

The needs for laboratory data for understanding the plasma environment of solar, stellar, and interstellar objects are vast. In addition to providing cross sections to the modeling community accurate, measured absolute cross sections are critical to benchmarking results of calculations. Not all cross sections, lifetimes, branching fractions, collision rates, *etc.* can be measured, and hence the most accurate theories must be used to calculate missing data.

The combination of the ESR and REBIT , and the use of the REBIT in a single-pass system, will provide a universe of experimental capabilities. Some of these classes of experiments are as follows:

- measurements of absolute electron-impact cross sections at energies of threshold to 5× threshold for up to helium- and hydrogen-like species
- absolute single and multiple charge-exchange cross sections for the ring-cooled, ground-state HCIs
- absolute direct and indirect ionization cross sections of HCIs
- accurate measurements of HCI fluorescence lifetimes ($10^{-9}$-$10^{-7}$ sec) and isotope shifts by tunable laser absorption
- measurements of lifetimes in the $10^{-6}$ to $10^{-3}$ sec range for the excited states of HCIs
- measurement of negative-ion lifetimes in diatomic and polyatomic negative ions, in the absence of magnetic-field mixing and black-body (photodetaching) radiation
- absolute direct and dielectronic recombination cross sections in HCIs
- laser photodissociation of prevalent ISM ions such as $H_2^+$, $H_3^+$, $H_3O^+$, $CH_3^+$, with product distributions

It is clear that a properly-configured experimental atomic and molecular physics laboratory will of essence provide experimental data that encompass a broad range of astrophysical applications and missions. The ESR and REBIT combination described herein will provide measurement capabilities in which there is no “wavelength barrier” or “ion barrier”! Transitions from the infrared to the hard X-ray regions; and targets from polyatomic negative ions to hydrogen-like HCIs will be accessed. It will also benefit from the presence of an accomplished capability and personnel already at work at JPL/Caltech.

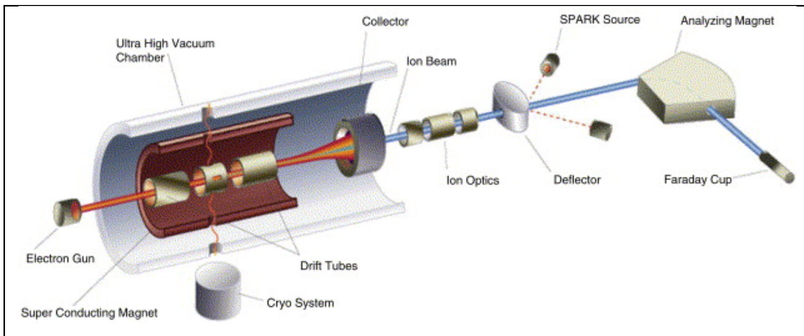


**Figure 6a: Schematic of the Refrigerated Electron Beam Ion Trap (REBIT).** Practically any charge state of any ion can be generated, with ample particle current for use in the ESR (McDonald & Schneider 2005).

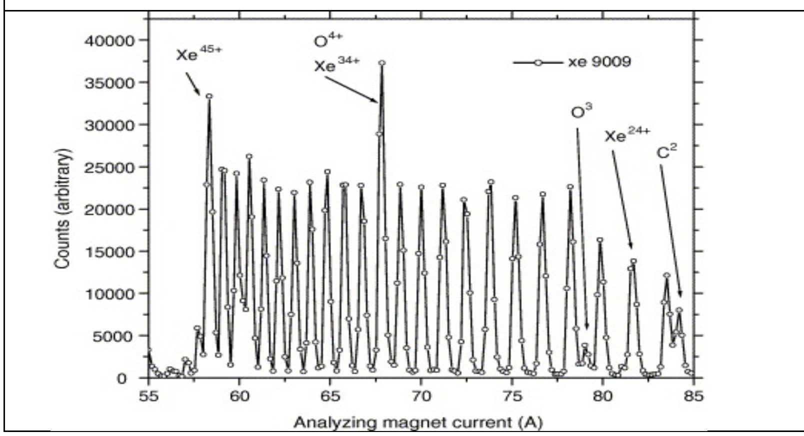


**Figure 6b: Ion Charge States Using the REBIT.** Generation of fully-stripped Fe ions is possible. The ions and charge states generated will cover an extremely broad range of ions presently observed and anticipated in astrophysical objects.

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