

INVITED TALK

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Laboratory Astrophysics: Enabling Scientific Discovery and Understanding

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ABSTRACT

NASA's Science Strategic Roadmap for Universe Exploration lays out a series of science objectives on a grand scale and discusses the various missions, over a wide range of wavelengths, which will enable discovery. Astronomical spectroscopy is arguably the most powerful tool we have for exploring the Universe. Experimental and theoretical studies in Laboratory Astrophysics convert "hard-won data into scientific understanding". However, the development of instruments with increasingly high spectroscopic resolution demands atomic and molecular data of unprecedented accuracy and completeness. How to meet these needs, in a time of severe budgetary constraints, poses a significant challenge both to NASA, the astronomical observers and model-builders, and the laboratory astrophysics community. I will discuss these issues, together with some recent examples of productive astronomy/ lab astro collaborations.

1. Introduction

As demonstrated by the many invited and contributed papers at this meeting, the field of Laboratory Astrophysics is incredibly diverse and fascinating. Whether one considers the Cold Universe or the Hot Universe, Laboratory Astrophysics plays a pivotal role in both discovery and understanding.

This is an exciting but extremely challenging time for our field. The NASA Science Strategic Roadmap, released in May, 2005, articulated a grand vision of Universe Exploration, consisting of two major program elements: Beyond Einstein – exploring extreme conditions in the Universe; and Pathways to Life – focusing on the formation and evolution of galaxies, stars and planets. As new missions develop better capabilities for spectroscopy with improved photon sensitivities and higher spectroscopic resolution, exciting new phenomena in our universe will be revealed. Laboratory Astrophysics will be a necessary element in making these discoveries. It is a challenging time because the funding to sustain this field

is so small, and has in fact declined in this program over the last year. In addition, the research itself is often very difficult, requiring the fastest computer facilities available and laboratory instruments which may be unique or may not even exist in the United States.

The plenary speaker of four years ago (NASA LAW, May 2002), Martin Harwit, ended his talk: “Without laboratory astrophysics there can be no astronomical science!” The science examples which I have chosen to discuss in this talk will illustrate this point. Whereas this quote is generally accepted in the LabAstro community, it needs to be more widely recognized throughout the Astronomy community. The potential for LabAstro to really challenge the astrophysics can only be realized once the uncertainties in the atomic, molecular and solid state parameters have been reduced to a negligible level. Astronomers need to be more critical of the LabAstro data that they use and more aware of how issues such as accuracy, outdated cross sections, and old approximations can seriously corrupt the interpretations of their observations and lead to false astrophysical conclusions.

2. Sustainability Concerns

The sustainability of the Laboratory Astrophysics enterprise is greatly threatened. Although NASA is to be congratulated for having a program in LabAstro (no other agency does), this program is small and getting smaller. Ground-based astronomy needs LabAstro just as much as space astronomy, so there need to be additional sources of funding beyond NASA for this field.

The reason that Laboratory Astrophysics is so poorly funded at this point is due to the historical fact that much of the research in atomic and molecular collisions and spectroscopy (the vast majority of the LabAstro research) used to be funded by the Atomic and Molecular Physics programs at the National Science Foundation (NSF) and Department of Energy (DOE). Astronomy benefited, but did not have to fund this work from astronomy programs. Now, however, the funding priorities for Atomic, Molecular and Optical (AMO) Physics programs have changed and new forefront areas of AMO Physics, such as the study of Bose-Einstein Condensation, generation of ultra-fast light pulses, quantum control, and quantum information science have commanded most of the resources in these programs.

Now is the time to argue for new sources of funding for LabAstro at NSF (Astronomy), DOE and NIST – the agencies singled out for significant budgetary increases in the recent State of the Union address (January, 2006). Although these agencies have very different missions, each could play a unique role in support of LabAstro. Not only would the field be strengthened by a diversity of funding sources, but also the NASA Laboratory Astrophysics program would benefit from the synergism.

There are other sustainability issues as well – but each concern can be traced back to lack of funding. The training of students and postdocs in Laboratory Astrophysics research is absolutely essential if the field is to continue. Young people are the “life-blood” of the field. There are almost no faculty or research staff appointments in the field of LabAstro – either

in physics, chemistry, or astronomy departments. New positions are usually not created in areas of research that are extremely under-funded. Finally laboratory research facilities are aging and need to be updated and maintained, with funds for new instrumentation and equipment. Despite these very serious issues, the science itself continues to be as compelling as ever.

3. Scientific Examples

There are so many examples I could have chosen to highlight from the broad array of scientific papers submitted to this workshop. From spectroscopic studies of PAHs and laboratory simulations in ices and minerals, to astrochemistry in the interstellar medium and in sites of star formation, to measurements of spectral lines and oscillator strengths of heavy elements such as Samarium in order to better understand nucleosynthesis scenarios, the work is of exceptional quality and value to the field of astronomy.

3.1. Understanding the Origin of Cometary X-rays

While the cometary x-ray story is not new, the reason to re-tell it in this setting is to emphasize that the solution to the origin of the x-rays rests exclusively with an atomic collision process, and that as astronomers and laboratory astrophysicists study this in more detail this process is proving to be the explanation for the x-rays seen in a variety of solar system settings, and potentially even beyond.

In 1996 Lisse and collaborators reported on observations of x-ray and EUV emissions from the comet Hyakutake, as it approached the sun. Observations were made using ROSAT and the Rossi X-ray Timing Explorer, with such low resolution that essentially no lines were discernible. Subsequently a number of other comets were found to exhibit x-ray emission as well. The source of these x-rays was a mystery.

Without an adequate spectrum several possible mechanisms for x-ray production were proposed and dismissed. Thermal bremsstrahlung was ruled out because the flux of energetic electrons was not high enough, by several orders of magnitude, to account for the detected intensity. Fluorescent scattering of solar x-rays by material in the comet's coma was rejected because generally x-rays do not scatter strongly. It was Cravens in 1997 who suggested that highly-charged ions in the solar wind were colliding with neutral molecules in the cometary atmosphere, capturing electrons in a process known as “charge exchange”. A valence electron is captured from the neutral species into a highly excited level of the ion, and as the electron decays to the lowest available energy level the ion emits radiation at x-ray and EUV wavelengths. Because this radiation is characteristic of the emitting ion, the spectrum contains valuable information about the original ions present in the solar wind.

The Chandra satellite has afforded the opportunity to resolve a number of spectral fea-

tures. Figure 1 shows a Chandra x-ray spectrum of Comet McNaught-Hartley (open circles) and a model of the emission over the range from 0.5 to 1.0 keV. The narrow dark lines are the spectral lines from theoretical calculations and experimental measurements. When the model spectra are convolved with the Chandra spectroscopic resolution, and the abundances of the solar wind ions are included as adjustable parameters, an excellent fit to the Chandra data can be obtained, as shown by the red line in Figure 1. Theorists were also able to predict the presence of a line of Ne^{8+} which the astronomers were able to identify subsequently.

The charge exchange mechanism is thought to be the major contributor to the heliospheric diffuse soft x-ray background, as well as explaining many of the x-ray observations of planets such as Jupiter, Mars and Saturn. This mechanism is not confined to solar system objects, however. Charge exchange may occur wherever there is the interaction of a highly-ionized plasma with a surrounding gas of neutral material, such as might be found close to the center of Active Galactic Nuclei.

In the future, with increasingly high resolution spectra available with new and planned x-ray telescope facilities, better experiment and theoretical calculations, it is anticipated that cometary x-ray spectra could be used as important diagnostics of the solar wind composition.

3.2. Fe XVII: Diagnostic of Collisionally-ionized Plasmas

The topic of collisionally-ionized plasmas is large, so I will just focus on one important but powerful diagnostic, the 3C/3D line ratio in Fe XVII. Recent work on this line ratio exemplifies the productive way that astrophysical modelers, laboratory experimenters and theorists can work together to determine critical data with high accuracy.

Stellar coronae and supernova remnants are among the many x-ray sources that are thought to be collisionally-ionized plasmas. The collisional models require a detailed understanding of atomic collision processes over a wide range of temperatures, as well as large amounts of data including: line identifications, line strengths, electron impact ionization and excitation cross sections, dielectronic and radiative recombination cross sections, and proton impact excitation and ionization cross sections. The challenges for both the modelers and the labastro scientists are the completeness and consistency of the atomic data, as well as the accuracy.

Line intensity ratios can be powerful diagnostics of astrophysical plasmas, allowing one to deduce temperature, electron density, ion abundances and opacity from the observations of spectral lines. Neon-like iron is a very abundant ion in objects with temperatures in the range of $2-6 \times 10^6 \text{K}$. In particular, the 3C resonance line at 15.01 Å is the strongest line in the solar x-ray spectrum. The 3C line is due to a dipole-allowed transition ($2p^5 3d^1 P_1^o \rightarrow 2p^6 \ ^1S_o$) and the 3D at 15.26 Å is a spin- forbidden intercombination line ($2p^5 3d^3 D_1^o \rightarrow 2p^6 \ ^1S_o$).

Historically there has been a problem with the 3C/3D line ratio, in that solar observations gave values considerably smaller than the early theoretical calculations by factors of 2 to 5. To account for these discrepancies, astrophysical effects, such as opacity and resonant

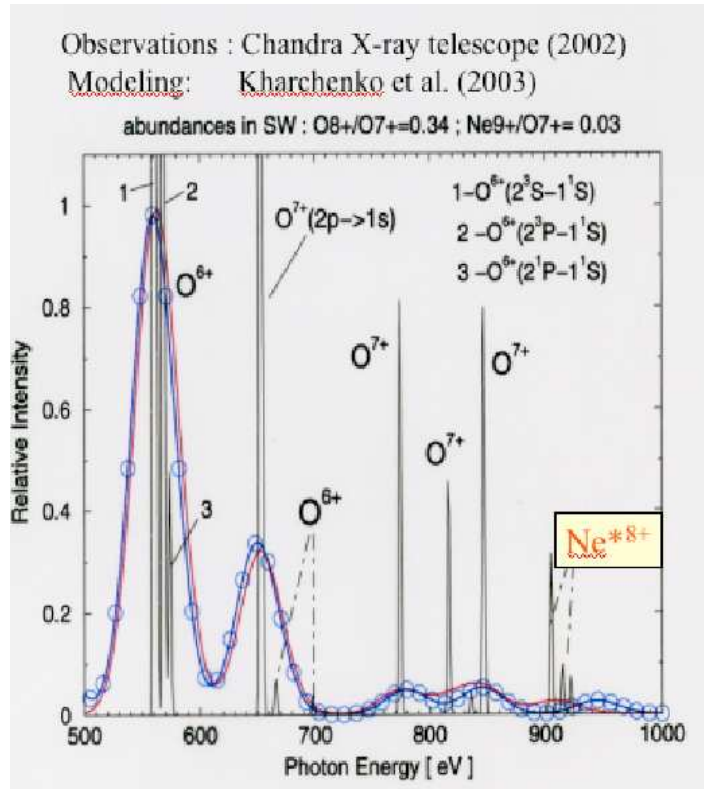


Fig. 1.— Chandra X-ray observations (open circles) of Comet McNaught-Hartley together with model spectra obtained from theory and experiment convolved at the spectral resolution of Chandra, using solar wind (SW) abundance ratios as listed at the top of the figure. (Courtesy of V. Kharchenko)

scattering, were posited as being responsible. It should be noted however that the early theoretical calculations used the distorted wave approximation that neglects channel coupling and resonances. It is known that forbidden and intercombination transitions, such as 3D, are more sensitive to the neglect of resonances than the dipole-allowed transitions.

Fortunately, experimental measurements of these transitions were made. The group at the LLNL EBIT (Brown, Beiersdorfer et al.) measured 3C/3D at several selected beam energies and obtained values more in harmony with the solar observations. Similar values were also reported by the NIST EBIT group (Laming et al.) in 2001. The laboratory measurements were absolutely critical in motivating theorists to look again at this problem. Chen and Pradhan (2002) carried out large-scale relativistic close-coupling calculations using the Breit-Pauli R-matrix method, including atomic levels up through $n=4$. They demonstrated the significant enhancement of the 3D collision strength due to the inclusion of resonances, bringing their 3C/3D ratio into better agreement with the EBIT measurements. They estimated the accuracy of their calculation to be at the 15-20% level.

Recently Chen (2006) has significantly improved on the calculation of Chen and Prad-

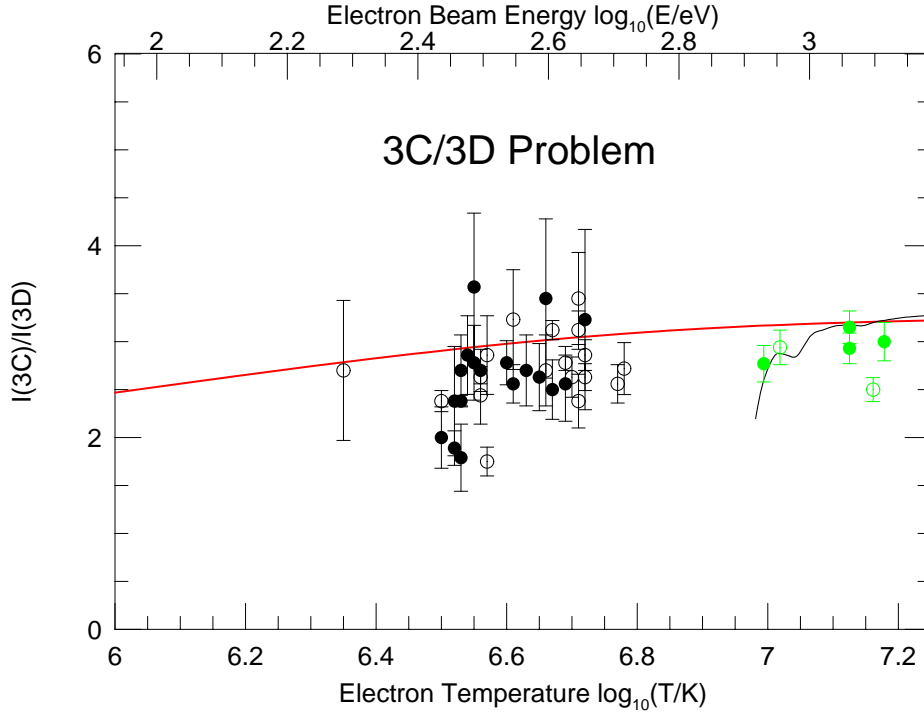


Fig. 2.— The Fe XVII 3C/3D line ratio as a function of electron temperature. The filled and open circles in the center of the figure are Chandra and XMM Newton observations for various stellar and cosmic sources. The EBIT measurements appear as filled and open circles at the far right-hand side of the graph. The Maxwellian-averaged theoretical calculations appear as the solid line, and a Gaussian average of the theoretical calculations (FWHM = 30 eV) is the wavy solid line going through the EBIT points. (Courtesy of G.X.Chen)

han by using a fully relativistic multi-configuration Dirac Fock R-matrix method, including levels up through $n=5$. He has demonstrated convergence in his calculations, and estimates an error of about 5% in the calculated line ratio. When the new theoretical results are Maxwellian-averaged, the solid line in Figure 2 is obtained. If, however, a Gaussian average of these same theoretical values is performed, using a full-width half maximum (FWHM) of 30 eV, the wavy curve lying on top of the EBIT measurements is obtained. (The EBIT measurements are the filled and open circles on the right-hand side of the graph; a Gaussian average is most appropriate for describing the EBIT electron distribution function.)

It is clear from Figure 2, that if one needs a Maxwellian average, the theoretical calculations are absolutely essential, as the EBIT experiments are best described by a Gaussian averaged electron distribution function, and the line ratios obtained for each kind of average are quite different. More discussion of the electron impact excitation cross sections of Fe

XVII at the Livermore EBIT are being reported (E9¹) at this meeting (Brown et al.). The NIST EBIT group (E33) is extending its work on Fe XVII to other neon-like ions (J. Tan et al.) Also in these Proceedings, N. Brickhouse (M1) will discuss why the 3C/3D line ratio has been so low in solar observations.

3.3. Line-broadening Diagnostics of Brown Dwarfs and Extrasolar Planets

Over the last ten years, the continuing discovery and the increasingly accurate characterization of brown dwarfs and extrasolar giant planets have created an exciting frontier in stellar and planetary astronomy. Brown dwarfs and extrasolar giant planets can be grouped together as substellar mass objects (SSMOs) in that they have significant overlap in terms of the parameter space of atmospheric temperatures, densities, and thus similar chemistries as well. The development of accurate spectral diagnostics and the refinement of the theoretical models to describe these objects are among the most important challenges for the future.

In the optical and near-infrared spectra of L-dwarfs and T-dwarfs the resonance lines of sodium (at 589 nm) and potassium (at 770 nm) appear as prominent absorption features, profoundly broadened due to collisions with the most abundant neutral species in the atmospheres of these objects: molecular hydrogen and He. The broadening is such that the line wings extend as much as 100 nm either side of line core. Although no full spectrum of an extrasolar planet has yet been observed, theoretical models of certain classes of exoplanets also predict these broadened absorption resonance lines to be prominent features in the visible and near-infrared.

At the Harvard-Smithsonian Center for Astrophysics we have a joint theoretical and experimental program to provide accurate line profiles for the resonance lines of K and Na, broadened by collisions with H₂ and He. We have found it advantageous to benchmark theory at particular temperatures and pressures obtainable in the laboratory, and then theory can be used to explore other parameter spaces. In brief, the double-beam absorption spectroscopy experiment features a Mach-Zehnder interferometer which provides the optical arrangement for the double-beam absorption paths, and a 3 m Czerny-Turner grating spectrograph, fitted with an array detector which disperses and records the spectra from 360 nm to 900 nm. The theoretical calculations focus on the line wings of the alkali-perturber systems, which are sensitive to the details of the interaction potentials. Densities are low enough that we can use the binary approximation. The line-broadening results from the change in transition energy of the system during the course of the collision, as described by the energy difference between the 4s- and 4p-type potential curves. Of particular interest are "satellite" features which arise at extrema of the difference potentials, and can be very sensitive to the temperature. Thus satellites can be very useful diagnostics.

A paper in this Proceedings will give more details regarding the theoretical calculations

¹Editorial note: Presentation codes are given in Appendix B, p. 306

and experimental details (Shindo et al., E6) on this work. Another paper by Lillestolen and Hinde (T3) reports on independent theoretical calculations of the line-broadening of K and Na by collisions with He.

4. Concluding Remarks

The close-coupling of Astronomy and Laboratory Astrophysics is particularly important in times of severe budgetary constraints. Astrophysics must help set the priorities regarding the LabAstro research that is needed, but astronomers must understand the necessity of testing new theoretical methods and experimental techniques on systems which are most tractable, before larger, more complex systems can be treated with confidence.

There is room for considerable improvement at the interfaces between the LabAstro researchers (“data providers”) and the databases, the modelers and the observers. Much can be lost at each of these interfaces. The lack of support for the development, updating and maintaining of databases is very serious. In addition, there is a tremendous need for critically evaluated data, which can help to identify areas in which new LabAstro research is necessary.

Finally, there are a number of challenges for the Astronomy community. The first is understanding the accuracy (or lack thereof) of LabAstro “data”, and appreciating how this impacts the astrophysical interpretations. The second is addressing the question as to whether LabAstro databases should become part of the National Virtual Observatory (NVO). And ultimately, it is essential that astrophysicists, realizing the importance of LabAstro to their science, support more funding for this research from within Astronomy programs, particularly at NASA and at NSF.

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