

# PROGRAM and ABSTRACTS



Washington, DC skyline at night. © Shutterstock/fstockfoto

## Eighth International Conference on Atomic and Molecular Data and Their Applications: ICAMDATA-8

September 30 - October 4, 2012  
*National Institute of Standards and Technology (NIST)*  
*Gaithersburg, MD, USA*

## Local Conference Committee

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John Curry, NIST  
Jeff Fuhr, NIST  
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## Important Information and Contact Numbers

Please be aware that access to the NIST grounds is restricted. Registrants are cleared for access M-Th through the main gate on Route 117 (West Diamond Avenue, which is the extension of Clopper Road) by presenting a government-issued photo ID (passport or U.S. Driver's License, for example). After 5PM registrants will need a NIST escort to enter the grounds. Participants in the Satellite meetings on Friday, who have not already done so, must contact one of the Satellite Meeting Chairs in advance to have their gate pass extended through Friday.

Phone numbers:

Police/Fire/Medical Emergency:

from NIST internal phone: 2222

from private phone: 911

NIST Police (non-emergency): 301-975-2805

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Mary Lou Norris: 301-975-2002

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See back cover for color block diagram of conference schedule



## Detailed Schedule

Sunday, September 30.

Reception (6:00 PM-8:00 PM) and Registration (4:00 PM-6:00PM) at the Marriott Washingtonian Center Hotel, 9751 Washingtonian Boulevard (Gaithersburg, MD). Note that there is a second Marriott nearby. If you are staying at the Courtyard Marriott, it is a short walk to the Marriott Washingtonian Center. Registration will also be available on subsequent days at NIST outside of the Green Auditorium.

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Monday, October 1.

All talks are held in the Green Auditorium of the NIST Administration Building (Bld 101). Map provided in this booklet.

8:15 AM. Bus departs from Marriott Washingtonian Center for NIST. You may also drive in by private car through gate A and park by the Administration Building (Bld 101) or take a taxi to the Visitor's center at gate A.

8:50 AM. Welcome by Dr. Willie E. May, Associate Director of Laboratory Programs, NIST (introduced by John Gillaspay, Chair of the ICAMDATA Local Conference Committee).

Session Chair: Wolfgang Wiese, NIST

Note: talk times listed below include 5 minutes for questions and answers.

9:00-9:30 AM. Stefan Schippers, Giessen University, Germany  
Storage-Ring Measurements of Hyperfine Induced and Two-Photon Transition Rates in Berylliumlike Ions

9:30-10:00 AM. James Colgan, Los Alamos Laboratory, USA  
Light element opacities of astrophysical interest from ATOMIC

10:00-10:30 AM. Juliet Pickering, Imperial College London, UK  
New laboratory atomic spectroscopic measurements with applications from astrophysics to industrial analytical applications.

10:30-11:00 AM. Coffee break (outside Green Auditorium)

Session Chair: Craig Sansonetti, NIST

11:00-11:30 AM. Gordon Drake, University of Windsor, Canada  
High Precision Atomic Data as a Measurement Tool for Halo Nuclei: Theory

11:30-12:00 AM. Wilfried Nörtershäuser, Johannes Gutenberg-Universität Mainz and GSI, Germany

High precision atomic data for halo nuclei and related nuclear structure

12:00-1:30. Lunch in the NIST Cafeteria (turn right as you exit the back of Green Auditorium). Lunch tickets are provided in your registration packet.

Session Chair: Marie-Lise Dubernet-Tuckey, LPMAA, Université Pierre et Marie Curie, France

1:30-2:00. Eberhard Tiemann, Leibniz Universität Hannover, Germany  
Renaissance in diatomic spectroscopy

2:00-2:30. Holger S. P. Müller, Universität zu Köln, Germany  
The CDMS View on Molecular Data Needs of *Herschel*, SOFIA, and ALMA

2:30-3:00. Andreas Wolf, Max Planck Institute for Nuclear Physics, Germany  
Storage Ring Experiments on Electron–Molecular-Ion Interactions

3:00-3:30. Zoran Lj. Petrović, Institute of Physics University of Belgrade, Serbia  
Data for Modeling of Positron Collisions and Transport in Gases

3:30-4:00. Coffee Break.

4:00-6:00. Poster Session A (Session Chair: Yuri Podpaly, NIST)

6:00. Bus leaves for hotel

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Tuesday, October 2.

All talks are held in the Green Auditorium of the NIST Administration Building (Bld 101). Map provided in this booklet.

8:15 AM. Bus departs from Marriott Washingtonian Center for NIST. You may also drive in by private car through gate A and park by the Administration Building (Bld 101) or take a taxi to the Visitor's center at gate A.

8:50 AM. Announcements.

Session Chair: Nirmol Podder, U. S. Department of Energy

9:00-9:30. Steve Lisgo, ITER Organization, France  
Atomic, Molecular, and Surface-Interaction Data Needs for ITER

9:30-10:00. Thomas Pütterich, Max Planck Institut für Plasma Physik Garching, Germany  
Spectroscopic Diagnostics of Highly Charged, Heavy Metal Impurities

10:00-10:30. Shigeru Morita, NIFS, Japan  
A Study of tungsten spectra using Large Helical Device and Compact Electron Beam Ion Trap in NIFS

10:30-11:00. Coffee break (outside Green Auditorium)

Session Chair: Alfred Müller, Justus-Liebig-University, Giessen, Germany

11:00-11:30. N. Nakamura, University of Electro-Communications (Tokyo)  
EBIT Spectroscopy of Highly Charged Heavy Ions Relevant to Hot Plasmas

11:30-12:00. Ronald Phaneuf, University of Nevada  
Cross-Section Measurements With Interacting Beams

12:00-12:15. Group photograph.

12:15-1:30. Lunch in the NIST Cafeteria (turn right as you exit the back of Green Auditorium).  
Lunch tickets are provided in your registration packet.

Session Chair: David Schultz, University of North Texas

1:30-2:00. Laurence Rothman, Harvard-Smithsonian Center for Astrophysics, USA  
The HITRAN Molecular Database

2:00-2:30. Yizhi Qu, Graduate University of Chinese Academy of Sciences Beijing, China  
Charge Transfer Cross Section Calculations and Evaluations

2:30-3:00. Stuart Loch, Auburn University, USA  
Propagation of uncertainties in atomic data through collisional-radiative models

3:00-3:30. Adam Foster, Harvard-Smithsonian Center for Astrophysics, USA  
AtomDB: Atomic Data for X-ray Astrophysics

3:30-4:00. Coffee break (outside Green Auditorium)

4:00-5:00. Panel 1: "Future Opportunities" (Chair: Yuri Ralchenko)

Panelists:

1. James Van Dam, Director of Research Division, Office of Fusion Energy Sciences, U.S. Department of Energy.
2. Marie-Lise Dubernet-Tuckey, Directrice, Molecular Physics Laboratory for the Atmosphere and Astrophysics (LPMAA), CNRS/University Pierre & Marie Curie, Observatory of Paris.
3. Arati Dasgupta, Plasma Physics Division, U. S. Naval Research Laboratory.
4. David Schultz, Chair of the Department of Physics, University of North Texas.

5:00-6:00 Database Demonstrations (Chair: Alexander Kramida, NIST).

6:00. Bus leaves for hotel.

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Wednesday, October 3.

All talks are held in the Green Auditorium of the NIST Administration Building (Bld 101). Map provided in this booklet.

8:15 AM. Bus departs from Marriott Washingtonian Center for NIST. You may also drive in by private car through gate A and park by the Administration Building (Bld 101) or take a taxi to the Visitor's center at gate A.

8:50 AM. Announcements.

Session Chair: Nancy Brickhouse, Harvard-Smithsonian Center for Astrophysics

9:00-9:30. Tim Kallman, NASA Goddard Space Flight Center, USA  
Data Needs for X-ray Satellites

9:30-10:00. Ehud Behar, Technion Israel Institute of Technology, Israel  
The Role Of Atomic Data In X-Ray Astrophysics

10:00-10:30. Jelle Kaastra, SRON Utrecht, The Netherlands  
Spectral Modeling and Diagnostics In Various Astrophysical Environments

10:30-11:00. Coffee break (outside Green Auditorium)

Session Chair: Michael Crisp, NIST

11:00-11:30. Oleksandr Marchuk, Forschungszentrum Juelich, Germany  
Atomic data for beam-stimulated plasma spectroscopy in fusion plasmas

11:30-12:00. Hajime Tanuma, Tokyo Univ., Japan  
Charge Exchange Spectroscopy of Multiply Charged Ions of Industrial and Astrophysical Interest

12:00-1:30. Lunch in the NIST Cafeteria (turn right as you exit the back of Green Auditorium).  
Lunch tickets are provided in your registration packet.

Session Chair: Glenn Wahlgren, NASA Headquarters

1:30-2:00. Daniel Savin, Columbia University, USA  
Laboratory Studies of Primordial Chemistry and Implications for First Star Formation

2:00-2:30. Laurence Campbell, Flinders Univ., Australia  
Data Needs For Simulations Of Electron-driven Processes In Planetary And Cometary Atmospheres

2:30-3:00. Jonathan Tennyson, University College London, UK  
Molecular Line Lists For Exoplanets and Other Atmospheres

3:00-3:30. Coffee break (outside Green Auditorium)

Special Session in Honor of Charlotte-Froese Fischer and Joseph Reader, two active long-term members of the NIST Atomic Spectroscopy Group.

Session Chair: John Curry, NIST

3:30-4:00. Per Jönsson, Malmö University, Sweden  
Accurate Transition Probabilities from Large-scale Multiconfiguration Calculations

4:00-4:30. David Leckrone, NASA HQ, USA

Laboratory Spectroscopy and Space Astrophysics: A Tribute to Joe Reader and Friends

4:30-6:00. Poster Session B (Session Chair: Rodrigo Ibacache, NIST).

6:00. Bus leaves for hotel

6:30-7:00. Cash Bar at Marriott Washingtonian Center before the Banquet.

7:00-. Banquet at the Marriott Washingtonian Center.

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Thursday, October 4.

All talks are held in the Green Auditorium of the NIST Administration Building (Bld 101). Map provided in this booklet.

8:15 AM. Bus departs from Marriott Washingtonian Center for NIST. You may also drive in by private car through gate A and park by the Administration Building (Bld 101) or take a taxi to the Visitor's center at gate A.

8:50 AM. Announcements.

Session Chair: John Gillaspy, NIST

9:00-9:30. Fumihiro Koike, Saga University, Japan  
Data of Heavy Elements for Light Sources in EUV and XUV lithography and Other Applications

9:30-10:00. Igor Kaganovich, Princeton Plasma Physics Lab., USA  
Data Needs for Low Temperature Plasmas and Accelerator Applications

10:00-10:30. Satoshi Hamaguchi, Osaka University, Japan  
Chemically reactive species in liquids generated by atmospheric-pressure plasmas and their roles in plasma medicine

10:30-11:00. Coffee break (outside Green Auditorium)

Session Chair: Bastiaan Braams, International Atomic Energy Agency (IAEA).

11:00-11:30. Hyun-Kyung Chung, IAEA, Vienna, Austria  
Coordinated Activities on Evaluation of Collisional Data for Fusion Applications

11:30-12:30. Panel 2: "Assessment of the Accuracy of Data" (Chair: Bas Braams)

Panelists:

1. Klaus Bartschat, Drake University
2. Gordon Drake, University of Windsor
3. Phillip Stancil, University of Georgia
4. Jonathan Tennyson, University College London

12:30-1:30. Business Meeting in Green Auditorium.

1:30. Bus leaves for hotel (and subway). For those wishing to do some sightseeing in Washington DC this afternoon, some members of the Local Organizing Committee will be available to offer advice and escort you downtown via the subway.

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Friday, October 5.

Two Satellite Meetings are scheduled to take place from 9AM-5PM:

*Symposium on Atomic Structure Calculations* (Chair: Charlotte Froese-Fischer)

*VAMDC-USA* (Chair: Yuri Ralchenko)

Access to NIST on Friday for the Satellite meetings requires advance signup in order to arrange gate clearance. If you wish to attend but have not already been in touch with one of the Satellite Meeting Chairs listed above, please do so immediately.

## Satellite Meetings

### *Symposium on Atomic Structure Calculations*

Chair: Charlotte Froese Fischer

Time: October 5, 2012 9AM-5PM

Location: Lecture Room B

The purpose of this symposium is to discuss recent work on advanced computational methods for atomic properties. Those wishing to present a talk on this subject should contact the person below by email, specifying the subject of the talk.

Contact Person:

Charlotte Froese Fischer

Charlotte.Fischer@nist.gov

### *VAMDC-USA*

Chairs: Yuri Ralchenko and Marie-Lise Dubernet

Time: October 5, 2012 9AM-5PM

Location: Lecture Room A

The purpose of this meeting is to expose Virtual Atomic and Molecular Data Center VAMDC to the US community and vice versa as well as to initiate collaborations between database providers and users with VAMDC. Those wishing to present a talk on this subject should contact the person below by email, specifying the subject of the talk.

Contact Person:

Yuri Ralchenko

yuri.ralchenko@nist.gov

Abstracts—Invited  
(in order of presentations)



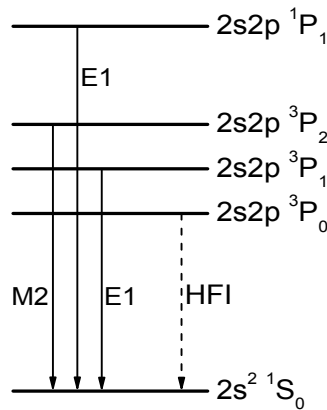
# Storage-Ring Measurements of Hyperfine Induced and Two-Photon Transition Rates in Berylliumlike Ions

Stefan Schippers

*Institute for Atomic and Molecular Physics, Justus-Liebig-University Giessen,  
Leihgesterner Weg 217, 35292 Giessen, Germany*

**Abstract.** Extremely long lived atomic states are highly sensitive to correlations within the atomic shell and even to the nuclear structure of the ions. An example of this is the lowest excited state in beryllium-like ions, i.e., the  $2s2p\ ^3P_0$  state, which cannot decay via a one-photon transition. However, the hyperfine interaction can quench the  $2s2p\ ^3P_0$  state if the nucleus has nonzero magnetic moment.

Theoretical calculations [1-5] of hyperfine induced (HFI) transition rates in beryllium-like ions disagree significantly with the until recently only available experimental result [6]. The measured results were obtained from an experiment with  $^{47}\text{Ti}^{18+}$  ions at the Heidelberg heavy-ion storage ring TSR. In order to broaden the experimental data base, HFI lifetime measurements with other beryllium-like ions are currently carried out at the TSR. Most recently, new results were obtained for  $^{33}\text{S}^{12+}$  ions [7]. These results will be presented and compared with corresponding theoretical calculations which predict a HFI  $2s2p\ ^3P_0 \rightarrow 2s^2\ ^1S_0$  transition rate of  $0.093\ \text{s}^{-1}$  [2,3] for this ion. Perspectives for measurements of the the competing E1M1 two-photon transition rate in beryllium-like ions [8] will be discussed as well.



Simplified level diagram of a beryllium-like ion. The one-photon transitions are labeled E1 (electric dipole), M2 (magnetic quadrupole), and HFI (hyperfine induced). Numbers in square brackets denote powers of 10. In case of nonzero nuclear spin the hyperfine induced  $^3P_0 \rightarrow ^1S_0$  transition rate  $A_{\text{HFI}}$  acquires a finite value.

## References

- [1] J. P. Marques *et al.*, Phys. Rev. A **47**, 929 (1993).
- [2] K. T. Cheng *et al.*, Phys. Rev. A **77**, 052504 (2008).
- [3] M. Andersson *et al.*, Phys. Rev. A **79**, 032501 (2009).
- [4] J. Li and C. Dong, Plas. Sci. Technol. **12**, 364 (2010).
- [5] J. Li *et al.*, Phys. Lett. A **375**, 914 (2011).
- [6] S. Schippers *et al.*, Phys. Rev. Lett. **98**, 033001 (2007).
- [7] S. Schippers *et al.*, Phys. Rev. A **85**, 012513 (2012).
- [8] D. Bernhardt *et al.*, J. Phys.: Conf. Ser. (in press).

# Light element opacities of astrophysical interest from ATOMIC

J. Colgan\*, D. P. Kilcrease\*, N. H. Magee, Jr\*, G. S. J. Armstrong\*, J. Abdallah, Jr.\* , M. E. Sherrill\*, C. J. Fontes†, H. L. Zhang† and P. Hakel†

\*Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

†Computational Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

**Abstract.** We present new calculations of local-thermodynamic-equilibrium (LTE) light element opacities from the Los Alamos ATOMIC code [1] for systems of astrophysical interest. ATOMIC is a multi-purpose code that can generate LTE or non-LTE quantities of interest at various levels of approximation. Our calculations, which include fine-structure detail, represent a systematic improvement over previous Los Alamos opacity calculations using the LEDCOP legacy code [2]. The ATOMIC code uses *ab-initio* atomic structure data computed from the CATS code, which is based on Cowan's atomic structure codes [3], and photoionization cross section data computed from the Los Alamos ionization code GIPPER. ATOMIC also incorporates a new equation-of-state (EOS) model based on the chemical picture [4]. ATOMIC incorporates some physics packages from LEDCOP and also includes additional physical processes, such as improved free-free cross sections and additional scattering mechanisms. Our new calculations are made for elements of astrophysical interest and for a wide range of temperatures and densities. Selected comparisons of our new opacity calculations with several other sets of calculations will be presented at the meeting. In particular, we will present detailed comparisons of Rosseland-mean opacity calculations with Opacity Project (OP) [5] and OPAL calculations [6] for hydrogen, helium, and iron. For iron, we also compare our monochromatic opacity calculations with recent work [7].

**Keywords:** opacity, astrophysics

## ACKNOWLEDGMENTS

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## REFERENCES

1. N. H. Magee et al, *14th Topical Conference on Atomic Processes in Plasmas*, Eds: J. S. Cohen, S. Mazevet, and D. P. Kilcrease, (New York: AIP), pp 168-179 (2004).
2. N. H. Magee et al, *Astronomical Society of the Pacific Conference Series* **78**, 51 (1995).
3. R. D. Cowan, *The Theory of Atomic Structure and Spectra*, Berkeley, CA: University of California Press, 1981.
4. P. Hakel and D. P. Kilcrease, *14th Topical Conference on Atomic Processes in Plasmas*, Eds: J. S. Cohen, S. Mazevet, and D. P. Kilcrease, (New York: AIP), pp 190-202 (2004).
5. N. R. Badnell et al, *Mon. Not. R. Astron. Soc.*, **360**, 458 (2005); M. J. Seaton and N. R. Badnell, *Mon. Not. R. Astron. Soc.* **354**, 457 (2004).
6. F. J. Rogers and C. A. Iglesias, *Ap. JS*, **79**, 507 (1992).
7. D. Gilles et al, *High Energy Density Physics* **7**, 312 (2011).

# **New laboratory atomic spectroscopic measurements with applications from astrophysics to industrial analytical applications.**

Juliet C. Pickering, M. Ruffoni, A.P. Thorne and F. Liggins

*Blackett Laboratory, Physics Department, Imperial College London, London SW7 2BZ, UK*

**Abstract.** New measurements of atomic and molecular data for applications ranging from astrophysics, atmospheric physics to industrial analytical applications will be represented.

High resolution iron group atomic spectra recorded by Fourier transform spectroscopy (FTS) in the visible-VUV at Imperial College, and IR-visible at NIST have been analysed, and are being combined with level lifetimes collaborating with J Lawler (Wisconsin), to give accurate new transition probabilities in the IR for the APOGEE and GAIA projects, aimed at understanding Galactic Evolution.

Term analysis projects for V II, Mn II, Ni II are giving accurate new energy levels and wavelength data for use in astrophysics applications, such as stellar spectrum synthesis.

UV FTS measurements of isotopologues of SO<sub>2</sub> have been completed resulting in the first accurate photoabsorption cross sections. These accurate measurements are vital for understanding the proxy used for oxygen levels in the early Earth's atmosphere, sulphur mass independent fractionation.

Relative intensities of spectral lines of elements were measured by FTS in studies aimed at understanding the line intensities observed in glow discharge (GD) spectra when trace gases are present. Glow discharge optical emission spectroscopy GD-OES is an analytical technique used in a wide variety of industrial applications, for determination and testing of material composition, for example in steel manufacturing, coatings, and even nano technology. It relies on a database of relative line intensities of elements observed in standard GD operating conditions. However, the presence of trace gases in the source, such as oxygen, changes the line intensities and leads to erroneous analytical results. Our involvement in investigations of the effect of trace gases on GD spectra will be discussed.

# High Precision Atomic Data as a Measurement Tool for Halo Nuclei: Theory

G.W.F. Drake

*<sup>a</sup>Department of Physics, University of Windsor, Windsor, Ontario, Canada N9B 3P4*

**Abstract.** Halo nuclei were first discovered by Tanihata in 1987. They are a form of atomic nucleus having a halo of excess planetary neutrons surrounding a tightly bound core. The atomic isotope shift method is now well established as the only effective method to determine their nuclear charge radius. The method depends on a comparison between theory and experiment for high-precision laser resonance measurements of atomic transition frequencies. Accuracies at the level of  $\pm 10$  kHz are required for both theory and experiment. Three broad series of measurements are now available for light nuclei, extending all the way from  $^3\text{He}$  to the halo nuclei  $^6\text{He}$  and  $^8\text{He}$ ,  $^6\text{Li}$  to the halo nucleus  $^{11}\text{Li}$ , and  $^7\text{Be}$  to the single-neutron halo nucleus  $^{11}\text{Be}$ . The results are particularly significant because they are able to discriminate amongst various theoretical models for the effective interaction potential between nucleons. By studying systems that fall apart easily, we learn about the forces holding them together. The principle of the method will be discussed in terms of the atomic structure calculations that are required to extract the nuclear charge radius from the isotope shift. The principal theoretical challenges are (a) to obtain sufficient accuracy in the lowest order nonrelativistic and relativistic contributions to the isotope shift, and (b) to calculate the mass dependence of the higher-order QED contributions, such as the Lamb shift. The current status of theory will be reviewed, and compared with experiment, as discussed in the companion paper by W. Nördershäuser. In view of the recently announced discrepancy in the proton radius, a comparison between muonic and electronic helium becomes particularly relevant and interesting.

# High precision atomic data for halo nuclei and related nuclear structure

Wilfried Nörtershäuser<sup>a,b</sup>

<sup>a</sup> *Institut für Kernchemie, Universität Mainz, Fritz-Straßmann-Weg 2, 55128 Mainz, Germany*

<sup>b</sup> *GSI Helmholtzzentrum, Planckstrasse 1, 64291 Darmstadt, Germany*

**Abstract.** The interest on high-accuracy atomic data of short-lived isotopes of the lightest elements has grown strongly during recent years. This is related to new possibilities to extract nuclear data from such measurements by combining their results with high-accuracy atomic physics calculations, as will be discussed in the talk by Gordon Drake. Few-nucleon systems, up to about  $^{12}\text{C}$  are the only nuclei for which *ab-initio* nuclear structure calculations are currently available. These calculations start out from  $N$  nucleons and try to construct the corresponding nucleus based on realistic two- and three-nucleon interactions. For these theories, nuclear data extracted from atomic physics measurements provides some the most reliable benchmark tests available.

Isotope shifts, hyperfine structure splitting and absolute transition frequencies have been determined for all isotopes of helium, lithium and beryllium with the exception of the isotope  $^{14}\text{Be}$  in several experiments at various on-line facilities world-wide. Among these isotopes, the so-called halo nuclei  $^{6,8}\text{He}$ ,  $^{11}\text{Li}$  and  $^{11}\text{Be}$  are of special importance since they exhibit one of the most intriguing nuclear structures of all known nuclei, namely the formation of a “halo” of dilute nuclear matter surrounding a compact core with the usual nuclear matter density. Atomic physics measurements have considerably contributed to our knowledge and our picture of these exotic systems.

In my talk I will provide an overview on the experimental techniques that have been applied and the obtained accuracy for the atomic and nuclear observables extracted from the measurements. Finally, an outlook will be given how a technique similar to that used for beryllium could be employed to perform high-accuracy measurements on the proton-halo nucleus  $^8\text{B}$ .

# Renaissance in diatomic spectroscopy

Eberhard Tiemann and Horst Knöckel

*Institute of Quantum Optics, Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany*

**Abstract.** New technological developments resulted in several periods of renaissances of spectroscopy, like microwaves and later lasers, and lead to developments of new models for description of observations, thus to understanding the underlying physics. Today, the exciting period of cold molecules has started and demands for new data from molecular spectroscopy and completion in their modeling.

This contribution will describe the status of understanding before the era of "cold molecules" and note open questions when entering the field of cold molecules. Because large varieties of cold molecules are studied, like deeply bound (about 1eV) or very weakly bound (less than 1 $\mu$ eV) ones, the spectroscopic tools and the theoretical descriptions have to be largely extended. We will describe recent success regarding different molecules of diatomic alkali- and alkaline-earth atoms as examples and will learn how to use the often huge body of spectroscopic data for obtaining predictions for optimal paths to produce ultra cold molecules in a desired molecular state.

It is very exciting to combine the results of spectroscopy and of studies of ultra cold ensembles which are influenced by their atom-molecule changeover. This allows already to complete the understanding of the electronic structure of atomic pairs from infinite internuclear separation to the range of strongly overlapping electronic distribution in some cases (e.g. KRb or KCs), but asks for enhanced effort for describing quantitatively the discoveries, already published or expected, like a contribution to the field of time dependence of fundamental constants. For molecules with their rotational and vibrational motion the ratio of electron-to-nuclear mass as a fundamental constant shows up as an obvious attraction for spectroscopic studies.

**The CDMS View on Molecular Data Needs of *Herschel*,  
SOFIA, and ALMA**

Holger S. P. Müller, C. P. Endres, J. Stutzki, S. Schlemmer

I. Physikalisches Institut, Universität zu Köln,  
Zùlpicher Str. 77, 50937 Köln, Germany  
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The catalog section of the Cologne Database for Molecular Spectroscopy, CDMS, contains mostly rotational transition frequencies, with auxiliary information, of molecules observable in space. The frequency lists are generated from mostly laboratory data employing established Hamiltonian models. The CDMS has been available online publicly for more than 10 years ([www.cdms.de](http://www.cdms.de)) [1, 2]. Initially constructed as ascii tables, its inclusion into a database environment within the Virtual Atomic and Molecular Data Centre (VAMDC, [www.vamdc.org](http://www.vamdc.org)) has begun in June 2008. A test version of the new CDMS should be released prior to this conference.

The CDMS activities have been part of the extensive laboratory spectroscopic investigations in Cologne. Moreover, these activities have also benefit from collaborations with other laboratory spectroscopy groups as well as with astronomers.

In the first part of the presentation, we will provide some basic information on the CDMS and its participation in the VAMDC project. In the second part, some recent detections of molecules [3, 4] will be discussed to evaluate data needs of *Herschel*, SOFIA, and ALMA in terms of light hydrides, complex molecules, and metal containing species.

[1] H. S. P. Müller et al., *Astron. Astrophys.* **370**, L49-L52 (2001)

[2] H. S. P. Müller et al., *J. Mol. Struct.* **742**, 215-227 (2005)

[3] E.g. *Astron. Astrophys.* special issue sections on *Herschel* (**518** (2010)), *Herschel/HIFI* (**521** (2010)), and SOFIA/GREAT (**542** (2012))

[4] See also <http://www.astro.uni-koeln.de/cdms/molecules>

# Storage Ring Experiments on Electron–Molecular-Ion Interactions

A. Wolf<sup>a</sup>, A. Becker<sup>a</sup>, H. Buhr<sup>a</sup>, M. Grieser<sup>a</sup>, C. Krantz<sup>a</sup>, O. Novotný<sup>b</sup>,  
R. Repnow<sup>a</sup>, D. W. Savin<sup>b</sup>, S. Schippers<sup>c</sup>, A. Shornikov<sup>a</sup>, K. Spruck<sup>c</sup>,  
J. Stützel<sup>a,b</sup>, S. Vogel<sup>a</sup>, and Bian Yang<sup>a,d</sup>

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**Abstract.** In ion storage rings, high-velocity ion beams are recirculated in an ultrahigh vacuum using a lattice of magnetic or electric deflection elements. With magnetic devices, this is applied to molecular ion beams of typical kinetic energies of 1–3 MeV. Using photocathode electron beams [1], the phase space of stored molecular ion beams can be cooled efficiently ensuring well-controlled kinematics for collision studies. By storing the ions various means arise to control their internal excitation. At the Max Planck Institute for Nuclear Physics, we are operating the magnetic storage ring TSR (to be taken out of service at the end of 2012). It will be replaced by an electrostatic ring (CSR) for 20–300 keV· $q$  ions, currently under construction [2]. It will provide a cryogenic environment for heavy-molecule and cluster ion beams and implement ion phase-space cooling by a cold low-energy electron beam.

Here we report on collision studies in velocity-matched merged beams of electrons and stored molecular cations, where collision energies down to  $\sim 1$  meV are realized. Observed processes are ro-vibrational cooling of the molecular ions and their dissociative recombination (DR). For the latter, fragments are counted and kinematically analyzed by coincidence imaging detectors. The measurements yield collision energy dependent, absolute DR cross sections, product branching ratios, and the excitation states of the products (including their ro-vibrational excitation). The measured fragment energies also probe molecular dissociation energies.

Recent studies have focused on dissociative recombination occurring in interstellar molecular clouds and planetary ionospheres and included nitrogen and halide hydrides ( $\text{HN}^+$ ,  $\text{HCl}^+$ ,  $\text{D}_2\text{Cl}^+$ ,  $\text{D}_2\text{F}^+$ ,  $\text{HF}^+$ ) and the deuterated forms of protonated species ( $\text{D}_3\text{O}^+$ ,  $\text{DCND}^+$ ) [3, 4]. An outlook will be given to upcoming merged-beams electron–ion collision studies at CSR. Among others, these studies aim at dissociative recombination cross sections and branching ratios for molecular ions at low-temperature ( $\sim 10$  K) radiative equilibrium (often rotational ground states); moreover, recombination cross sections between a wide range of atomic mono-cations and low-energy electrons will become accessible for merged-beams measurements.

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# Data for Modeling of Positron Collisions and Transport in Gases

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**Abstract.** We review the current status of positron cross sections for collisions with atoms and molecules from the standpoint of modeling of positron transport in gases, vapours, liquids and human tissues. Recent results obtained by binary collision experiments, especially those based on measurements in a Penning- Malmberg-Surko trap, have been successful in producing the data with an accuracy that now matches that for electrons. The data include those for rare gases, some molecular gases (eg. N<sub>2</sub>, H<sub>2</sub>, CO<sub>2</sub>, CF<sub>4</sub>) and in particular the data for organic molecules and molecules relevant for applications in medicine (water, formic acid THF, pyrimidine). Based on the newly accumulated cross section data it has become possible to assemble the cross section sets necessary to model transport in gases, which are complete in terms of number, momentum and energy balance. However no single source is able to provide all the important data with equal accuracy. In such a case for electrons the completeness of the set is tested by comparing calculated and measured transport data, but for positrons the transport coefficients were rarely measured in the past. Thus we have only shown that the present stage in understanding of charged particle transport is sufficient to interpret old experiments and we advocate building of new experiments. We also analyze kinetic phenomena generated by the very large positronium (Ps) formation cross section which is associated with a process that is non-conservative (number changing). Studies of positron transport allow kinetic theorists an opportunity to analyze the largest observed effect of non-conservative collisions on transport. Finally we show how the data are used to model applications in medicine and, for that purpose, the analysis of collisions and tracks in the human body (consisting mainly of water) may be now performed on the basis of elementary binary processes. Some modifications have to be made for studies in liquids but it turns out that significant changes in the cross sections occur for liquids only below the threshold for Ps formation. In addition the accumulated data and complete sets allow us to model the gas-filled traps used in the experiments and optimize their thermalization and overall performance. New methods of cooling may also be explained based on the knowledge of the binary positron molecule data.

# Atomic, Molecular, and Surface-Interaction Data Needs for ITER

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**Abstract.** Research related to the production of energy from the fusion of atomic nuclei has proceeded steadily for the last half century. One approach is to confine a high-temperature plasma with a magnetic field so that the thermal velocities of the particles are sufficient to overcome the Coulomb repulsion between ions. The “tokamak” has emerged as the preferred research configuration due to a strong performance scaling with size, and the ITER device under construction in France will be a definitive test for thermonuclear (“burning”) plasma physics and reactor-scale engineering. During operation, fuelling, particle beam heating, the introduction of non-fuel elements into the plasma for energy dissipation, and interactions between the plasma and the inner wall of containment vessel can all contribute to atomic, molecular and surface-interaction (AMSI) processes. It is very important, therefore, to have a complete and high quality AMSI data set for use with simulation codes when designing in-vessel plasma-facing components, diagnostic systems, and operational scenarios. An ITER overview will be presented, followed by a discussion of data generation requests for all elements of interest (H, He, Be, C, N, Ne, Ar, Fe, W) for which the current data set is incomplete.

**Keywords:** ITER, fusion, plasma, tungsten

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# Spectroscopic Diagnostics of Highly Charged, Heavy Metal Impurities

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**Abstract.** Tungsten (W) is an important candidate material for a future fusion reactor. Its application as a first wall material is investigated in today's fusion experiments and its diagnosis is developed simultaneously. The latter offers many challenges, which need to be overcome in order to provide a reliable interpretation of the complex W spectra. For the plasma core these challenges are given by the large number of relevant ionization stages, of levels within each ion and of the emitted spectral lines. Experimentally, these spectral lines cannot be separated in all cases, such that hundreds of them form spectral features that are often called quasicontinua. The spectra typically result from integration along a line of sight crossing regions with a wide variety of electron temperatures and densities making an interpretation rely on the knowledge of the ionization and recombination equilibrium of W. The emissions of W between about 500-20000eV measured in today's fusion devices are presented and corresponding model calculations are compared to them. These investigations focus on W-ions with charge stages from about 20+ to 65+. Along with well known spectral signatures of W also puzzling issues in the W spectra are presented in order to document current interests of the tokamak based research on W spectroscopy.

## **A Study of tungsten spectra using Large Helical Device and Compact Electron Beam Ion Trap in NIFS**

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Tungsten spectra have been observed from Large Helical Device (LHD) and Compact electron Beam Ion Trap (CoBIT) in wavelength range of visible to EUV. An impurity pellet (cylindrical carbon with tungsten) is injected to LHD plasmas for observing the tungsten spectra. Radial profiles of EUV spectra from highly ionized tungsten ions have been measured and analyzed with impurity transport simulation code to examine the ionization balance determined by ionization and recombination rate coefficients. In order to observe the tungsten spectra from lower-ionized stages, which can give useful information on the tungsten influx in fusion plasmas, the ablation cloud of the impurity pellet is directly measured with visible spectroscopy. A lot of spectra from neutral and singly ionized tungsten are observed and some of them are identified. A magnetic forbidden line from highly ionized ions of high-Z elements including tungsten observed from LHD plasmas has been analyzed for reconstruction of the atomic structure model in addition to the diagnostic use for D-T burning plasmas. The EUV spectra of tungsten ions, e.g.,  $W^{+24-26}$ , measured from LHD plasmas are compared with those measured from plasmas of CoBIT with monoenergetic electron beam ( $\leq 2\text{keV}$ ). The data are analyzed with collisional-radiative model.

# EBIT Spectroscopy of Highly Charged Heavy Ions Relevant to Hot Plasmas

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**Abstract.** An electron beam ion trap (EBIT) is a versatile device for studying highly charged ions. We have been using two types of EBITs for the spectroscopic studies of highly charged ions. One is a high-energy device called the Tokyo-EBIT, and another is a compact low-energy device called CoBIT. Complementary use of them enables us to obtain spectroscopic data for ions over a wide charge-state range interacting with electrons over a wide energy range. In this talk, we present EBIT spectra for elements relevant to hot plasmas, such as tungsten, iron, gadolinium, etc., after introducing the devices. Tungsten is considered to be the main impurity in the ITER plasma, and thus its emission lines are important for diagnosing and controlling the ITER plasma. We present many previously unreported lines of moderately charged tungsten. Iron is one of the main components of the solar corona, and its spectra are used to diagnose temperature, density, etc. The diagnostics is usually done by comparing observed spectra with model calculations. An EBIT can provide spectra under a well-defined condition; they are thus useful to test the model calculations. Laser-produced gadolinium plasma is a candidate of the 6.7 nm light source for the future EUV lithography. An EBIT has a narrow charge state distribution; it is thus useful to disentangle the spectra of laser-produced plasma containing ions with a wide charge-state range.

# Cross-Section Measurements With Interacting Beams

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**Abstract.** Interacting beams were first employed to determine absolute cross sections for atomic processes nearly a half century ago. Significant advances in many technologies have improved the precision and sensitivity of such experiments to the degree that the high quality of those early measurements seems remarkable today. Despite their early successes and these continuing advances, interacting beams experiments and the determination of absolute cross sections and rate coefficients from them remain a challenge. This presentation will concentrate on one large-scale technical advance, the synchrotron light source, which has facilitated interacting-beams measurements of cross sections for photoionization of atomic and molecular ions. Third-generation electron synchrotrons with insertion devices provide intense, continuously tunable and highly collimated beams of light at extreme ultraviolet wavelengths for which tunable lasers are currently unavailable. Such a photon beam may be merged with an ion beam to determine absolute photoionization cross sections for atomic and molecular ions. Typical results will be presented from such a setup at the Advanced Light Source (ALS), Lawrence Berkeley National Laboratory for free atomic and molecular ions. The  $C_{60}$  molecule has an empty spherical cage structure with a diameter of nearly 1 nm, within which an atom may be trapped, forming a so-called endohedral fullerene molecule. The 4d subshell photoionization of a Xe atom inside  $C_{60}$  ( $Xe@C_{60}$ ) has been predicted theoretically to produce so-called “confinement resonances” that significantly redistribute the Xe 4d oscillator strength relative to that for a free Xe atom. Their origin is multipath interference of photoelectron waves due to possible reflection by the  $C_{60}$  cage. This fundamental phenomenon was observed experimentally for the first time using the merged-beams setup at the ALS with a  $Xe@C_{60}^+$  ion beam current of less than 1 picoampere ( $< 10^7$  ions/second). This measurement is believed to set a record for the sensitivity of a merged-beams experiment.

# The HITRAN Molecular Database

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**Abstract.** This presentation provides an overview of the updates and extensions of the HITRAN molecular spectroscopic absorption database.<sup>1</sup> The new significantly improved parameters for the major atmospheric absorbers (for instance H<sub>2</sub>O and O<sub>2</sub>) have been given particular attention. For most of the molecules, spectral parameters have been revised and updated. The new edition also features many new spectral bands and new isotopic species. The cross-section part of the database has also been significantly extended by adding new species as well as more temperature-pressure sets for existing species. In addition, HITRAN now provides the collision-induced absorption parameters, including those relevant to the terrestrial atmosphere: N<sub>2</sub>-N<sub>2</sub>, N<sub>2</sub>-O<sub>2</sub>, O<sub>2</sub>-O<sub>2</sub>.<sup>2</sup>

The study of the spectroscopic signatures of planetary atmospheres is a powerful tool for extracting detailed information concerning their constituents and thermodynamic properties. The HITRAN molecular spectroscopic database has traditionally served researchers involved with terrestrial atmospheric problems, such as remote sensing of constituents in the atmosphere, pollution monitoring at the surface, and numerous environmental issues. In collaboration with laboratories across the globe, an extensive effort is currently underway to extend the HITRAN database to have capabilities for investigating a variety of planetary atmospheres. Spectroscopic parameters for gases and spectral bands of molecules that are germane to the studies of planetary atmospheres are being assembled. These parameters include the types of data that have already been considered for transmission and radiance algorithms, such as line position, intensity, broadening coefficients, lower-state energies, and temperature dependence values.

A number of new molecules, including H<sub>2</sub>, CS, C<sub>4</sub>H<sub>2</sub>, HC<sub>3</sub>N, and C<sub>2</sub>N<sub>2</sub>, are being incorporated into HITRAN, while several other molecules are pending. For some of the molecules, additional parameters, beyond those currently considered for the terrestrial atmosphere, are being archived. Examples are collision-broadened half widths due to various foreign partners, collision-induced absorption, and temperature dependence factors. Collision-induced absorption data for H<sub>2</sub>-H<sub>2</sub>, H<sub>2</sub>-N<sub>2</sub>, H<sub>2</sub>-He, H<sub>2</sub>-CH<sub>4</sub>, CH<sub>4</sub>-CH<sub>4</sub>, O<sub>2</sub>-CO<sub>2</sub> and N<sub>2</sub>-CH<sub>4</sub> were recently released.<sup>2</sup> Partition sums, that are necessary for applications at a wide range of temperatures, have also been calculated for a variety of molecules of planetary interest,<sup>3</sup> and form an integral part of the HITRAN compilation.

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# Charge Transfer Cross Section Calculations and Evaluations

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**Abstract.** Charge transfer processes in collisions of multi-charged ions with atoms have been subject to extensive theoretical and experimental studies during the last five decades. The important role of these processes in many laboratory and astrophysical plasmas stems from their large cross sections (proportional to the ionic charge) and pronounced final-state-selectivity. With increasing the ionic charge the higher and higher excited states are populated in the electron transfer process the radiation from which can serve as a useful plasma diagnostic tool, such as the widely used charge-exchange-recombination spectroscopy diagnostics in magnetic fusion plasmas. The electron capture processes of multiply charged impurity ions with the neutral hydrogen species are also important in the studies of impurity transport in the edge and divertor plasma regions. By using the full quantal molecular orbital close-coupling, the two-center atomic-orbital close-coupling and the solving time-dependent Schrodinger equation methods, we have calculated the charge transfer processes for numbers of systems, including proton with alkali atoms,  $\text{Be}^{q+}$ ,  $\text{B}^{q+}$  and  $\text{C}^{q+}$  with H,  $\text{N}^{q+}$  with He,  $\text{O}^{q+}$  with H, He and  $\text{H}_2$ , and obtained the radiative and non-radiative total and state-selective charge transfer cross sections for the single- and double-electron capture processes. As an example, we also evaluated the total and state-selective cross section data in the collisions of  $\text{Be}^{q+}$  ( $q = 1-4$ ) with H in a wide collision energy range, and the validity of different methods and the recommended data are presented.



# Propagation of uncertainties in atomic data through collisional-radiative models

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**Abstract.** The demand for meaningful uncertainties on theoretical atomic data has increased in recent years, with a focus on determining and improving the accuracy of spectral diagnostics in a number of key areas. We present an overview of two methods for the generation of such uncertainties on electron-impact excitation, ionization and recombination rate coefficients. These two methods are referred to as 'baseline' and 'method sensitivity' data. From either method the uncertainties can be carried through collisional-radiative models to produce uncertainties on excited populations, photon emissivities and effective ionization/recombination rate coefficients. Baseline data provides a generous estimate of the uncertainties and reflects the likely spread of values in existing databases, or between two approaches. We show some examples of baseline uncertainties for  $O^{6+}$ , and explore issues of distribution functions in the input data and correlation in the derived coefficients. We also discuss possible techniques for the generation of method sensitivity data. Method sensitivity data provides a much tighter constraint on the uncertainties produced by one particular method and includes information on the correlation in the input dataset. We illustrate the potential use of these approaches using some common line ratio diagnostics.

# AtomDB: Atomic Data for X-ray Astrophysics

A. R. Foster

**Abstract.** The AtomDB project collects atomic data from a wide range of theoretical and experimental sources, converts them into useful formats for X-ray astronomers, and provides tight integration with spectral fitting codes to enable easy use of our data by observers in the X-ray band and the wider community.

The project's focus is on collisionally ionized, as opposed to photo-ionized, plasmas. In the latest version we have focused in particular on processes relevant to plasmas which are not in ionization equilibrium, such as shocked material in a supernova remnant, or in coronal flares. Enabling observers to model these features well requires not just a range of new data, such as inner shell excitation and state-selective recombination, but also reorganization of the database and construction of a range of new models for existing spectral fitting codes to enable this expanded data set to be used in without become prohibitively slow.

We present an outline of the changes we have made, combined with examples of the effect of the new data and models on interpretation of spectra from several sources.

# Data Needs for X-ray Satellites

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**Abstract.** In this talk I will review the current status of atomic data for X-ray astronomy satellites. This includes some of the astrophysical issues which can be addressed, current modeling and analysis techniques, computational tools, the limitations imposed by currently available atomic data, and the validity of standard assumptions. I will also discuss ideas for the future: challenges associated with future missions, computational opportunities, and goals for atomic data collection.

# The Role Of Atomic Data In X-Ray Astrophysics

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**Abstract.** Atomic spectroscopy has been one of the main achievements of the X-ray astrophysical missions of the 21<sup>st</sup> century, e.g., *Chandra* and *XMM-Newton*. Consequently, the knowledge of atomic data has played a major role in determining our ability to carry out high precision measurements using X-ray astrophysical observations. A special challenge to observers and to modelers has been ionized Fe, whose emission and absorption spectra have been investigated only to a small degree until about a decade ago. I will review the progress in the availability of Fe atomic data and indicate the few places where I believe we are still lacking. In particular, I will stress the importance of inner-shell absorption spectroscopy, e.g. [1] with an emphasis on Fe K-shell transitions that will be nicely resolved for the first time with the microcalorimeter on board the *Astro-H* mission (to be launched in 2014). I will also describe the difficulties to model Fe L-shell emission from photo-ionized plasmas in active galactic nuclei that have been ongoing since the first measurements of such spectra [2].

**Keywords:** X-Ray Astrophysics, Spectroscopy, Photoionized Plasma

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# Spectral Modeling And Diagnostics In Various Astrophysical Environments

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**Abstract.** In this contribution I discuss various complex astrophysical environments and tools to derive the physical parameters of these environments. Multi-temperature plasmas in extended sources like clusters of galaxies present a challenge in the proper balance between simplicity and detail of the temperature structure, while biases in derived parameters like chemical abundances need to be avoided. Resonance scattering, in particular in Fe XVII lines, is another challenge because of uncertainties in atomic cross sections. I will also discuss recent highlights in modeling the galactic foreground absorption from the mixture of dust, cold and hot gas that is present in our galaxy. The last topic will be photo-ionized plasmas in active galactic nuclei. I will discuss models for the absorption measure distribution as well as time-dependent photo-ionization in these sources. Examples will be given using the SPEX package that was developed at SRON.

# Atomic data for beam-stimulated plasma spectroscopy in fusion plasmas

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Energetic neutral beams of hydrogen and deuterium are extensively used for heating and diagnostics of fusion plasmas. The excited states of hydrogen atoms are strongly affected by the strong fields in the plasma. The Zeeman effect for spectral lines of cold atoms emitted at the plasma edge and the motional Stark effect (MSE) for the injected high-energy atoms put forward new demands on the atomic (primarily collisional) data for the field-modified states of neutrals.

We present the current status of collisional atomic data for the parabolic states of hydrogen atoms which are required for the accurate modeling of MSE. Unlike the field-free emission of hydrogen lines, where only atomic data averaged over the magnetic numbers  $m$  are needed, calculation of collisional data in a translational electric field is more complicated. It is shown that the collisional data require knowledge of the density matrix of excitation including the off-diagonal matrix elements. Comparison between atomic-orbital close-coupling method and eikonal, Glauber and Born approximations is presented. For excitation from the ground state the data are in agreement for higher energies (higher than 100-200 keV/u) while at lower energies significant discrepancies are found.

The new atomic data between the parabolic states of atomic hydrogen were utilized in a collisional-radiative model for H parabolic states extended to  $n=10$ . In addition to proton- and electron-impact excitations and radiative processes, collisional and field-induced ionizations were included as well. The ratio between the  $\sigma$ - and  $\pi$ - components and beam-emission rate coefficients were calculated in a quasi-steady state approximation. A good agreement with the experimental data from JET was found which points out to strong deviations from the statistical distribution for the  $m$ -component populations. The non-statistical effects will also be discussed in detail.

# Charge Exchange Spectroscopy of Multiply Charged Ions of Industrial and Astrophysical Interest

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**Abstract.** As extreme ultra-violet (EUV) light sources for the next generation semiconductor lithography, laser produced plasmas (LPP) and discharge produced plasmas (DPP) of Xe and Sn have been investigated intensively in this decade. In these plasmas, multiply charged Xe and Sn ions emit the radiation near 13.5 nm. However, the emission lines from individual charge states of ions were understood until the emission spectra from charge-selected these ions with charge exchange spectroscopy were observed.

The solar wind charge exchange (SWCX) means the electron capture of multiply charged ions constituting the solar wind in collisions with neutral matters within the heliosphere and has been regarded as a dominant mechanism of the soft X-ray emission in the solar system. In order to analyze the X-ray spectra observed with satellites quantitatively in detail, the X-ray emission cross sections of the SWCX processes are needed by astrophysicists.

Multiply charged ions were produced in a 14.25 GHz electron cyclotron resonance (ECR) ion source with introduction of source gases, namely Xe, O<sub>2</sub>, N<sub>2</sub>, and C<sub>2</sub>H<sub>4</sub> (or CH<sub>4</sub>). For Sn ions, we inserted pellets of sintered tin oxide (SnO<sub>2</sub>) into a plasma chamber in which oxygen plasma had been produced. The ions were fed into a collision chamber after the charge-state separation, and the photon emission following the charge exchange collisions of ions with He, H<sub>2</sub>, and CH<sub>4</sub> gases was observed with spectrometers. A compact flat-field grazing-incident spectrometer (GIS) equipped with a liquid-nitrogen-cooled CCD camera had been used to observe optical radiation in the EUV region (5–38 nm) of Xe and Sn ions at a collision energy of 20 keV/charge. On the other hand, soft X-ray emission spectra in the photon energy range of 400–1000 eV had been observed with a window-less Si(Li) detector at 90° to the ion beam direction and a window-less silicon drift detector (SDD) at a magic angle of 54.7° for C, N, and O ions at collision velocity similar to that of the solar wind.

In the EUV spectra of lower charge Xe ions, individual emission lines have been identified, and it was found that four lines of Xe VII, eight lines for Xe VIII, and nine lines for Xe IX correspond to newly observed transitions. On the other hand, the unresolved transition arrays (UTAs) corresponding to 4d-4p, 4d-4f, and 4d-5p transitions have been observed in the EUV region for Xe X–Xe XVIII and Sn V–Sn XX, and a comparison with calculations using the Hebrew University Livermore Laboratory Atomic physics Code (HULLAC) has been carried out. The theoretical analysis indicates strong interactions between  $4p^6 4d^{k-1} 4f$  and  $4p^5 4d^{k+1}$  configurations, even though the experimental and theoretical results on the wavelengths of UTAs show significant discrepancy in the 4d–4f transition.

Soft X-ray emission spectra in collisions of bare and hydrogen-like C, N, and O ions with neutral target gases show dominant peaks corresponding to  $1s-2p$  and  $1s^2-1s2p$  transitions, respectively. Also, the  $1s-np$  and  $1s^2-1snp$  ( $n = 3 - 5$ ) transitions have been observed with smaller intensities. According to both the classical over-the-barrier model and the quantal atomic orbital close coupling (AOCC) calculations, the dominant capture levels in highly charged ions are higher than  $n = 3$ . This fact means that the cascade processes from higher states to the  $2p$  states are quite significant. We also measured the total single electron capture cross sections using a different experimental setup with the retarding method to separate the charge-state of ions after the collisions. Therefore the intensity ratios and the capture cross sections give the emission cross sections for each  $1s-np$  and  $1s^2-1snp$  transition of hydrogen-like and helium-like ions.

# Laboratory Studies of Primordial Chemistry and Implications for First Star Formation

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## **Abstract.**

During the epoch of protogalaxy and first star formation,  $\text{H}_2$  was the dominant coolant for collapsing primordial clouds at temperatures below 8,000 K. Hence, a reliable model of  $\text{H}_2$  formation and abundance is critical for our understanding of structure formation in the early Universe. The dominant  $\text{H}_2$  formation mechanism during this epoch is initially the associative detachment (AD) reaction  $\text{H}^- + \text{H} \rightarrow \text{H}_2 + \text{e}^-$ . There are a number of reactions, however, which limit the  $\text{H}^-$  abundance available to form  $\text{H}_2$ . One of the most important of these is the mutual neutralization (MN) reaction  $\text{H}^- + \text{H}^+ \rightarrow \text{H} + \text{H}$ . As a cloud continues to collapse and the density increases, the cloud converts to fully molecular, largely through the three body association (TBA) process  $\text{H} + \text{H} + \text{H} \rightarrow \text{H}_2 + \text{H}$ . The energy released by TBA formation of  $\text{H}_2$  heats the cloud and can delay collapse of the cloud. Uncertainties in the rate coefficients for all three of these reactions have limited our understanding of structure formation in the early Universe. Here we will report recent measurements which largely remove the uncertainties for the AD and MN reactions. We will also discuss the experimental challenges of attempting to measure the TBA reaction. This work is supported in part by the NSF Division of Astronomical Sciences Astronomy and Astrophysics Grants program.



# Data Needs For Simulations Of Electron-driven Processes In Planetary And Cometary Atmospheres

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**Abstract.** Sunlight causes photoionization of atoms and molecules in planetary and cometary atmospheres, producing photoelectrons. These cause further ionization, yielding secondary electrons. Electrons in the solar wind, often accelerated by magnetospheric processes, also produce ionization and secondary electrons. In each case the secondary electrons lose energy in further interactions, including dissociation and electronic and vibrational excitation. Radiative decay of the excited species produces light emissions, such as dayglow, nightglow and aurora. Excitation energy can also be lost in collisions between excited molecules and neutral species, sometimes initiating chemical reactions. Thus electron-driven processes are important in determining both the energy balance and composition of planetary and cometary atmospheres.

Simulation of these processes requires accurate atomic and molecular data, such as electron impact cross sections for ionization and excitation, radiative transition probabilities and collisional reaction rates. This will be illustrated by several examples of our recent work in which updated measurements [1-4] or theoretical calculations [5] of atomic and molecular data were applied to simulations of electron cooling by CO<sub>2</sub> at Mars [6], the abundance of CO in comet Hale-Bopp [7], electron heating rates in the atmosphere of Titan [8], infrared emission rates from CO in the atmospheres of Mars and Venus [9], and 630.0-nm emissions in the atmosphere of Europa [10]. Finally, ongoing simulations of emissions from hydrogen in the atmosphere of Jupiter will be described.

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# Molecular Line Lists For Exoplanets and Other Atmospheres

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**Abstract.** At elevated temperatures the spectra of polyatomic molecules become extremely complicated with millions, or even billions, of transitions potentially playing an important role. The atmospheres of cool stars and "hot Jupiter" extrasolar planets are rich with molecules in the temperature range 1000 to 3000 K and their properties are strongly influenced by the infrared and visible spectra of these molecules. So far there are extensive, reliable lists of spectral lines for a number species including some stable diatomics, water, ammonia. However data is almost completely lacking for many key species such as methane.

The ExoMol project ([www.exomol.com](http://www.exomol.com)) aims to construct line lists of molecular transitions suitable for spectroscopic and atmospheric modelling of cool stars and exoplanets [1]. At elevated temperatures it is necessary to consider many millions, even billions, of lines for a single species. Line lists therefore are computed on the basis of robust theoretical models tested against available laboratory data rather than constructed experimentally. Illustrative examples will be discussed and as will progress on obtaining the full set of molecular data. Given the sheer volume of data it is also necessary to consider data representation and storage issues.

## ACKNOWLEDGMENTS

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# Accurate Transition Probabilities from Large-scale Multiconfiguration Calculations

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**Abstract.** The quality and resolution of solar, stellar, and other types of plasma observations, has so improved that the accuracy of atomic data is frequently a limiting factor in the interpretation of these new observations. An obvious need is for accurate transition probabilities. Laboratory measurements, e.g. using ion/traps, beam-foil or laser techniques, have been performed for isolated transitions and atoms, but no systematic laboratory study exists or is in progress. Instead the bulk of these atomic data must be calculated. Multiconfiguration methods, either non-relativistic with Breit-Pauli corrections (MCHF+BP) or fully relativistic (MCDHF), are useful to this end. The main advantage of multiconfiguration methods is that they are readily applicable to excited and open-shell systems, including open  $f$ -shells, across the whole periodic table, thus allowing for mass production of atomic data. The accuracy of these calculations depends on the complexity of the shell structure and on the underlying model for describing electron correlation. By systematically increasing the number of basis functions in large-scale calculations, as well as exploring different models for electron correlation, it is often possible to provide both transition energies and transition probabilities with some error estimate.

The success of the calculations also depends on available computer software. In this talk we will describe a collaborative effort to continue the important and acclaimed work of Prof. Charlotte Froese Fischer and to develop state-of-the-art multiconfiguration codes. In the latest versions of the non-relativistic (ATSP2K) and relativistic (GRASP2K) multiconfiguration codes angular integration is performed using second quantization in the coupled tensorial form, angular momentum theory in three spaces (orbital, spin and quasispin), and a generalized graphical technique that allows open  $f$ -shells. In addition it is possible to transform results given in the relativistic  $jj$ -coupling to the more useful  $LSJ$ -coupling. Biorthogonal transformation techniques are implemented and initial and final states in a transition can be separately optimized. The main parts of the codes are also adapted for parallel execution using MPI. Results from recent large-scale calculations using these codes will be presented for systems of different complexity. Of special interest are spectrum calculations, where all states up to a certain level are computed at the same time. Finally, we look at new computational developments that allow basis functions in multiconfiguration methods to be built on several independent and non-orthogonal sets of one-electron orbitals. Initial calculations indicate that the increased flexibility of the orbital sets allows transition energies, as well as other atomic properties, to be predicted to a much higher accuracy than before.

**PACS:** 31.15.am; 31.15.vj; 31.15.xr; 32.70.Cs

## **Laboratory Spectroscopy and Space Astrophysics: A Tribute to Joe Reader and Friends**

D. Leckrone

Beginning with the launch of the Copernicus Satellite in 1973, and continuing with the International Ultraviolet Explorer (IUE), and the state-of-the-art spectrographs on the Hubble Space Telescope (GHRS, FOS, STIS and COS), astrophysics has experienced dramatic advancements in capabilities to study the composition and physical properties of planets, comets, stars, nebulae, the interstellar medium, galaxies, quasars and the intergalactic medium at visible and ultraviolet wavelengths. It became clear almost immediately that the available atomic data needed to calibrate and quantitatively analyze these superb spectroscopic observations, obtained at great cost from space observatories, was not up to that task. Over the past 3+ decades, Joe Reader and his collaborators at NIST have provided, essentially “on demand”, laboratory observations and analyses of extraordinary quality to help astrophysicists extract the maximum possible physical understanding of objects in the cosmos from their space observations. This talk is a one scientist’s grateful retrospective about these invaluable collaborations.

# Data of Heavy Elements for Light Sources in EUV and XUV and Other Applications

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The spectra of photoemissions due to the transitions between the sub-shell levels in N-sub-shell open atomic ions are of interest for the strong influence from the interactions between the electronic state configurations with different constituent orbitals. The spectral narrowing of the unresolved transition array (UTA) [1] is advantageous for extreme ultraviolet (EUV) light sources. For shorter wavelength light sources, we should investigate the heavier elements. The wavelengths of the 4d - 4f transitions are reported to be, for example, 7.9 nm for Nd ( $Z=60$ ), 7.0 nm for Eu ( $Z=63$ ), and 6.8 nm for Gd ( $Z=64$ ) [2]. Recently, the 4d-4f transitions of Tb at 6.5 nm have been investigated theoretically by Sasaki et al [3].

The photoemissions from W atomic highly charged ions have recently also drawn a strong attention because W has been considered as one of the wall materials in magnetic confinement fusion (MCF) devices. In intermediate stages of ionizations W ions also have open N-sub-shells and exhibit complex emission spectra due to configuration interaction.

Data of atomic ionic states and transition properties of the elements with the atomic numbers  $Z$  ranging 50 ~ 80 are indispensable for the development of the devices using the plasmas containing such heavy elements. We will review the data production and compilations and investigate the current status of the study in this field. We also discuss the recent spectroscopic measurement for W, Gd, and Nd using Large Helical Device (LHD) [4].

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# Data Needs for Low Temperature Plasmas and Accelerator Applications

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**Abstract.** I will describe the needs for scattering, ionization and charge exchange cross sections for the modeling of low temperature plasmas and accelerator applications. These applications require wide range of data in an approximate form that can be used in Monte Carlo procedures. Examples of such description are given in Ref.1 for low temperature plasmas for differential electron scattering in He and Ref.2 for accelerator applications for charge changing (stripping and ionization) collisions between a fast ion and an atom. An analytical approximation for differential cross-section of electron scattering on helium atoms is introduced [1]. It is intended for Monte Carlo simulations, which, instead of angular distributions based on experimental data (or on first-principle calculations), usually rely on approximations that are accurate yet numerically efficient. The approximation is based on the screened-Coulomb differential cross-section with energy-dependent screening. For helium, a two-pole approximation of the screening parameter is found to be highly accurate over a wide range of energies. The values of ion-atom ionization and stripping cross-sections are frequently needed for many applications that utilize the propagation of fast ions through matter. When experimental data and theoretical calculations are not available, approximate formulae are frequently used. Reference [2] briefly summarizes the most important theoretical results and approaches to cross-section calculations in order to place the discussion in historical perspective and offer a concise introduction to the topic. Based on experimental data and theoretical predictions, a new fit for ionization cross-sections is proposed. The range of validity and accuracy of several frequently used approximations (classical trajectory, the Born approximation, and so forth) are discussed using, as examples, the ionization cross-sections of hydrogen and helium atoms by various fully stripped ions. A formulary of analytical approximations for cross-sections is presented.

## ACKNOWLEDGMENTS

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# Chemically reactive species in liquids generated by atmospheric-pressure plasmas and their roles in plasma medicine

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**Abstract.** Plasmas whose gas temperatures are close to room temperature may be generated in ambient air or a gas at atmospheric pressure with the use of low-frequency high voltage or low-power radio-frequency (RF) or microwave power applied to electrodes. Such plasmas can serve as a powerful source of free radicals and/or chemically reactive species that arise from atoms and molecules of the ambient gas. Recently use of such plasmas for medical purposes has attracted much attention as they can be implemented in possible medical devices that can cause blood coagulation, heal wounds, facilitate angiogenesis, sterilize surgical devices as well as living tissues without harming healthy animal cells, and selectively inactivate cancer cells. Especially of interest among reactive species generated by atmospheric-pressure plasmas (APP) are reactive oxygen species (ROS) and reactive nitrogen species (RNS) that are generated in liquid phase. Since most living tissues and cells are immersed in liquids (such as blood or culture media), reactive species generated by APPs in the gas phase are transported to the liquid phase and possibly converted to different types of reactive species therein before causing some influence on the tissues or cells. In this study, we solve rate equations to evaluate concentrations of various reactive species in pure water that are originated by plasma reactions in atmosphere and discuss possible effects of such species (including ROS/RNS) on living tissues and cells.

# Coordinated Activities on Evaluation of Collisional Data for Fusion Applications

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**Abstract.** The research to create sustainable fusion reactions for energy generation is highly inter-disciplinary and requires extensive sets of data on atomic, molecular and plasma-surface interaction (AM/PSI) properties used for modeling the confined plasma and the evolution of the plasma-facing materials. Data are needed for the main plasma species and a variety of impurity elements and molecules and their ions over a wide range of plasma conditions and for plasma interaction with different pure and mixed wall materials. In many cases the uncertainty in the collisional data is poorly known and many data sets have not been critically evaluated due to the technical difficulties and the lack of researchers to carry out data evaluation. However, the need is greatly increasing for evaluated data, and ultimately for a standard reference library for fusion relevant data.

It is the role of the Atomic and Molecular (A+M) Data Unit of the International Atomic Energy Agency to review progress and achievements in the production of AM/PSI data for fusion program, and to encourage international cooperation in measurement, compilation and evaluation of AM/PSI data for fusion. Since 1978 the A+M Data Unit has supported the International Atomic and Molecular Data Centre Network (DCN) where a number of institutions coordinate the production, exchange, compilation, dissemination and evaluation of fusion relevant data. Until recently, DCN activities were focused on producing, compiling and disseminating new data sets in response to demands for non-existing data from the fusion community. With the increasing requests from the fusion community for evaluation of the quality of available data sets, the DCN members discussed on the international coordination and effort to verify and validate the AM/PSI data sets relevant to fusion applications.

The DCN meeting and subsequent Consultancy meetings identified important issues that must be addressed to support data evaluation and, in the longer run, the development of an internationally recommended standard library for AM/PSI data for fusion. A technical meeting on data evaluation is held in Daejeon, Korea, from 4 to 7 September 2012. Approximately 30 people from 11 countries participate to discuss relevant issues: 1) Error Propagation and Sensitivity Analysis, 2) Current Status of Evaluated Data bases, 3) Uncertainty Estimates of Theoretical Data, 4) Experimental Data Evaluation, 5) Data Evaluation Methods and Semi-Empirical Fits and 6) Establishment of Evaluators' Network.

In the present meeting the summaries of the Technical Meeting, the recommendations and conclusions of the Data Centre Network meeting and the Consultancy meetings on data evaluation activities will be presented and the long-term goal to establish the IAEA standard library of fusion relevant atomic, molecular and plasma-material interaction data will be discussed.



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# High Resolution Spectrum of La-Ar Hollow Cathode Lamp in Near-Infrared Region

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**Abstract.** The atomic emission spectra of La-Ar plasma have been recorded using a high-resolution *Bruker IFS-125 HR* Fourier transform (FT) spectrometer with a resolution of  $0.05\text{ cm}^{-1}$  at the Laser Centre of the University of Latvia in Riga. The rare-earth metal lanthanum ( $Z=57$ ) has only one stable isotope,  $^{139}\text{La}$ , with a natural abundance of 99.911%.

For the first time, a systematic analysis of the spectrum of an La-Ar plasma in the near-infrared spectral range is presented. The aim of this work is the classification of spectral lines and a comprehensive study of lanthanum lines covering the region from 833 nm to 1665 nm ( $6000\text{ cm}^{-1}$ - $12000\text{ cm}^{-1}$ ). The classification of spectral lines is done with a classification program [1], which shows all suggestions of possible transitions for the particular wavelength of a spectral line, taking into account the selection rules for electric dipole radiation. The center of gravity wave number of spectral lines could be determined with an accuracy better than  $0.01\text{ cm}^{-1}$ . Because the La spectrum is very dense (which means exhibiting many lines per wavelength interval), the hyperfine structure of La is needed as a "fingerprint" to choose the correct classification for unknown transitions.

In total, 2385 hyperfine structure patterns have been observed in the FT spectra. Of these, 710 are new lines, which are not listed in commonly used wavelength lists [2-7]. We have assigned 418 unclassified lines as atomic La lines and 8 lines as singly ionized La. Further, 199 lines are assigned as atomic Ar lines and 85 lines as singly ionized Ar. Additionally, we have observed 223 lines which have hyperfine structure patterns in FT spectra, but none of them have transition suggestions in the classification program [1]. These transitions should be related to new, as yet unknown energy levels.

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# Electron collisions with hydrogen – data available for applications

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**Abstract.** There are many applications in the astrophysics and plasma physics where data from electron-atom and electron-molecule collision calculations are necessary. Our work has been motivated by astronomers' need for accurate and detailed scattering data. Though electron-atom collisions are almost routinely simulated in many laboratories and institutes around the world, the freely available outcome is still scarce, whether we mean numerical data or free computer program packages. Our aim is to create a universal interface which would provide the astronomers and other physicists with an intuitive tool to retrieve the various cross sections and related quantities for processes of interest without a deep knowledge of underlying atomic codes and methods.

We believe that

- (1) present situation in availability and usability of scattering data requires nontrivial understanding of the atomic physics computations, and substantial effort has to be spent to get relevant data, which makes an astronomer's life difficult,
- (2) freely available scattering data even for such a basic process as the e-H collision are far from satisfactory – they are often too coarse and lack detailed structures such as resonances which can play an important role in applications,
- (3) results of freely available computing packages do not necessarily agree with each other and are often difficult to use.

We addressed these deficiencies in the following way:

- (1) appropriate methods (e.g. exterior complex scaling with the B-spline basis for low energies, higher order distorted wave Born approximation for high energies) has been implemented to judge among existing published programs and available data, they can even be used as a primary source of reliable data,
- (2) fine enough data from which all necessary cross sections and other quantities can be obtained can be precomputed and stored in an appropriate format because obtaining these data is time consuming,
- (3) finally an intuitive interface to get the data of interest from the precomputed data has been created for a casual black-box usage.

ATOMIC DATA FOR THE CHIANTI DATABASE, A. K. Bhatia, NASA/GSFC and E. Landi, University of Michigan

The CHIANTI spectral code consists of an atomic database and a suite of computer programs to calculate the optically thin spectrum of astrophysical objects and to carry out spectroscopic plasma diagnostics. The database includes atomic energy levels, wavelengths, radiative transition rates, collisional excitation, ionization and recombination rate coefficients, as well as data to calculate free-free, free-bound and two-photon continuum emission.

In recent years, we have been pursuing a program to calculate atomic data for ions whose lines have been observed in astrophysical spectra but have been neglected in the literature, and to provide CHIANTI with all the data necessary to predict line intensities.

There are two types of such ions: those for which calculations are available for low-energy configurations but not for high-energy configurations (i.e., C-like, N-like, O-like systems), and ions that have never or only seldom been studied. This poster will summarize the current status of this project and indicate the future activities.

# Computational Atomic Structure

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**Abstract.** There is an increasing demand for accurate atomic data due to advancements in experimental techniques and investments in large scale research facilities. In astrophysics the quality and resolution of solar and stellar spectra has so improved that the accuracy of atomic data is frequently a limiting factor in the interpretation. Accurate atomic data are also required in plasma physics and in other emerging areas such as laser spectroscopy on isotope separators, X-ray lithography, and lighting research. The needs include accurate transition energies, fine- and hyperfine structures, isotope shifts as well as parameters related to interaction with external magnetic fields. Also there is a constant need for transition rates between excited states. Data are needed for a wide range of elements and ionization stages.

To meet the demands for accurate atomic data the COMPUTational Atomic Structure (COMPAS) group has been formed. The group is involved in developing state of the art computer codes for atomic calculations in the non-relativistic scheme with relativistic corrections in the Breit-Pauli approximation [1] as well as in the fully relativistic domain. Here we describe new developments of the GRASP2K relativistic atomic structure code [2, 3]. We present results for a number of systems and properties to illustrate the potential and restriction of computational atomic structure. Among the properties are hyperfine structures and hyperfine quenched rates, Zeeman splittings in intermediate fields, isotope shifts and transition rates [4]. We also discuss plans for future code developments.

**Keywords:** multiconfiguration Hartree-Fock, multiconfiguration Dirac-Hartree-Fock, transition rates, energy structure

**PACS:** 31.15.am; 31.15.vj; 31.15.xr; 32.70.Cs

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# Role of M2 and E3 Transitions for $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ Configurations Level Lifetimes

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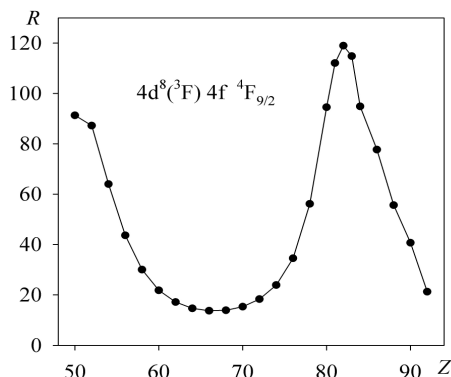
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Theoretical investigation of spectral parameters for multicharged tungsten ions with an open 4d-shell [1] has demonstrated that electric octupole E3 transitions from some levels of the excited configurations  $4p^5 4d^{N+1}$  and  $4p^6 4d^{N-1} 4f$  to the ground configuration  $4p^6 4d^N$  play very important role in determining their lifetimes. This is caused by fact that these are metastable levels with high values of total momentum  $J$ . Hence electric dipole E1 transitions to the ground configuration are forbidden. Furthermore, if magnetic dipole M1 or electric quadrupole E2 transitions from these levels are weak, their radiative lifetimes are strongly influenced by magnetic quadrupole M2 and E3 transitions to the ground state.

In present work we investigate the influence of M2 and E3 transitions on the radiative lifetimes of metastable levels in extended isoelectronic sequences. We use parameter  $R = \tau_{E2+M1}/\tau_{TOT}$  as a measure, where  $\tau_{TOT}$  is a lifetime determined from all (E2, M1, E3, M2) transition probabilities (E1 transition is forbidden),  $\tau_{E2+M1}$  is a lifetime determined from transitions inside configuration. The ratio  $R$  shows how much a lifetime decreases when M2 and E3 transitions are included. The calculations were performed in quasirelativistic approximation [2]. Preliminary calculations have proved that correlation corrections are not important for the studied parameter  $R$ . Therefore the ground configuration  $4p^6 4d^N$  was investigated in a single-configuration approximation; only interaction between two excited configurations  $4p^5 4d^{N+1}$  and  $4p^6 4d^{N-1} 4f$ , which is very strong in multicharged ions, was included for the odd states.

In figure we present dependence of parameter  $R$  on nuclear charge  $Z$  for the  $4d^8 4f^4 F_{9/2}$  level. It is evident that M2 and E3 transitions can reduce calculated radiative lifetimes significantly. If M2 transitions are allowed, they give the main contribution to value of parameter  $R$ . Behaviour of  $R$  presented in this figure is quite representative. Curve bending is caused by different  $Z$ -dependence of non-relativistic and relativistic energy contributions inside and between the configurations. This significantly affects transition probabilities. There is a prominent break of curve when  $Z > 82$ . This behaviour is caused by the situation when investigated level energy becomes higher comparing to other levels of the same parity. Therefore new M1 and E2 transitions become available and their probabilities are increasing.

During calculations we additionally investigated tendencies of interaction between excited configurations along the isoelectronic sequences. Performed investigation confirmed that forbidden M2 and E3 transitions must be included along with transitions inside configurations when the radiative lifetimes of metastable energy levels are determined. We plan to place these transition probability values into our newly created atomic database for astrophysical, technological and laboratory plasma modelling.



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# Assessing The Accuracy Of Spectroscopic Atomic Data For S II Lines

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Absorption-line spectroscopy is a powerful tool used to estimate element abundances in the nearby as well as distant universe. The accuracy of the abundances thus derived is, naturally, limited by the accuracy of the atomic data assumed for the spectral lines. Unfortunately, atomic data such as oscillator strengths or transition probabilities are fairly uncertain for most elements beyond Mg. To improve this situation, we have recently started a project to improve the atomic data used for optical/UV spectral lines using state-of-the-art quantal codes, and incorporate them into the plasma simulation code Cloudy [1]. Here we demonstrate our approach by focussing on S II, an ion used to estimate metallicities for Milky Way interstellar clouds as well as distant damped Lyman-alpha (DLA) and sub-DLA absorber galaxies. We report new improved calculations of a large number of energy levels and the oscillator strengths for all S II electric dipole, magnetic dipole, electric quadrupole, and electric octupole transitions.

Our calculations are based on the configuration interaction (CI) method within a numerical Hartree-Fock framework and Breit-Pauli (BP) approach to include relativistic corrections. We implement significant additions to the multiconfiguration Hartree-Fock code used in previous calculations by adopting the transformed radial orbitals (TRO) [2] to describe radial functions of the electrons in virtually excited configurations with the principal quantum number  $n > 3$ . In parallel, we perform similar calculations using original quasirelativistic Hartree-Fock method (QRHF) [3] with TRO in order to assess the accuracy of generated atomic data because a very similar set of configurations is implemented in both BP and QRHF calculations.

The results of these improved atomic calculations are then incorporated into Cloudy and applied to a typical DLA, for illustrative purposes. Our calculations agree closely with those from previous works, and imply only modest changes ( $\approx 0.04$  dex) to the metallicity estimated from S II in past studies.

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# IAEA Projects on Atomic, Molecular and Plasma-material Interaction Data for Fusion

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**Abstract.** The IAEA Atomic and Molecular Data Unit, part of the Nuclear Data Section, has the mission to support the development of fusion energy by providing internationally evaluated and recommended data for atomic, molecular and plasma-material interaction (A+M+PMI) processes. The Unit organizes various technical meetings and coordinates an international A+M Data Centre Network (DCN) and an international Code Centre Network (CCN). Currently the IAEA activities involving the DCN and CCN are primarily focused on data evaluation as is described in the presentation by H.-K. Chung at this conference. In addition the Unit organizes Coordinated Research Projects (CRPs), for which the objectives are mixed between development of new data and evaluation and recommendation of existing data. The ongoing and new CRPs are briefly described here and in the poster.

The Unit manages 3 active CRPs on atomic and molecular processes. The CRP on “Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions” (2009-2013) is focused on collisional data for elements H-O and their hydrides in fusion edge plasma. The CRP on “Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV” (2010-2014) aims to provide comprehensive recommended data for tungsten impurity in core and edge plasma. The CRP on “Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma” has the objective to develop a comprehensive database for the main species in divertor and edge plasma. These 3 CRPs were described in more detail already at the 2010 ICAMDATA meeting.

The Unit’s new and planned CRPs are all in the area of plasma-material interaction. The wall materials of most interest in current fusion devices are beryllium, tungsten and various carbon-based materials. However, graphite and CFCs look unattractive for a reactor due to their propensity to absorb tritium. ITER will operate with a Be-W wall and since about a year the JET experiment is operating with a Be-W “ITER-Like Wall”. For beryllium the main concerns are wall lifetime (gross erosion) and tritium retention whereas for tungsten in ITER the main concern is plasma contamination. For tungsten in a reactor there are concerns associated with radiation damage and transmutation and their effect on tritium retention that need to be understood. Beyond ITER some low activation steels are seen as candidates for the main wall instead of beryllium. With this in mind the Unit is starting a CRP on “Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials” set to have its first meeting 26-28 September 2012. We anticipate a CRP on “Plasma-wall Interaction for Irradiated Tungsten and Tungsten Alloys” to start early in 2014. Tentatively the next CRP to start after that is one on “Plasma-wall Interaction with Low-activation Steel Surfaces”, but this would be only in 2015 and plans are subject to change.

# Light Polarization And Quantum Interference Effects In Unresolvable Atomic Lines Applied To A Precise Measurement Of The $^{6,7}\text{Li}$ D<sub>2</sub> Lines

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**Abstract.** Precise measurement of the isotope shift of the lithium  $2s \rightarrow 3s$  and  $2s \rightarrow 2p$  (D) lines has been proposed [1] and subsequently used [2] as a sensitive probe of nuclear charge radii, including halo nuclei in unstable isotopes. Despite this success, large discrepancies have remained among observations of D lines of the stable isotopes. We find that when the excited state splittings are of order the excited state natural linewidths, as is the case for the D<sub>2</sub> line of lithium, light-polarization-dependent quantum interference modifies the lineshape and represents an overlooked but significant systematic effect. We present expressions for the corrected line shapes and demonstrate that they yield consistent line centers for arbitrary polarization of the excitation laser.

In our experiment Doppler free spectra were collected using a tunable single-frequency diode laser referenced to a frequency comb [3]. We analyze spectra of the  $^{6,7}\text{Li}$  D<sub>2</sub> lines taken at various excitation laser polarizations and show that failure to account for the quantum interference changes the inferred line strengths and shifts the fitted line centers by as much as 1 MHz, a systematic effect large enough to account for discrepancies between previous measurements. We obtain revised values for the absolute transition frequencies of the unresolvable  $^{6,7}\text{Li}$  D<sub>2</sub> features. Combining these with our previous results for the D<sub>1</sub> lines [3], we derive the  $^{6,7}\text{Li}$  excited state fine structure intervals, the  $2s \rightarrow 2p$  isotope shift, the splitting isotope shift and the relative nuclear charge radii [4]. This analysis should also be important for precise spectral measurements in a number of other species including partially resolved D<sub>2</sub> lines in hydrogen, lithium, potassium, francium, and singly-ionized beryllium and magnesium.

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# Analysis of Matrix Absorption Effects for Fe via WDXRF and EDXRF

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**Abstract.** In the present work, the matrix effects in X-ray fluorescence analyses have been investigated for Fe using both EDXRF (energy dispersive X ray fluorescence) and WDXRF (wave length dispersive X ray fluorescence). The absorption matrix effects of Fe element have been obtained and these effects have been corrected using appropriate correction methods.

All the samples which were prepared appropriately for measurements have been pressed using a Spex (Cat. B25) pressing machine to form pellet samples. These samples have been analyzed in EDXRF and WDXRF spectrometers. In the present study, the  $K\alpha$  X ray fluorescence spectra of Fe have been analyzed in all samples. The characteristic spectra of Fe have been obtained by transferring the data obtained from these systems in to demo version of OriginPro 7.5 computer program. Consequently, these data were then used to obtain the absorption effects curves for  $K\alpha$  lines of Fe and the matrix corrections have been done using an appropriate method.

The obtained results have been evaluated statistically. Moreover, the use of different techniques have been compared using the obtained results since two different system (EDXRF and WDXRF) have been used in the study.

**Keywords:** Matrix effect, absorption, enhancement, WDXRF, EDXRF.



# Ab Initio Approach To The Study Of Transient States And Ultra-Fast Processes

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**Abstract.** Recent advances in attosecond XUV pulse generation pave the way for time-resolved investigation and control of electron wave-packets [1]. The interpretation of this as well as of similar experiments often relies on single-particle models where the interaction of the photoelectron with the remaining electrons in the atom is approximated by a local static potential. The assumptions at the basis of these models, however, come with two major limitations: they do not account for the underlying many-electron processes that unfold on the same time-scale as the photoelectron emission, and they do not properly enforce the exclusion principle.

In this contribution, we report on the development of a package that aims at integrating the Time-Dependent Schrödinger Equation (TDSE) including many-body effects, as well as providing reliable ab initio data of use in atomic attophysics, e.g. photoelectron phases – which relate to so-called photoionization time delays –, multi-photon ionization cross-sections, and resonance properties. We follow a configuration interaction approach with orbitals expanded on B-spline basis sets. For dealing with the complicated angular integration involved in computing matrix elements, we use the Atomic Structure Package (ATSP2K) [2]. In order to avoid problems due to the finite box, in time independent computations, we solve the many-body problem along complex radial coordinates, i.e. using the (exterior) complex scaling method.

Photoionization cross-sections and resonance widths are reported using (i) time-independent perturbation theory combined with complex scaling, and (ii) integration of the TDSE. We also present photoelectron phases obtained using exterior complex scaling.

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# E1 transitions in Ni II

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**Abstract.** We have undertaken an extensive CI calculation of E1 transitions between all levels of the  $3d^9$ ,  $3d^84s$ ,  $3d^74s^2$  and  $3d^84p$ ,  $3d^74s4p$  configurations of Ni II. Many of these lines are observed in a variety of astronomical objects, and so atomic data is needed, with a good level of accuracy, for the analysis of the observational data. To date, only a limited number of extensive calculations have been undertaken for this ion [1,2] while experimental [3,4,5] or observationally derived [6,7] atomic data are limited to an even smaller selection of lines.

In this work, we have used the general CI code CIV3 [8] in which relativistic effects are incorporated using the Breit-Pauli approximation. In addition, *ab initio* results are enhanced by our fine-tuning process which seeks to bring the calculated energy levels into line with experimental levels.

For many of the lines studied, our results are in good agreement with those of [1,2]. But it is not always so. This is illustrated below for oscillator strengths (length form) of a very small selection of  $4s - 4p$  lines, with a common lower level.

Transition	Oscillator strengths		
	This work	[1]	[2]
$3d^8(^3P)4s\ ^2P_{0.5}^o - 3d^8(^3P)4p\ ^2P_{1.5}^o$	0.0870	0.2264	0.2511
$3d^8(^3P)4s\ ^2P_{0.5}^o - 3d^8(^1D)4p\ ^2P_{1.5}^o$	0.0602	0.0321	0.0271
$3d^8(^3P)4s\ ^2P_{0.5}^o - 3d^8(^3P)4p\ ^2D_{1.5}^o$	0.3904	0.3062	0.3008
$3d^8(^3P)4s\ ^2P_{0.5}^o - 3d^8(^3P)4p\ ^4S_{1.5}^o$	0.0098	0.0035	0.0002
Total	0.5474	0.5682	0.5782

so, although the total of the four f-values is almost the same, there is a significant variation in the distribution of the oscillator strength, due to different CI mixings in the upper levels. For example, for the  $3d^8(^3P)4p\ ^2P_{1.5}^o$  level, the main percentage compositions are

$$\begin{array}{ll} \text{Our work} & 45\%(3d^8(^3P)4p\ ^2P_{1.5}^o) + 29\%(3d^8(^1D)4p\ ^2P_{1.5}^o) + 14\%(3d^8(^3P)4p\ ^4S_{1.5}^o) \\ \text{Kurucz} & 69\%(3d^8(^3P)4p\ ^2P_{1.5}^o) + 15\%(3d^8(^1D)4p\ ^2P_{1.5}^o) + 9\%(3d^8(^3P)4p\ ^2D_{1.5}^o) \end{array}$$

Further results and discussion will be presented at the conference.

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# FLYCHK At NIST : The Population Kinetics Modeling Capability

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**Abstract.** Plasma spectroscopy plays an important role in the diagnosis and design of laboratory plasma experiments. With the development of novel plasmas, which access physical regimes in extreme conditions, a general plasma modeling capability is required. This capability is needed to assist in design and analysis of spectroscopic data for a wider range of plasma conditions than previously considered. As a response we have developed FLYCHK [H.-K. Chung, M. H. Chen, W L Morgan, Y. Ralchenko and R. W. Lee, HEDP **1**, 3 (2005)] which is a simple, generalized, non-LTE population kinetics and spectrum generator that provides charge state distributions and synthetic spectra. FLYCHK has been benchmarked against experiments and other kinetics codes and found to provide charge state distributions comparable with both measurements and calculations for most laboratory conditions. At present, an initial version of FLYCHK is implemented at NIST making it widely available to the community with a simple, easy-to-use, fast, and portable interface. Currently, we have 55 users from 14 countries who apply FLYCHK in the area of plasma spectroscopy. We present benchmarked results of FLYCHK, the current status of the code implementation at NIST, and plans for future developments.

**PACS:** 52.25Jm; 52.25Os;52.40Db;52.70-m

# The IRON Project, The Iron Opacity Project, and Astrophysical Diagnostics

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**Abstract.** The aims of the Iron Project are detailed study of radiative and collisional processes of astrophysically abundant atoms and ions, mainly iron and iron-peak elements, over a wide energy range, from infra-red to X-rays, and application to astrophysical problems. The project has been extended to the Iron Opacity Project to study the solar opacity problem. The discrepancy in the solar iron opacity in the convection zone due to particularly the iron ions from Fe~XVI to Fe XX is being investigated in collaboration with the experimental group at Sandia National Lab. We will report progress on the work including hitherto neglected atomic physics of resonances which are largely treated as lines in existing opacities calculations.

With inclusion of higher order relativistic effects in the Breit-Pauli R-matrix (BPRM) codes, under the Iron Project, high accuracy collision strengths are being computed for second row elements for astrophysical diagnostics in nebular plasmas. One of the most fundamental astrophysical problem has been the discrepancy in the abundances of these elements obtained from collisionally excited lines (CEL) and those from recombination lines (REL). Using the BPRM method, we find significant effects due to fine structure couplings in the low energy region. There are resonances produced only from fine structure, but not allowed in LS coupling. We present highly resolved collision strengths of Ne V for 10 low lying transitions in the infrared transitions that are used as temperature and density diagnostics of nebular as well as dust obscured astrophysical objects. Fine structure transitions among the ground state levels  $1s^2 2s^2 2p^3 P_{0,1,2}$  give rise to the well-known 14.3  $\mu\text{m}$  and 24.3  $\mu\text{m}$  lines. We will illustrate the effect of improved collision strengths on temperature and density sensitive line ratios of these lines. The study of the fine structure effects in low energy will be extended to the recombination process.

# Branching Ratios For The Radiometric Calibration Of EUNIS-2012

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**Abstract.** The Extreme Ultraviolet Normal Incidence Spectrograph (EUNIS) sounding rocket instrument is a two-channel imaging spectrograph that observes the solar corona and transition region with high spectral resolution and a rapid cadence made possible by unprecedented sensitivity. The upcoming flight will incorporate a new wavelength channel covering the range 524–630 Å, the previously-flown 300-370 Å channel, and the first flight demonstration of cooled active pixel sensor (APS) arrays. The new 524–630 Å channel incorporates a Toroidal Varied Line Space (TVLS) grating coated with B<sub>4</sub>C/Ir, providing broad spectral coverage and a wide temperature range of 0.025 to 10 MK. Absolute radiometric calibration of the two channels is being performed using a hollow cathode discharge lamp and NIST-calibrated AXUV-100G photodiode. Laboratory observations of He I 584 Å and He II 304 Å provide absolute radiometric calibrations of the two channels at those two respective wavelengths by using the AXUV photodiode as a transfer standard. The spectral responsivity is being determined by observing line pairs with a common upper state in the spectra of Ne I-III and Ar II-III. Calculations of *A*-values for the observed branching ratios are in progress.

# Fast beam experiments on XUV and soft-X-ray photofragmentation of molecules

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**Abstract.** In harsh radiative environments, molecules can be broken following the production of valence or inner-shell vacancies. For polyatomic structures, the molecular breakup patterns generated by photofragmentation comprise smaller, charged and neutral molecules and atoms, which are characteristic for the specific potential surfaces created by the initial photoexcitation or ionization step. Beside the initial electronic transition, the molecular breakup pattern in particular reflects the propagation of the nuclei or molecular sub-units on the relevant potential surfaces (as well as the ones becoming relevant by dynamical couplings to other electronic states on the fragmentation pathway). While such unimolecular reaction data are required in various fields – astrochemistry, planetary and atmospheric research, radiation biochemistry, and others – experimental results, especially for neutral fragments and fragment radicals, are often not available and reliable theoretical predictions often not in reach.

At the free electron laser FLASH (HASYLAB, DESY, Hamburg) [1], we have developed the ion beam infrastructure TIFF [2,3] to study molecular photofragmentation by XUV and soft-X-ray photons in multi-fragment coincidence measurements in the crossed-beams geometry. In recent measurements, we obtained the main fragmentation channels triggered by ~30–100 eV photons for protonated water [3,4], protonated water clusters [4,5], the water (H<sub>2</sub>O<sup>+</sup>) cation [6], and others. The fragmentation momenta were used to obtain kinetic energy releases, fragmentation angular distributions, and angular geometries for three-body fragmentation channels. Moreover, we identified the photofragmentation channels, determined their branching ratios, and the absolute photofragmentation cross section. Recently, also first results were obtained for photoelectron energies which reveal the molecular vacancy states created by the incident XUV and soft-X-ray radiation. Further measurements are planned to study polyatomic photofragmentation and molecular structures of interest in astrochemistry and other fields.

This work was partly supported by the Max-Planck Working Group (ASG) at the Centre for Free Electron Lasers, Hamburg, Germany, and the Lundbeck Foundation.

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# Estimation of total radiation of $C^{2+}$ - $C^{5+}$ ions in Large Helical Device based on VUV and EUV spectroscopy

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Carbon is only an abundant impurity in recent fusion devices. In order to investigate the carbon radiation loss, the resonance transitions of CIII (977.03Å:  $2s^2\ ^1S_0-2s2p\ ^1P_1$ ), CIV (1550Å:  $2s\ ^2S-2p\ ^2P$ ), CV (40.27Å:  $1s^2\ ^1S_0-1s2p\ ^1P_1$ ) and CVI (33.73Å:  $1s\ ^2S-2p\ ^2P$ ) are measured from high-temperature plasmas in Large Helical Device (LHD) since such transitions occupy a large part of the radiation loss in each ionization stage. Absolute intensities of the CV and CVI resonance transitions are observed by an extreme ultraviolet (EUV) spectrometer and those of the CIII and CIV resonance transitions are observed by vacuum ultraviolet (VUV) spectrometers. All the spectrometers are absolutely calibrated based on bremsstrahlung continuum emitted from the LHD plasma. The total radiation power from  $C^{2+}$  to  $C^{5+}$  ions are calculated by the collisional-radiative (CR) model based on the measured resonance line intensities. The calculated result shows that the radiation loss from  $C^{2+}$  and  $C^{3+}$  ions increases with electron density, whereas the radiation loss from  $C^{4+}$  and  $C^{5+}$  ions almost keeps constant with the electron density. It indicates the impurity screening induced by stochastic magnetic field layer called 'ergodic layer' existing in the outside of main plasma with well-defined magnetic surfaces in LHD. The radiation loss from  $C^{3+}$  ion is two times bigger than that from  $C^{2+}$  ion, but it is negligible compared with that from  $C^{5+}$  ion. The total radiation losses from  $C^{4+}$  and  $C^{5+}$  ions are around 50kW in the present LHD plasma, which is much smaller than the total input power, e.g., 10-20MW. The total radiation is also compared among each ionization stage. The result is discussed with carbon transport and edge plasma parameters.

# NIST Atomic and Molecular Databases on the World Wide Web

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**Abstract.** At the National Institute of Standards and Technology (NIST), the Information Office coordinates and facilitates the electronic dissemination of information for the Physical Measurement Laboratory (PML). The Information Office is responsible for PML World Wide Web (WWW) pages at <http://physics.nist.gov> and the Information Office is engaged with PML Divisions and the NIST Standard Reference Data Program in developing physical reference databases for WWW dissemination. A list of available databases can be found at <http://physics.nist.gov/data>.

In collaboration with the Atomic Physics Division the following databases are available online:

- Atomic Spectra Database
- Fundamental Physical Constants Database
- Electron-Impact Ionization Cross Section Database
- Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibrations
- Ground Levels and Ionization Energies for the Neutral Atoms
- Bibliographic Databases are available for Atomic Transition Probabilities, Atomic Spectral Line Broadening and Shifts, Atomic Energy Levels and Spectra, and Fundamental Constants.

An Elemental Data Index provides access to the holdings of online Physical Reference Data organized by element. The Elemental Data Index is designed to simplify the process of retrieving online scientific data for a specific element. Additional databases of interest include the Atomic Weights and Isotopic Compositions Database and a variety of molecular spectroscopic databases.

NIST's Information Office has been involved in developing an XML (eXtensible Markup Language) schema, called UnitsML, for encoding measurement units in XML. Adoption of this schema will allow for the unambiguous exchange of numerical data over the World Wide Web.



# BASECOL2012: A Collisional Database Repository and Web Service within VAMDC

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The BASECOL2012 [1] database (<http://basecol.obspm.fr>) is a repository of collisional data and a web service within the Virtual Atomic and Molecular Data Centre [2, 3] (VAMDC, <http://www.vamdc.eu>). Basecol contains rate coefficients for the collisional excitation of rotational, ro-vibrational, vibrational, fine and hyperfine levels of molecules by atoms, molecules and electrons, as well as fine structure excitation of some atoms, which are relevant to interstellar and circumstellar astrophysical applications. Additional features are provided such as information on and critical evaluation of the rate coefficient calculations, fitted functions for many available rate coefficients and a section for community information.

In addition BASECOL2012 provides spectroscopic data queried from the Cologne Database for Molecular Spectroscopy database (CDMS <http://www.astro.uni-koeln.de/cdms>) [4], the Jet Propulsion Laboratory catalogue (JPL, <http://spec.jpl.nasa.gov/>) [5], the High-resolution TRANsmission molecular absorption database (HITRAN, <http://www.cfa.harvard.edu/hitran/>) [6] using the VAMDC technology. These spectroscopic data are conveniently matched to the in-house collisional excitation rate coefficients using the SPECTCOL software package [7,8] (<http://vamdc.eu/software>) and the combined sets of data can be downloaded from the BASECOL2012 website. Being a partner of the VAMDC, BASECOL2012 is accessible from the general VAMDC portal (<http://portal.vamdc.eu>) and from user tools such as SPECTCOL.

## Acknowledgements

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# Virtual Atomic and Molecular Data Centre: An interoperable infrastructure

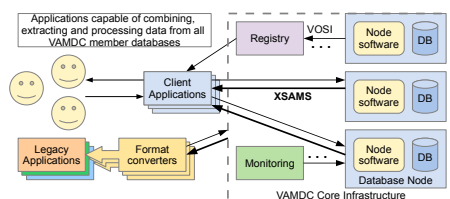
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The Virtual Atomic and Molecular Data Centre (VAMDC, <http://www.vamdc.eu>) is an international Consortium that combines the expertise of existing Atomic and Molecular (A&M) databases, data producers and service providers with the specific aim of creating an interoperable e-science infrastructure that is easily tuned to the requirements of a wide variety of users in academic, governmental, industrial or public communities. It has started thanks to a major European initiative (FP7 ERA funding) with the aim to build a unified, secure, documented, flexible and interoperable e-science environment-based interface to existing A&M data. The VAMDC defines standards for the exchange of atomic and molecular data, develop reference implementation of those standards, deploys registries of internet resources (“yellow pages”), designs user applications in order to meet the user needs, builds data access layers above databases to provide unified outputs from these databases, cares about asynchronous queries with workflows and connects its infrastructure to the grid.

The paper describes the current ‘Level 3’ service deployment of the VAMDC data infrastructure across



our 20 databases.

Note: The VAMDC satellite meeting (<http://physics.nist.gov/Icamdata/index.php?view=meetings>) will expose VAMDC to the US community and vice versa and will aim to initiate collaborations between database providers and users with VAMDC.

## Acknowledgements

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# Multiconfiguration Dirac-Hartree-Fock energy levels, wavefunction compositions, and transition probabilities for W XXXVIII

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## Abstract.

Energies, lifetimes, and wave function compositions have been computed for all levels of  $4p^64d$ ,  $4p^64f$ , and  $4p^54d^2$  configurations. Single- and double excitations were used to generate expansions for the multiconfiguration Dirac-Hartree-Fock (MCDHF) approximation from an active set of orbitals with maximum  $nl$  quantum numbers of  $4f$ ,  $5g$ ,  $6h$ , respectively. For the even states, the excitations were from  $4s^24p^64d$  with an inactive Ni-like core, but for odd levels the excitations were from both  $4s^24p^64f$  and  $4s^24p^54d^2$ . Orbitals were optimized in groups of levels specified by  $J$  and parity.

A newly extended version [1] of the general relativistic atomic structure package, GRASP2K [2], was used to deal with configuration state functions with as many as six open shell and with configurations containing as many as three  $f$ -electrons in a subshell. Also included in this package is a new JJ2LSJ program that rapidly transforms a specified portion of the wavefunction from  $jj$ -coupling to intermediate LSJ-coupling. The present calculations were a test-case for this code for complex, relativistic atomic systems.

Calculations were performed systematically so that the convergence of the levels could be monitored as a function of the increasing size of the orbital sets used in the expansion. Configuration interaction calculations were performed to include Breit and QED corrections.

The E1, E2, M1 transition probabilities between all these levels and their computed and lifetimes will be presented. Results will be compared with other theory [3] and with experiment [4], when available. The present wavelengths are in good agreement with experiment although there is a discrepancy in the composition for the upper level with the highest transition to the ground state.

**Keywords:** multiconfiguration Hartree-Fock, multiconfiguration Dirac-Hartree-Fock, transition rates, energy structure

**PACS:** 31.15.am; 31.15.vj; 31.15.xr; 32.70.Cs

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# Computation Of Atomic Transition, Ionization and Recombination Properties

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**Abstract.** During the past decade, the RATIP program has been developed to calculate the electronic structure and properties of atoms and ions. The design and implementation of the program is presented, and selected applications are discussed.

The RATIP program has been developed during the past years to calculate the electronic structure and properties of atoms and ions [1]. Today, these tools provide a powerful platform for studying atomic processes of open-shell atoms and ions at storage rings, ion traps as well as in plasma and intense radiation fields, including photo excitation, ionization and Auger processes. Although the main focus in developing these tools has been paid on processes with just one electron in the continuum, recent emphasis was placed also on second-order processes as well as those properties for which different types of (many-electron) amplitudes need to be combined in order explain complex spectra. Here, I present and discuss the present capabilities of the RATIP tools of which a major part now became public [2]. Recent applications of the code refer to the radiative [3] and di-electronic recombination [4] as well as the Coulomb excitation of multiple and highly charged ions [5].

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# Energies for States of the $2s^22p^5$ and $2s2p^6$ in Fluorine-like Ions Between Si VI and W LXVI

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**Abstract.** Energies from relativistic configuration interaction (RCI) calculations are reported for the states of the  $(1s^2)2s^22p^5$  and  $2s2p^6$  configurations in all fluorine-like ions between Si VI and W LXVI. Valence, core-valence, and core-core correlation effects were accounted for through single-double expansions to increasing sets of active orbitals.

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The experimental energy levels and computed energies from the largest RCI calculations including QED corrections are displayed in Table 1. The computed energies agree very well with experimental values. Starting from Si VI the energy differences rapidly goes down to a few hundred  $\text{cm}^{-1}$ , which corresponds to an error of around 0.02 %.

From Sr XXX to Sn XLII experimental energies are given with error bars between 1000 and 2000  $\text{cm}^{-1}$ . The calculated values are within the stated experimental error bars except for Cd XL and Sn XLII. The reason for the difference in these two ions is not known. Experimental data for ions from Sb XLIII to Ta LXV are not available. For the W LXVI ion, the differences between theoretical and experimental transition energies are a few thousand  $\text{cm}^{-1}$ . As discussed by Kramida [1] the total uncertainties of the measured energies in W LXVI were dominated by the calibration uncertainties and varied in the range 1.0 - 2.3 eV, which translates to 8000 - 20000  $\text{cm}^{-1}$ . Based on the comparison between theory and experiment for the lighter ions as well as for W LXVI we estimate that the errors in the calculated transition energies for ions in the range Sb XLIII - Ta LXV, for which no experimental data are available, are less than 0.08 %.

**TABLE 1.** Energy levels in  $\text{cm}^{-1}$

Level	$J$	Si VI			W LXVI		
		Calc.	Obs. [2]	Diff.	Calc.	Obs. [2]	Diff.
$2s^22p^5\ ^2P^o$	3/2	0			0		
	1/2	5093.02	5090.00	3.02	11203964.89	11201971.55	1993.34
$2s2p^6\ ^2S$	1/2	407480.13	406497.00	983.13	15049974.97	15054000.00	-4025.03

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# The Structure of Atom

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**Abstract.** Rutherford's Gold foil experiment has proved that an atom has a positively charged nucleus and most of the mass of an atom is concentrated in the nucleus alone. However, even though his experiment did not provide any information about the state of electrons in atoms, he proposed that, electrons are moving around the nucleus at high speed. To explain peaked absorption and emission lines produced by atoms of different elements, Bohr proposed that, electrons can travel around the nucleus only in well defined energy levels or orbitals. When an electron absorbs a photon of light, it jumps from an inner low-energy level to an outer high-energy level. He believed that an atom emits a photon of light when an electron jumps from a high-energy level to a low-energy level. Keeping in mind this motion of electrons around the nucleus, de Broglie proposed his matter wave hypothesis. Later, Davisson- Germer and G.P. Thomson performed experiments with artificially created electron beams, proved that matter in motion demonstrates a wavelike behavior, which eventually led to the development of the present wave mechanical (or atomic orbital) model of atom. But in reality, there is no experiment has ever proved that electrons are moving around the nucleus. Volume of atoms and elastic nature of atoms (e.g. gas atoms move randomly and bounce when they collide with other atoms or its container) indicate that, the nucleus of an atom is surrounded by a form of elastic matter. Since the space inside an atom is filled with this matter, we can call this matter as 'space matter'. Atom of an element produces unique emission spectrum when it is excited, and in cold state, the same atom produces absorption spectrum with exactly matching wavelengths of the emission spectrum indicate that electrons in an atom are situated in some kind of resonant columns. Since the nucleus of an atom is enveloped by space matter, we can conclude that, these resonant columns are formed by space matter. Electron configuration in an atom is determined by three factors: a) attraction from the nucleus, b) repulsion between electrons and c) force exerted by space matter, i.e. the buoyant force. Buoyant force is the only force which prevents the innermost electrons of an atom from collapsing in to the nucleus. For the electrons other than one nearest to the nucleus, buoyant force exerted by space matter and repulsion with the electrons from the inner region keep the electrons in its respective positions.

# Electron Impact Excitation of Mg VIII

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Mg VIII emission lines are present in the solar corona and are a common feature in the spectra of Seyfert galaxies [1]. For example, the [Mg VIII] 3.03  $\mu\text{m}$  line has been detected in the planetary nebula NGC 6302 as well as NGC 5548, 5929 and 1068 [2]. Accurate data for Mg VIII is important since it helps in the understanding of the coronal line region in active galactic nuclei.

In the present work collision strengths were calculated for all 7750 transitions between 125  $jj$  levels of Mg VIII, extending the work of Zhang et al. (1994) [3] and Bhatia & Thomas (1998) [4]. The 125 fine-structure levels included in the calculation arise from the  $2s^22p$ ,  $2s2p^2$ ,  $2p^3$ ,  $2s^23s$ ,  $2s^23p$ ,  $2s^23d$ ,  $2s2p3s$ ,  $2s2p3p$ ,  $2s2p3d$ ,  $2p^23s$ ,  $2p^23p$  and  $2p^23d$  configurations. The latest RMATRIXII suite of codes [5] was employed for the internal region R-matrix calculation to yield  $LS$  coupled results. The results were transformed into intermediate coupling via the code FINE which requires the use of term coupling coefficients. The external region STGF code [6] was utilised to obtain the final set of fine-structure collision strengths.

The collision strengths have been averaged over a Maxwellian distribution of electron velocities to yield the astrophysically important effective collision strengths. The results will be presented at the conference.

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# An in-depth correlation study of the ground term transition in Ag-like tungsten and its isoelectronic neighbours

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Tungsten, because of its excellent thermo-mechanical properties and its very low erosion under various physical and chemical conditions, is considered as a strong candidate for the plasma facing material for future fusion devices. But as a heavy element, it exhibits very high radiation power, so a small fraction of W atoms in a fusion plasma could lead to dramatic effects on the plasma temperature and thereby degrade the plasma performance.

We present an experimental and theoretical study of the  ${}^2F_{5/2} - {}^2F_{7/2}$  fine structure energy in Ag-like W ( $W^{27+}$ ). The experimental energy was obtained through measuring the wavelength of the  ${}^2F_{5/2} - {}^2F_{7/2}$  M1 transition using the Shanghai permanent magnet EBIT. The theoretical value was obtained using the GRASP2K [1] set of computer codes and included a comprehensive correlation study, including core valence correlation of all core sub-shells and an estimate of core-core correlation in all shells. The experimental M1 wavelength was measured as  $3377.4 \pm 0.26 \text{ \AA}$  ( $3378.4 \text{ \AA}$ , vacuum wavelength). We performed two different calculations resulting in  $3378.0$  and  $3381.8 \text{ \AA}$ , which is in excellent agreement with the experiment. This shows the importance of fully understanding the electron correlation effects to predict the energy of the fine structure even in this, for tungsten, relatively simple case.

The presence of tungsten ions in a fusion plasma will also form other atomic species. We have therefore extended the analysis of the ground term transition in Ag-like tungsten to include some of its closest isoelectronic neighbours.

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# Spectroscopy of Highly Charged Ions Isolated in Compact Penning Traps

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**Abstract.** Unitary-architecture Penning traps, built around rare-earth NdFeB permanent magnets, provide a very compact and well-controlled environment to isolate highly-charged ions (HCI) for spectroscopy and for experiments with exotic states. Following charge-state selection and careful slowing, ions extracted from an electron beam ion trap (EBIT) source are captured in a unitary Penning trap with the resulting thermal energy reduced by a factor of order one hundred, compared to temperatures typically found in an EBIT. HCIs are confined in the unitary traps with storage lifetimes exceeding one second for a room-temperature apparatus, sufficiently long for a variety of ongoing and planned investigations of interest to astrophysics, plasma diagnostics, and fundamental metrology. Holes positioned along the trap mid-plane provide optical access for light collection and future laser spectroscopy of trapped HCI. As a first demonstration, radiative lifetimes of metastable excited states are measured by detecting visible fluorescence emitted by trapped B-like Ar XIV (441 nm,  $2p\ ^2P_{3/2} \rightarrow 2p\ ^2P_{1/2}$ ) and K-like Kr XVIII (637 nm,  $3d\ ^2D_{5/2} \rightarrow 3d\ ^2D_{3/2}$ ). A second apparatus, currently under construction, incorporates an electron gun along with unitary NdFeB structures to form a room-temperature ion source, an extraction beamline, and a compact ion trap to isolate low-Z HCIs. A beam of Rydberg rubidium atoms, also under development, is designed for charge exchange with trapped bare nuclei. An initial goal is the production of hydrogen-like ions in Rydberg states of high angular momentum, an attractive system for precision metrology and tests of atomic structure theory.

# Laboratory Astrophysics for Near-Infrared Astrophysical Applications

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**Abstract.** Astronomical near-infrared (NIR) observations are attracting more interest, and telescopes are being equipped with high-resolution NIR spectrographs. The next generation telescopes will have optimal performance in the nIR and high-resolution instrumentation.

The scientific interest for the NIR has several reasons, among them the interest in cooler stars having intensity peaks in this region, and also studies of obscured regions where the extinction prevents studies in short wavelength regions. In addition, several atomic and molecular species in astronomically interesting sources also have optimal transitions for abundance studies in the NIR.

Judging from the available atomic data bases, there are few known atomic transitions in the infrared region. Part of the explanation for this is the lack of interest from the atomic physics community. Motivated by this, we are running a program to improve the amount and accuracy of atomic transition data in the nIR with priorities from astronomical observations. The CRIRES-POP program on VLT/CRIRES will be a source for these priorities.

Parameters of interest are wavelengths, oscillator strengths and line profiles (hyperfine and isotopic structure). Measurements are complemented by atomic structure calculations where applicable. Current studies include the measurements of Y I, Sc I and La I, which all have strong, low-excitation lines appearing in the atmospheric transmission bands.

The Edlen laboratory at Lund Observatory is equipped with a high-resolution FTS optimized for the infrared region. At Lund High Power Laser facility, a laboratory dedicated to radiative lifetime measurements is being adopted for NIR measurements.

**Keywords:** <Enter Keywords here>

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# Charge Changing Collision Cross Sections of Tungsten Ions

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**Abstract.** We have measured electron capture cross sections for  $W^+$  and  $W^{2+}$  ions colliding with He, Ne, Ar, Kr,  $H_2$ ,  $D_2$ ,  $N_2$ ,  $CH_4$ ,  $C_2H_6$ , and  $C_3H_8$  atoms and molecules at collision energy between 5 and 15 keV. Measured cross sections show power-law dependence on the target first ionization potential, as have been demonstrated in collisions of light or medium-heavy element ions of Be, B, C, Fe, Ni and so on, implying a possibility that electron capture for heavy and “warmly-clothed” ions might be understood as distant collisions of potential particle with neutral targets. Electron capture cross sections for  $H_2$ ,  $D_2$ , and He targets are compared with theoretical calculations based on the hidden crossing method and remarkable threshold behavior on collision energy will be discussed. Our new plan for producing ionization, electron capture and loss cross sections for  $H + W^{q+}$  collisions at NBI energy (up to 1 MeV/u) will also be presented.

# New Capabilities for X-ray Transition Energy and Relative Intensity Determinations using TES Microcalorimeter Detectors

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**Abstract.** The x-ray microcalorimeter detector using a transition-edge sensor (TES) is a versatile detector that covers a broad energy range and possesses a demonstrated energy resolution of  $E/\Delta E \approx 2000$ . It operates on the principle of measuring the temperature change due to absorption of single x-ray photons. This type of detector is capable of determining relative intensities of x-ray lines as well as transition energies over an energy range far greater than diffractive studies. The detectors will permit combined measurements of K, L, and M x-ray lines in single spectra. TES detectors covering various energy ranges and resolutions are currently being developed at NIST.

# Reduced-Density-Operator Description for Single-Photon and Multi-Photon Processes in Many-Electron Atomic and Molecular Systems

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**Abstract.** A reduced-density-operator formulation is developed for single-photon and multi-photon processes in quantized many-electron systems, taking into account environmental collisional and radiative interactions. A fundamental microscopic quantum-mechanical description for the spectral line shapes is provided, which is based on the derivation of precise expressions for the tetradic matrix elements of the frequency-domain Liouville-space self-energy operator occurring in the general expression for the Liouville-space transition operator. Using a perturbation expansion of the frequency-domain Liouville-space self-energy operator, the spectral-line widths and shifts are systematically evaluated in the isolated-line, short-memory-time (Markov), and lowest-order (Born) approximations. The general reduced-density-operator formulation can also be employed in the more difficult spectral description that is applicable to overlapping lines. Applications of interest include spectral simulations for atomic and molecular systems. In addition to the standard data sets consisting of collisional cross sections and radiative transitions rates, the corresponding transitions matrix elements may also be required.

This investigation has been supported by the Office of Naval Research.

# Theoretical study of electron-impact ionization of $W^{25+}$

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Tungsten as facing material in nuclear fusion devices can withstand the high temperatures and heavy bombardments by particles. Nevertheless tungsten penetrates as intrinsic impurity in the thermonuclear plasma. Thus it is up-and-coming to investigate formation of ionized ions due to interaction with electrons.

In this work electron-impact ionization of  $W^{25+}$  ion from the ground state has been investigated performing level to level calculations. Theoretical treatment of the ion is complicated by the presence of open  $f$  shell. Excitation-autoionization and direct ionization processes are responsible for the formation of ions in the next ionization stage. The direct single ionization and electron-impact excitation cross-sections are obtained in relativistic distorted wave approximation. The calculations are performed using Flexible Atomic Code [1]. Previous investigations [2] using configuration-average model show that radiative damping of excited configurations starts to be important up from  $W^{45+}$ . For  $W^{25+}$  configuration-average autoionization branching ratios are close to one. Probability to remove an additional electron after electron-impact excitation or ionization due to shake-off process for the highly ionized ions is negligible [3].

Calculated ionization energy of 780.58 eV indicates that excited configurations produced by promotion of electrons from  $4s$ ,  $4p$  and deeper shells can decay further through Auger transitions. However excited configurations with the vacancies in  $4f$  or  $4d$  shells do not reach the ionization threshold. The dominant contribution to the total direct ionization gives  $4d$  shell. The ionization cross-section for this shell ( $1.6 \cdot 10^{-19} \text{ cm}^2$ ) is about 50 % larger than for  $4f$  shell ( $9.6 \cdot 10^{-20} \text{ cm}^2$ ) at twice the ionization threshold.

Calculated energy of double ionization equals 1611.19 eV. Only configurations with vacancies in  $3d$  or deeper shells have higher energies.

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# GRIDView: Analysis and Cataloging of Atomic Spectra for Galaxies

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**Abstract.** Data discovery in astrophysics has become increasingly dependent on rapid access to three dimensional data, catalogs, and spectral archives. Visualization of large data cubes is of vital importance for the success of large spectral line surveys in astrophysics. Extracting information from spectral lines for galaxies yields information on distances, rotations, dynamics, and kinematics that are important to galaxy luminosity and mass models. I will show examples of data visualization utilizing the *GRIDView* software package, which allows users to manipulate spectral line data cubes. Currently the package is mostly used for analyzing and cataloging atomic spectra of galaxies. The tools also incorporate Virtual Observatory client applications for overlaying database information in real time while moving through redshift space. The software has been used with great success for spectral line and continuum data sets obtained from large radio survey collaborations. More information about the software package can be found at: <http://www.cv.nrao.edu/~bkent/computing/gridview.html>

# Current Status of Atomic Spectroscopy Databases at NIST

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The NIST Atomic Spectroscopy Data Center maintains several online databases on atomic spectroscopy. These databases can be accessed via the <http://physics.nist.gov/PhysRefData> web page. Our main database, Atomic Spectra Database (ASD) has recently been upgraded to v. 5.0, which contains critically evaluated data for about 194,000 spectral lines and 106,000 energy levels of almost all elements in the periodic table. This new version has been expanded to include the ground states and ionization energies of all elements up to Ds ( $Z=110$ ) in all ionization stages with a new Web interface for displaying them. We continue to maintain and regularly update our bibliography databases, ensuring comprehensive coverage of current literature on atomic spectra, including energy levels, spectral lines, transition probabilities, hyperfine structure, isotope shifts, Zeeman and Stark effects. We continue to maintain other popular databases such as the Handbook of Basic Atomic Spectroscopy Data, searchable atlases of spectra of Pt-Ne and Th-Ne lamps, and non-LTE plasma-kinetics code comparisons.

## ACKNOWLEDGMENTS

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# Calculation of single Ionization fully differential cross section of hydrogen molecule using DWBA approach

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The charged particle impact ionization studies of fundamental atomic and molecular systems have been of great interest since the early days of quantum mechanics. Extensive theoretical and experimental investigations have been carried out to understand the electron impact single ionization (i. e. (e, 2e) processes) of various targets. [1-6]. Being able to provide the information about momentum vectors of both final state continuum electrons, the (e, 2e) processes are very important in understanding the dynamical behaviour of quantum mechanical systems and also provide the stringent tests of the theoretical models. Accurate cross sections for molecular target ionization by electron impact are very important for the understanding of the complex interactions involved in the process.

Most recently the (e, 2e) Fully differential cross section (FDCS) results have been reported in the low to intermediate incident energy ranges for relatively simple molecular systems [7-8]. We present in this communication the results of our calculation of (e, 2e) FDCS of hydrogen molecule. We calculate the FDCS in the Distorted Wave Born Approximation (DWBA) formalism in the framework of the Linear combination of atomic orbital (LCAO) approach in which the molecular wave functions are expressed as a sum of Slater type orbital (STO) for each atomic nucleus of hydrogen. We will apply this treatment to calculate the FDCS for variety of kinematic conditions and will discuss the salient features of the cross section for the hydrogen molecule.

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# The “Including All the Lines” Project

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**Abstract.** I present a progress report on including all the lines in the line lists, including all the lines in the opacities, and including all the lines in the model atmosphere and spectrum synthesis calculations. The increased opacity will improve stellar atmosphere, pulsation, stellar interior, asteroseismology, nova, supernova, and other radiation-hydrodynamics calculations. I also report on producing high-resolution, high-signal-to-noise atlases for use in verifying the line data and spectrum calculations, and as tools for extending laboratory spectrum analyses to higher energy levels. All the data are available on my website [kurucz.harvard.edu](http://kurucz.harvard.edu).

In updating previous calculations I generally compute three times as many levels, including all the most recent laboratory data, and produce ten times as many lines. With the addition of heavier elements that were not previously computed I expect to have more than one billion atomic lines. At this writing I have completed 62 ions, mostly iron group, that produced 260 million lines. I am also revising and adding to my diatomic molecular data. Large scale results will take one or two more years. I will produce a wavelength-sorted line list with all the lines for opacities and a second list with all the lines with accurate wavelengths for computing detailed spectra.

For each ion I save the least squares fits; energy level tables with E, J, identification, strongest eigenvector components, lifetime, A sum,  $C_4$ ,  $C_6$ , and Landé g; electric dipole, magnetic dipole, and electric quadrupole line lists. Eigenvalues are replaced by measured energies when data exist. Lines connecting measured levels have correct wavelengths, but most of the lines have predicted, uncertain wavelengths. Lines have radiative, Stark, and van der Waals damping constants, Landé g, and branching fractions. Hyperfine and isotopic splitting are included when laboratory data exist. Laboratory measurements of gf values and lifetimes are included. I have started to include measured or estimated widths of autoionizing levels and measured or estimated Shore parameters for Fano profile lines.

I already have production programs that can treat billions of lines. My program DFSYNTH can tabulate opacity spectra and opacity distribution functions (ODFs). Model atmosphere program ATLAS9 uses ODFs for opacity while ATLAS12 uses opacity sampling.

# Effective Atomic Number and Electron Density Studies in Some Water Equivalent Phantoms for MV X-Rays

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**Abstract.** A simple procedure has been presented for calculation of effective atomic numbers ( $Z_{\text{eff}}$ ) and electron densities ( $N_{\text{eff}}$ ) in some water equivalent phantoms namely PMMA, Polystyrene, Solid Water (WT1), RW3 and ABS for MV X-rays which are heterogeneous in energy. Firstly, effective atomic cross sections have been determined to obtain effective photon energies which were further used for calculation of  $Z_{\text{eff}}$  and  $N_{\text{eff}}$ . Similar procedure was adopted for Co-60 X-rays to check the validity of the present method. Results were found to be quite satisfactory. With the help of this method, it can be possible to obtain  $Z_{\text{eff}}$  and  $N_{\text{eff}}$  of different materials for MV X-rays.

# STRUCTURE AND INTERACTIONS OF ULTRACOLD Yb IONS AND Rb ATOMS

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**Abstract.** In order to study ultracold charge-transfer processes in hybrid atom-ion traps, we have mapped out the potential energy curves and molecular parameters for several low lying states of the  $\text{RbYb}^+$  system. We employ both a multi-reference configuration interaction (MRCI) and a full configuration interaction (FCI) approach. Turning points, crossing points, potential minima and spectroscopic molecular constants are obtained for the lowest five molecular states. Long-range parameters, including the dispersion coefficients are estimated from our *ab initio* data. The separated-atom ionization potentials and atomic polarizability of the ytterbium atom ( $\alpha_d=128.4$  atomic units) are in good agreement with experiment and previous calculations. We will present dynamical calculations for (adiabatic) scattering lengths for the two lowest ( $\text{Yb,Rb}^+$ ) channels that were carried out in our work. We find that the pseudo potential approximation is rather limited in validity, and only applies to nK temperatures. The adiabatic scattering lengths for both the triplet and singlet channels, are large and negative in the FCI approximation.

**Keywords:** Ultracold, potential curves, scattering lengths, molecular constants

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# Atomic Data Needs For Understanding Elemental and Isotopic Fractionation in the Solar Wind and Corona

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**Abstract.** The solar composition is now known to vary with location on the sun. The corona was first observed in 1963 to exhibit what has now become known as the “FIP Effect”. Elements with First Ionization Potential (FIP) less than about 10 eV are enhanced in their abundance relative to hydrogen by a factor of 3-4, relative to values in the solar photosphere. These low FIP elements include Fe, Si, Mg. Modern observations indicate that similar abundance anomalies apply in the corona and slow speed solar wind. High FIP elements are relatively less affected, but He and possibly Ne exhibit abundance depletions from their photospheric values. These fractionations are best explained within the context of a model where Alfvén waves generated within coronal loops interact with chromospheric ions, but not neutrals, through the ponderomotive force. This arises as the Alfvén waves reflect from loop footpoints to remain trapped in the coronal loop. The fractionation is thus reduced in open field structures such as coronal holes and the high speed solar wind emanating from them, in agreement with observations.

More recently, the Genesis mission has revealed isotopic fractionation between the fast and slow speed solar winds. Lighter isotopes of the same elements are relatively more abundant in the slow speed wind than in the fast wind. The simplest application of the ponderomotive force model, assuming chromospheric ionization balance independent of isotope, predicts isotopic fractionations of about the right magnitude but of the wrong sign. Lighter isotopes need to be relatively more ionized in the chromosphere for such fractionation to be explained by the ponderomotive force.

We will discuss the role that charge exchange reactions play in establishing the elemental charge states in the chromospheric, with reference to both FIP and isotopic fractionation. Reduced mass corrections between isotopes may lead to variation of the ionization balance, and allow us to speculate on whether the ponderomotive force can explain all fractionations, or whether different physics is required.

# Charge exchange measurements with an x-ray calorimeter at an EBIT

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**Abstract.** We present X-ray spectra recorded with the EBIT Calorimeter Spectrometer (ECS) following charge exchange reactions with highly charged ions produced and trapped with the electron beam ion trap EBIT I at LLNL. We have shown that, contrary to previous EBIT measurements of charge exchange spectra [1], significant variations in spectral hardness ratio can be produced by varying the ion species and neutral target gas [2]. We present new measurements that demonstrate further variation in hardness ratio for different ion and neutral species. Our new measurements also exclude the alternative possibility that variations in ion temperature can explain the observed variations in hardness ratio, thus confirming our previous results. We also report on efforts to develop atomic hydrogen injection for EBIT charge exchange experiments.

**Keywords:** -

**PACS:** -

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# Mass and Field Isotope Shift Parameters for the 2s - 2p Resonance Doublet of Lithium-like Ions

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**Abstract.** Dielectronic recombination measurements have been proven to be a sensitive tool for deducing changes in the nuclear mean-square charge radii of highly-charged lithium-like neodymium [1]. To make use of this method for other elements and isotopes, mass and field isotope shift calculations are required in order to derive information about the nuclear charge distributions. In this work, we estimate and discuss the relativistic mass and field isotope shift factors for the two  $2s\ ^2S_{1/2} - 2p\ ^2P_{1/2,3/2}$  transitions along the lithium isoelectronic sequence. Using the grasp2K package based on the multi-configuration Dirac-Fock method, the electron correlation and the Breit interaction are taken systematically into account in all the calculations.

Adopting the calculated electronic parameters of isotope shifts, we qualitatively analyze the competition between the mass and field shift contributions for the 2s-2p resonance doublet along the isoelectronic sequence, with the assistance of some empirical relations between  $Z$  and the nuclear properties. It is found that the mass shifts and the field shifts possess similar orders of magnitude in the  $Z < 40$  range, so that one should consider both of them for a relevant analysis of isotope shifts, especially for extracting the nuclear mean-square charge radii. The field shift contribution grows rapidly towards the high- $Z$  region and becomes quickly dominant.

Quantitative discussions are also made for the  $2s\ ^2S_{1/2} - 2p\ ^2P_{1/2,3/2}$  line isotope shifts in the case of  $^{150,142}\text{Nd}^{57+}$  for which experimental values are available. The present results show that the higher-order nuclear moments often neglected in the calculation of the field shift should be considered for very highly charged ions in order to extract the  $\delta\langle r^2 \rangle$  values from experiments. The consistency between grasp2K and MCDF-gme results will be illustrated.

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# Heavy Element X-ray Spectroscopy For Cancer Therapy and Diagnostics

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**Abstract.** Heavy high-Z (HZ) elements are commonly used in radiosensitizing agents for cancer diagnostics and treatment. The basic property of the HZ element being utilized is its interaction with the irradiating x-rays. Current x-ray sources in medical facilities, such as LINAC, produce broadband x-rays only part of which is absorbed by the reagent while the rest cause harm as they are absorbed and Compton scattered in the body tissue. Our proposed method *Resonant Nano-Plasma Theranostics*<sup>1-3</sup>, or RT in short, implements the spectroscopic resonant interaction of the x-rays with the HZ element for more effective and safer therapy and diagnostics (Theranostics). The production of electron which is ejected by photoionization during interaction and cause the destruction of the malignant cell can be increased through monochromatic x-rays targeted at the resonant energy. We show that while cross sections for photoionization rapidly decrease after the K-edge; strong resonant absorption of x-rays occur below the K-edge. We determine the resonant energy which is mainly due to K-L transitions and corresponding resonant cross sections which can be orders of magnitude higher than the background. Through initiation of Auger process by K-shell ionization, the process of theranostics could be enhanced considerably.

We will present study between X-ray radiotherapy in two energy ranges: (i)  $E < 100$  keV including HZ sensitization, and (ii)  $E > 100$  keV where sensitization is inefficient. We perform Monte Carlo numerical simulations of tumor tissue embedded with platinum compound and compute radiation dose enhancement factors (DEF) upon irradiation with 100 kV, 170 kV and 6 MV sources. Our results demonstrate that the DEF peaks below 100 keV and fall sharply above 200 keV to very small values. Therefore most of the X-ray output from LINACs up to the MeV range is utilized very inefficiently. We also describe experimental studies for implementation of low energy x-rays with Pt reagents and selected cancer cell lines. Resultant radiation exposure to patients could be greatly reduced, yet still result in increased tumoricidal ability.

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## Influence of dissociative recombination of $\text{Hg}_2^+$ on an inductively coupled Ar-Hg discharge

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*Domain:* Laboratory and industrial plasmas

This paper describes an important effect of  $\text{Hg}_2^+$  on the skin effect in an inductively coupled Ar-Hg discharge. A 2D plasma model coupled with the Maxwell equations is utilized for the analysis. The model includes all important plasma chemical reactions and loss mechanisms of particles. Plasma reactions rates are calculated based on the assumption that the electron energy distribution function (EEDF) is Maxwellian. Electron loss caused by dissociative recombination (DR) is expressed as  $K_{\text{DR}}n_e n_{\text{Hg}_2^+}$ , where  $K_{\text{DR}}$  is the reaction rate,  $n_{\text{Hg}_2^+}$  is number density of the  $\text{Hg}_2^+$  ion and  $n_e$  is electron density. Very few publications on  $n_{\text{Hg}_2^+}$  in discharge plasma exist to the best of our knowledge. However, this can be indirectly obtained by estimating the reaction cross sections. According to Ref. 1, the average cross section of associative ionization (AI) is about one fifth of the average chemi-ionization (CI) cross section. That means about one  $\text{Hg}_2^+$  is produced in every five CI reactions. In the present model, we assume that CI is responsible for 10%, 20%, and 50% of total electron production. Then,  $n_{\text{Hg}_2^+} = \alpha n_e$ , where  $\alpha = 0.02, 0.04, \text{ and } 0.1$ . Therefore, the loss term becomes  $K_{\text{DR}}n_e^2$ . According to Ref. 2 and Ref. 3,  $K_{\text{DR}}$  is on the order of  $10^{-13} \text{ m}^3/\text{s}$ . Here we use  $3 \times 10^{-13} \text{ m}^3/\text{s}$ . Simulation reveals that even with small amount of  $\text{Hg}_2^+$ , discharge will not become constricted. Furthermore, different densities of  $\text{Hg}_2^+$  do not significantly affect spatial distribution of the electric field. But density of excited Hg atoms is affected. As  $\text{Hg}_2^+$  density increases, the density of Hg  $6^3\text{P}_1$  atoms decreases due to smaller rates of excitation caused by rapid loss of electrons. Therefore, DR can be considered as an important mechanism of preventing the discharge from getting constricted. What we should note is that our model is based on a Maxwellian EEDF. Once non-Maxwellian EEDF is applied, frequent excitation and ionization of atoms caused by discharge constriction may quickly drain electrons with high energy. As a result, the process of discharge contraction can be stopped. Thus, depletion of high energy electrons may also be a factor to reduce discharge constriction.

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# Cross Sections for Inner-Shell Ionization by Electron Impact

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**Abstract.** Cross sections for the removal of atomic inner-shell electrons by electron impact are needed in many branches of physics including atomic physics, plasma physics, radiation physics, material analysis by electron-probe microanalysis, surface analysis by Auger electron spectroscopy, and thin-film analysis by electron energy-loss spectroscopy in the electron microscope. We have performed an analysis of measured and calculated cross sections for inner-shell ionization as well as of cross sections from a number of widely used predictive formulae [2-5]. The emphasis in our analysis is on the recent formulation of the distorted-wave Born approximation by Bote and Salvat [1] which has been used to generate an extensive database of cross sections for the ionization of the K shell and the L and M subshells of all elements from hydrogen to einsteinium ( $Z = 1$  to  $Z = 99$ ) by electrons and positrons with kinetic energies up to 1 GeV [6].

We will present examples of our analysis of measured and calculated cross sections for K-shell ionization. We used the calculated cross sections to assess whether the measured cross sections showed the expected energy dependences, as judged by Fano plots [7]. We identified 26 elements for which there were at least three sets of independent measurements that were consistent with each other and that showed energy dependences which were generally consistent with those expected from the calculated cross sections and the Bethe formula for inner-shell ionization [8]. Illustrative plots will be shown to indicate the degree of agreement between calculated and measured cross sections as well as the agreement between the calculated cross sections and those expected from the predictive formulae.

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# Status Report on the Low-Temperature Plasma Data Exchange Project (PDEP)

The LXCat team\*, presented by Oleg Zatsarinny<sup>1</sup>

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**Abstract.** The open-access, on-line databases available on [www.lxcat.net](http://www.lxcat.net) contain data relevant to electron and ion scattering and transport in low-temperature plasmas, in forms suitable for use in modeling such plasmas. The site was restructured in 2012, and data evaluation is a continuing activity.

**Keywords:** electron, ion, scattering, transport processes, low-temperature plasmas.

**PACS:** 34.80.Bm; 34.80.Dp; 52.20.Fs; 52.20.Hv; 52.25.Fi; 52.65.-y

The *GEC Plasma Data Exchange Project (PDEP)* is an informal, community-based project that was initiated as a result of a public discussion held at the 2010 Gaseous Electronics Conference (*GEC*), one of the leading international meetings for the *Low-Temperature Plasma* community. This project aims to address the well-recognized needs of the community to organize the means of collecting, evaluating, and sharing data for both modeling and interpreting the outcome of experiments.

At the heart of the *PDEP* is the open access website [www.lxcat.net](http://www.lxcat.net) developed by researchers at LAPLACE in Toulouse, France. *LXCAT* ([www.lxcat.laplace.univ-tlse.fr](http://www.lxcat.laplace.univ-tlse.fr)) (updated in 2012) distributes collections of data related to electron and ion scattering and transport in cold, neutral gases, which are critically important to modeling low-temperature plasmas. At present, 22 databases, contributed by groups around the world, can be accessed on *LXCAT*, with several others under development. On-line tools enable importing and exporting data, plotting and comparing different sets of data, and downloading data. In cases where “complete” sets of cross sections are available, the conversion to electron transport and rate coefficients can be accomplished with on-line or downloadable tools, including the Boltzmann equation solver, BOLSIG+. The steadily increasing number of contributors and users clearly demonstrates the utility and international enthusiasm for this site.

Data evaluation and authentication is key to PDEP, an activity requiring considerable community-based expertise. In a first effort, twelve researchers participated in a coordinated effort to review and evaluate data for electron-neutral scattering cross sections for rare gases. The work was reported at the *GEC 2011*. Presently under review are data related to electron scattering and transport in simple molecular targets. A review of data for more complex molecules will be undertaken in 2013. The rare-gas evaluations, to be published in 2013, are intended to serve as documentation for the on-line databases and as guidelines for the modeling community.

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# Radiative Cooling in Collisionally- and Photo-Ionized Plasmas

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**Abstract.** We discuss recent improvements in the calculation of the radiative cooling in both collisionally and photo ionized plasmas. We are extending the spectral simulation code Cloudy so that as much as possible of the underlying atomic data is taken from external databases, some created by others, some developed by the Cloudy team. This work focuses on recent changes in the treatment of many stages of ionization of iron, and discusses its extensions to other elements. The H-like and He-like ions are treated in the iso-electronic approach described previously. Fe II is a special case treated with a large model atom. Here we focus on Fe III through Fe XXIV, ions which are important contributors to the radiative cooling of hot ( $10^5 - 10^7$  K) plasmas and for X-ray spectroscopy. We use the Chianti atomic database to greatly expand the number of transitions in the cooling function. Chianti only includes lines that have atomic data computed by sophisticated methods. This limits the line list to lower excitation, longer wavelength transitions. We had previously included lines from the Opacity Project database, which tends to include higher energy, shorter wavelength, transitions. These were combined with various forms of the “g-bar” approximation, a highly approximate method of estimating collision rates. For several iron ions the two databases are almost entirely complementary. We adopt a hybrid approach in which we use Chianti where possible, supplemented by lines from the Opacity Project for shorter wavelength transitions. The total cooling differs from some previous calculations by significant amounts.

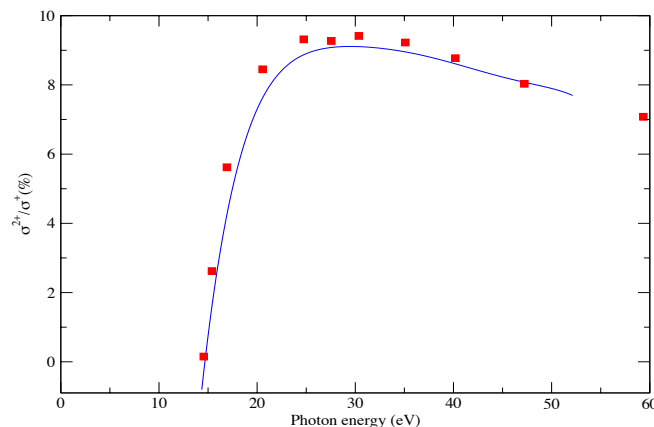
Supported by NSF (0908877; 1108928; and 1109061), NASA (07-ATFP07-0124, 10-ATP10-0053, and 10-ADAP10-0073), JPL (RSA No 1430426), and STScI (HST-AR-12125.01, GO-12560, and HST-GO-12309).

# An IERM approach to photoionisation with application to $H^-$ , He-like and Be-like ions

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**Abstract.** Recent experimental advances in the field of attosecond science and X-ray free-electron laser sources [1, 2] necessitate the availability of advanced theoretical models which can provide an accurate treatment of double-electron continua. As a first step towards the development of a multipurpose R-matrix code for multiple-electron ejection, we consider the recently developed intermediate energy R-matrix (IERM) approach to photoionisation [3, 4], to ascertain if such an approach could provide a suitable method of representing double-electron continua within an R-matrix framework. We investigate photodetachment and photo-double-detachment of  $H^-$ , and show that results are in excellent agreement with existing data (see Fig.1). In addition, we apply the IERM method for photoionisation to members of the He and Be isoelectronic sequences, studying both single and double ionisation processes. While scaling laws for the photo-double-ionisation cross section of He-like ions have been proposed [5], we seek also to determine a scaling law for the photo-double-ionisation of Be-like ions. Various ions of Ne and Ar are also being studied and the latest results will be presented at the conference.



**FIGURE 1.** Percentage ratio of double-ionisation to single-ionisation in the photodetachment cross section of  $H^-$ . Present results (solid line) and Kheifets and Bray [6] (squares).

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# ELECTRON COLLISIONS WITH SMALL MOLECULES

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## ABSTRACT

Electron collisions with small molecules opens the doorway to investigate a variety of collision processes such as vibronic excitation, dissociative electron attachment (DEA), dissociative recombination (DR) and photoionization. On going developments based on R-matrix methods implemented on parallel computing architectures have been used to perform detailed electron collision cross section calculations on a variety of species, such as; BeH, BeH<sub>2</sub>, C<sub>2</sub>, CH, CO and N<sub>2</sub>H and their cations [1- 5]. Where possible we compare our results with previous calculations and experiments. Such comparisons serve as the ultimate benchmark for our work in order to have confidence in the molecular data for applications in ultracold collisions, fusion physics [6-7] and astrophysics [8].

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# Integrating PAH databases in the VAMDC infrastructure

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**Abstract.** The Virtual Atomic and Molecular Data Centre (VAMDC) is a project funded by the European Union to build a unified access infrastructure to (virtually) all existing online databases of atomic and molecular data. Its aim is to offer a transparent, unified query interface to all available resources through a unique point of access (the VAMDC portal). Another part of the VAMDC infrastructure is the VAMDC registry, which keeps track of the databases which joined the infrastructure, what information they provide, the query capabilities they offer. VAMDC queries produce results in a unified format, namely the XML Schema for Atoms, Molecules and Solids, which is an international standard. Being written in XML, such results can be easily transformed in any desired format, using available libraries and tools to perform an XSL transformation. The minor drawback is that XSAMS, despite being extremely rich, due to its generality will never be able to accommodate **all** information in a specialised database. For this reasons, direct query interfaces of individual databases will continue to exist, for users requiring complete access to all available data. The possibility to simultaneously query multiple VAMDC resources, on the other hand, opens the way for (relatively) easy cross-correlation of databases.

The Cagliari/Toulouse PAH theoretical spectra database was one of the initial participants to the VAMDC project, and thus is part of the infrastructure since its initial release. This was used also as an early benchmark of the VAMDC-XSAMS format, making it possible to address some of its limitations for describing large polyatomic molecules. The preliminary release of the VAMDC interface to this database is described in this poster.

In addition, a new database of experimental data is being set up in Toulouse, which will hold (experimental) information partly overlapping but mostly complementary to that in the theoretical database. The tools developed in the VAMDC project make it a (relatively) trivial matter to turn any existing relational database into a VAMDC node (or even import a previously non-existent set of structured text dables into an automatically created, brand new relational database implemented in MySQL), and this is expected to be accomplished shortly. Preliminary information on this process is also presented, highlighting the prospective potential for cross-correlating, and merging information from, these two databases.

**PACS:** 31.15.-p, 33.15.-e, 33.20.-t, 89.20.Ff, 89.20.Hh, 95.30.Ky

# NORAD-ATOMIC-DATA for Radiative Processes at the Ohio State University

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**Abstract.** NORAD-Atomic-Data is an on-line database based at the Ohio State University containing data for radiative atomic processes, such as photoionization, electron-ion recombination, radiative transitions, lifetimes, etc. Significant part of the atomic data corresponds to new and improved work including relativistic effects under the international Opacity Project and the Iron Project. It contains large sets of energy levels, photoionization cross sections, recombination cross sections and rate coefficients, oscillator strengths and other transition parameters. It also gives lifetimes and some collision strengths for electron-impact excitations. The data sets consider large number of bound levels, typically going up to  $n=10$  for complete astrophysical models. The results are mainly from large scale R-matrix calculations by Nahar et al.. All files are in standard ascii character format for use in models and diagnostics of astrophysical and laboratory plasmas.. The database currently contains data for over 80 atomic species of elements H, He, C, N, O, F, Ne, etc going up to Ni.

The atomic data can be downloaded for direct applications. Spectroscopic information for all levels and transitions are provided. They are usually given in the energy tables and the numerical codes connect them to the transitions and levels in the cross section and rate coefficient files.

The x-ray K-alpha transition of elements, particularly of heavier ones, have been of great interest for various astronomical, biomedical, fusion plasma application. There are 112 K-L transitions possible for each element. A new addition to NORAD-Atomic-Data will be these transitions for a large number of elements.

NORAD-Atomic-Data can be accessed from various database pages, such as, at CfA-Harvard (<http://www.cfa.harvard.edu/amp/ampdata/databases.html>),

International Atomic Energy Agency:

(<http://www-amdis.iaea.org/databases.php>),

CFADC of Oak Ridge National Lab.

(<http://www-cfadc.phy.ornl.gov/databases.html>)



# Comprehensive Analysis of the Spectrum of Singly-Ionized Iron (Fe II)

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**Abstract.** In 1978, Sveneric Johansson published a comprehensive analysis of the spectrum of Fe II, consisting of about 3300 lines from 576 energy levels and covering the region 90 nm to 1120 nm. This analysis has been incorporated in many databases used in astronomical spectroscopy, including the NIST Atomic Spectra Database, the Vienna Atomic Line Database, and the synthetic spectrum codes of Kurucz. Since its publication, high resolution grating and Fourier transform (FT) spectrometers have increased the number of lines by a factor of over 4, extended the wavelength region up to 5500 nm, and reduced the uncertainty of the wavelengths by an order of magnitude. These spectra have been used in an analysis of the spectrum of Fe I, in the discovery of astrophysical lasers in Eta Carinae, and for the identification of very high-excitation spectral lines in HR 6000. However, although Prof. Johansson continued work on the analysis of Fe II, resulting in over 1000 known energy levels, this work remained uncompleted at the time of his death. Hence there has been no new comprehensive analysis of Fe II since 1978 and the majority of these data remain unpublished.

This poster presents the completion of the analysis of the Fe II spectrum. The spectrum has been recorded using high-resolution FT and grating spectroscopy over the wavelength range 90 nm to 5500 nm. The spectra were observed in high-current continuous and pulsed hollow cathode discharges using FT spectrometers at the Kitt Peak National Observatory, Tucson, AZ and Imperial College, London and with the 10.7-m Normal Incidence Spectrograph at the National Institute of Standards and Technology. Over 13 600 lines were classified using 1028 energy levels of Fe II that were optimized to the measured wavenumbers. The uncertainties of lines in the FT spectra range from  $10^{-4} \text{ cm}^{-1}$  ( $1.6 \times 10^{-4} \text{ nm}$ ) for strong lines around 4000 nm to  $0.05 \text{ cm}^{-1}$  ( $1.1 \times 10^{-4} \text{ nm}$ ) for weaker lines around 150 nm. The wavelength uncertainty of lines in the grating spectra is 0.0002 nm for moderately strong lines that do not saturate the photographic plate. The ionization energy of  $130\,655.4 \pm 0.4 \text{ cm}^{-1}$  was estimated from the  $3d^6(^5D)5g$  and  $3d^6(^5D)6h$  levels.

**Acknowledgement.** This work was partially supported by the National Aeronautics and Space Administration under the inter-agency agreement NNH10AH38I. Some of the spectra used in this work are from the National Solar Observatory digital Library.

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\*deceased

# SEARCHING QUANTUM LEVEL INTERFERENCE EFFECTS ON THE IONIZATION OF H<sub>2</sub> BY ELECTRON IMPACT

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Electron-Hydrogen molecule collisions have been studied for a long time, while cross sections have been reported in a wide variety of publications. In order to update a selection of the existing interference effects in the cross section results, we have measured the triple differential cross section (TDCS) of H<sub>2</sub> molecule by electron impact at various scattering angles. We have used (e, 2e) technique to measure TDCS for the electron impact ionization of H<sub>2</sub> at 250 eV incident electron energy in this work. The TDCSs of H<sub>2</sub> are measured at 50 eV ejected electron energy and for three different scattering angles of 7, 15 and 30<sup>0</sup>.

The present procedure has an advantage of being one of the first studied measurements over the scattering angle changes to see the effect of interference in the TDCS spectra of H<sub>2</sub> molecule itself. To stimulate more experimental work on interference argument in literature, current measurements are taken for single ionization of H<sub>2</sub> molecule at different kinematics. The results of our measurements will be discussed in details at the Conference.

**Acknowledgments:** This work was supported by TUBITAK in Turkey through grant 109T738.

# Electron-Impact Ionization of the Carbon Atom

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**Abstract.** Time-dependent close-coupling (TDCC) and time-independent distorted-wave (TIDW) methods are used to calculate the electron-impact ionization of the  $1s^2 2s^2 2p^2$  and  $1s^2 2s^2 2p 3\ell$  ( $\ell=0-2$ ) configurations of the carbon atom. Ionization of both the  $2s$  and  $2p$  subshells are included in the TDCC and TIDW calculations for the  $1s^2 2s^2 2p^2$  ground configuration. The TDCC results are in agreement with experiment [1], while the TIDW results are 20% higher. Ionization of the  $2s$ ,  $2p$ , and  $3\ell$  subshells are included in the TDCC and TIDW calculations for the  $1s^2 2s^2 2p 3\ell$  excited configurations. The ionization cross sections for the excited states are much larger than for the ground state. For example, the peak cross section for the  $1s^2 2s^2 2p 3p$  configuration is an order of magnitude larger than the peak cross section for the  $1s^2 2s^2 2p^2$  configuration. The TDCC results are again found to be substantially lower than the TIDW results. The ionization cross section results will permit the generation of more accurate generalized collisional-radiative (GCR) ionization coefficients needed for the modeling of moderately dense carbon plasmas.

[1] E. Brook, M. F. A. Harrison, and A. C. H. Smith, *J. Phys. B* **11**, 3115 (1978).

# Overview of Recent and Ongoing Research at the NIST EBIT

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**Abstract.** Ongoing and recent work at the NIST EBIT is presented for research applicable to fusion and basic science. Transition wavelengths have been generated for tokamak applications in order to be able to better characterize the core and divertor plasmas and infer plasma rotation and ion temperatures. Studied ions include fusion diagnostic elements such as krypton and xenon and possible intrinsic impurity elements such as tungsten, tantalum, hafnium, and gold. Furthermore, basic science work has included studies of precision QED effects in few electron ions, which will be presented as well.

This work supported in part by the Office of Fusion Energy of the US Department of Energy.

# Recent Progress in the Determination of Radiative Data for Lowly Charged Tungsten Ions (W I – W VI) of Interest in Fusion Research

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**Abstract.** A large amount of new radiative decay rates have recently been obtained for allowed (E1) and forbidden (M1, E2) transitions in tungsten ions from W I to W VI. Our calculations, motivated by strong interest for low-density plasmas and fusion research, illustrate in a convincing way the importance of core-valence correlation effects which substantially increase the lifetimes and, accordingly, decrease the transition probabilities of these heavy ions. The reliability of the theoretical  $A$ -values has been tested by comparison of numerical results obtained with independent methods such as the relativistic Hartree-Fock (HFR) approach including core-polarization corrections (HFR+CPOL), multiconfiguration Dirac-Fock (MCDF) method and the Flexible Atomic Code (FAC) well suited for investigating the atomic structure of heavy ions. For W I, W II and W III, our theoretical results have also been compared with available experimental lifetimes measured by laser spectroscopy. From detailed comparisons between these different approaches, it has been shown that some line strengths are particularly sensitive to level mixings which are expected to be better estimated when using semi-empirical methods. The new sets of radiative data obtained in the present work are stored in the DESIRE atomic database (<http://w3.umons.ac.be/astro/desire.shtml>).

# Atomic and Molecular Calibration Sources for High-Precision Astronomical Spectrometers

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**Abstract.** The search for extrasolar planets requires calibration sources with a weighted-average precision and accuracy of a few parts in  $10^9$  or better. While laser frequency combs easily achieve this requirement, such sources are too expensive and too complex for most astrophysical spectrometers. We have established and investigated potential and existing atomic and molecular calibration sources for the optical and near-infrared. These include commercial hollow cathode lamps of thorium argon (optical and near infrared) and uranium neon (near infrared), as well as a series of molecular gas cells ( $\text{H}_2\text{C}_2$ ,  $\text{H}^{13}\text{CN}$ ,  $^{12}\text{CO}$ ,  $^{13}\text{CO}$ , and  $\text{CO}_2$ ) that are utilized by the telecommunications industry ( $1.5\ \mu\text{m} - 1.65\ \mu\text{m}$ ). We present the current status of these sources and their applicability to current and future astrophysical spectrometers.

**Keywords:** <Enter Keywords here>

**PACS:** <Replace this text with PACS numbers; choose from this list: <http://www.aip.org/pacs/index.html>>

# Splatalogue - Database for Molecular Spectroscopy in the New Era of Astronomical Facilities

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**Abstract.** The next generation of powerful radio and millimeter/submillimeter observatories (e.g. Karl G. Jansky VLA, Robert C. ByrdGBT, ALMA) are now either in full operation or will be completing construction within the next 12 months. In addition to being the most sensitive facilities ever built for astronomical observations, each facility now has the capability to obtain broadband spectral line data (8 GHz of instantaneous bandwidth) at high spectral resolution (m/s velocity resolution). As such, these facilities will uncover a vast new array of molecular material never before seen in the universe and will require extensive resources to help identify spectral line transitions. We describe the compilation of the most complete spectral line database currently assembled for this purpose. The Splatalogue is a comprehensive transition-resolved compilation of observed, measured and calculated spectral lines. Splatalogue currently contains over 5.9 million spectral transitions over 8 different databases. Splatalogue also contains atomic and recombination lines, template spectra, and is completely VO-compliant, queryable under the IVOA SLAP standard. Splatalogue is used worldwide by astronomers preparing their observations using the ALMA Observing Tool and is integrated into the ALMA/VLA data reduction software CASA. Splatalogue can be used by 3rd party packages through the SLAP interface to model and view a host of spectral line data. The details of the database, how it is currently used and how users may access or add to the database through already accepted standards and data formats will be discussed.

# Observation of post-collision interaction in electron-impact excitation of the $4p^6$ subshell in Rb

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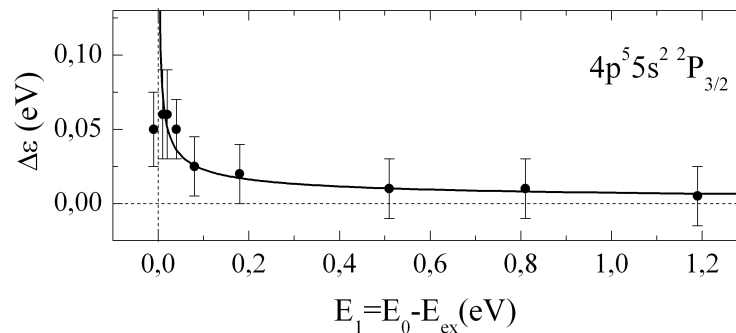
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**Abstract.** The first results on the PCI energy shift of the  $(4p^5 5s^2)^2P_{3/2,1/2}$  lines in Rb atoms are reported.

Negative ions influence essentially both excitation dynamics and PCI energy shift of autoionizing lines in ejected-electron spectra of alkali atoms. In particular, the energy shift of the  $(2p^5 3s^2)^2P_{3/2}$  and  $(3p^5 4s^2)^2P_{3/2}$  lines in Na and K spectra becomes of negative or positive sign depending on the presence or absence of negative-ion resonances in the excitation functions of corresponding autoionizing states. In contrast to these data, the energy dependence of the line shift for the  $(5p^5 6s^2)^2P_{3/2}$  state in Cs atoms possesses a simple asymptotic character.

In the present work, we report the first results on the PCI energy shift of the  $(4p^5 5s^2)^2P_{3/2,1/2}$  lines in Rb atoms. The measurements were performed with an incident-electron energy resolution of 0.2 eV over the impact energy range from the excitation threshold up to 17.5 eV. The data show an asymptotic character of the energy dependence of the PCI shift with the maximum values of 60 meV ( $^2P_{3/2}$ ) and 135 meV ( $^2P_{1/2}$ ) observed at threshold energies. From the fitting of the data by using the Barker–Berry formula  $\Delta\varepsilon=0.5\Gamma(R/E_1)^{0.5}$ , the energy width  $\Gamma$  of the  $(4p^5 5s^2)^2P_{3/2,1/2}$  states was estimated as 3.9 meV and 7.2 meV, respectively. The data are compared with the near-threshold excitation cross sections for the  $(4p^5 5s^2)^2P_{3/2,1/2}$  states.



**Figure 1:** The PCI energy shift for the  $(4p^5 5s^2)^2P_{3/2}$  autoionizing state in Rb atoms. The solid line presents the fitting result obtained by using the Barker–Berry formula.



# A Database on VUV absorption spectra of diatomic molecules using XSAMS

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**Abstract.** We present a database aiming to give the full absorption spectrum of molecular Hydrogen and its deuterated variants HD and D<sub>2</sub> as well as carbon monoxide CO. The data represent a compilation from various papers, both experimental and theoretical.

As far as H<sub>2</sub> isotopologues are concerned, values up to J = 30 are included in the database for plasma applications at temperatures of about 5000K. B-X, B'-X, C-X and D-X transitions are reported.

We have extended the J values of the CO spectrum as well and report absorption transitions within the fourth positive A-X band system as well as the transitions due to the intersystem a'-X, e-X, d-X bands. o-c values are provided when available.

The various quantum numbers and quantities such as transition wavenumber, transition wavelength, oscillator strength are described within xml language, following the Case by Case Schema for Molecular States in XSAMS v0.3 (<http://www.vamdc.org/documents/standards/dataModel/vamdcxsams/index.html>).

Validation procedures of the various symmetry properties and parity labels within the xml schema have been found very useful for checking their consistency.

**Keywords:**

**PACS:**

# Spectrum and Energy Levels of Singly-Ionized Chromium (Cr II): New Observations from the Vacuum Ultraviolet to the Infrared

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**Abstract.** Chromium is the third most abundant of the iron group elements and has a complex spectrum that is densely distributed over a wide spectral region. Lines of singly-ionized chromium (Cr II) are prominent in the spectra of a wide variety of astrophysical sources, and accurate laboratory data are essential for interpreting astronomical observations. Until recently the only comprehensive study of the Cr II spectrum in the literature was the six-decade old work of Kiess [1]. A large number of additional energy levels were located by S. Johansson of Lund University and are reported in a compilation of energy levels of the iron group elements [2]. Unfortunately, Johansson's work was never published. As a result no classified lines have been reported for 60% of the known energy levels and the uncertainty of the level values cannot be reliably determined.

We have re-observed the spectrum, emitted in Cr/Ne hollow cathode lamps, from 1130 Å to 5.5 μm using the NIST 10.7 m normal incidence vacuum spectrograph, the FT700 UV/Vis Fourier transform spectrometer (FTS), and the 2 m UV/Vis/IR FTS. We recently completed a description of the UV spectrum with new measurements of more than 3600 lines and re-optimization of 651 energy levels [3]. This work is being extended with new FT spectra covering the visible and IR regions that are now being analyzed. These spectra are of particular interest because new astronomical instruments on both space and ground-based telescopes have pushed the region of high-resolution astronomical spectroscopy to the red and IR. There are currently no lines of Cr II in the literature at wavelengths longer than 7311 Å, and Ritz wavelengths calculated from the Cr II energy levels cannot match the accuracy of the best astronomical observations.

From our present preliminary results, we estimate that we will identify about 800 additional Cr II lines at wavelengths longer than 3955 Å. These data will provide precise wavelengths for interpretation of astronomical spectra and allow further improvement in the accuracy of high lying energy levels. They will also provide the first precise values for levels of the high angular momentum configurations  $3d^45g$  and  $3d^46g$ , which have no observable transitions at shorter wavelengths. These configurations are expected to produce prominent lines in the infrared spectra of astrophysical objects.

**Acknowledgement.** This work is supported by the National Aeronautics and Space Administration under interagency agreement NNH10AN38I.

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**PACS:** 32.30.Jc, 32.30.Bv, 32.10.-f

# Diatomic Air Species Spectra From The Infrared To The Vacuum Ultra Violet

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**Abstract.** As part of the HyperRad Project for the Fundamental Aeronautics Program at NASA, we have carried out first principle calculations of the spectra of  $N_2$ ,  $N_2^+$ ,  $O_2$ ,  $O_2^+$ ,  $NO$ ,  $NO^+$ ,  $CO$ ,  $CN$ , and  $C_2$ . Many electronic states are considered so that we predict the spectrum from the infrared to the vacuum ultra violet. Rydberg states are explicitly included and high quality electronic wave functions are produced. Using these electronic wave functions, we compute the electric dipole, electric quadrapole and magnetic dipole transition moments as well as Spin-Orbit splittings and couplings. These are used in coupled ro-vib-electronic bound state calculations to produce bound-bound spectra. Above the lowest dissociation limit, the ro-vib-electronic levels become pre-dissociated, and we treat these levels using scattering theory to produce the bound-free and free-bound spectra. Novel diabatic states facilitate the nuclear dynamics calculations. All experimentally characterized bands are well reproduced, and a myriad of new states and bands are also predicted.

**PACS:** 31.15.ae, 31.15.ag, 31.15.aj, 31.15.vn, 31.15.xv, 31.50.Bc, 31.50.Df, 31.50.Gh, 33.13.Fm, 33.15.Kr, 33.15.Pw, 33.20.Bx, 33.20.Ea, 33.20.Kf, 33.20.Lg, 33.20.Ni, 33.20.Wr, 33.70.Ca, 33.80.Gj, 34.20.Cf.

# **Molecular Spectroscopy Data of Some Diatomic Metal Halides**

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## **ABSTRACT:**

**An extensive study of the available information of molecular structure and spectroscopy of diatomic halides of IIIA group metals (B, Al, Ga, In, Tl) and Copper has been performed. The literature survey extends till early 2012 and the experimental and theoretical data on molecular constants of ground state as well as excited states of these molecules will be presented. A brief discussion on the dissociation energies, ionization potentials, and the nature of bonding in the ground state alongwith the spectroscopic properties of the excited states will be given. The energy level diagram and potential energy curve as well as Transition probabilities, Einstein coefficients (for few rotational-vibration transitions) for these molecules will be also presented. Mechanism of Laser Transition in atomic Indium and Gallium due to ultraviolet photo dissociation in the diatomic Indium and Gallium halides will be discussed.**

# W XLV: atomic data for ITER diagnostics

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**Abstract.** Tungsten is a potential material for the lining of the walls of the divertor region of the International Thermonuclear Experimental Reactor (ITER), because of its low rate of erosion and hence long lifetime. A knowledge of decay rates of various ions of this element, both radiative and by electron collision, are important in analysing the impurities in the plasma.

To this end, we are investigating the properties of highly ionised Tungsten, specifically W XLV. We have used the CIV3 program [1] which incorporates relativistic effects via the Breit-Pauli Hamiltonian, to undertake configuration interaction calculations of the levels associated with configurations  $\{1s^2 2s^2 2p^6 3s^2 3p^6\} 3d^{10}[4s^2, 4s4p, 4s4d, 4s4f, 4p^2, 4p4d]; 3d^9[4s^2 4p, 4s^2 4d, 4s^2 4f, 4s4p4d]$ . The CI expansions also include the configurations  $3d^{10}[4p4f, 4d^2, 4d4f, 4f^2]; 3d^9[4s4p4f$  and  $4p4d4f]$  to allow for correlation effects.

The  $n=4$  orbitals were optimised by including the one-body mass correction and Darwin terms of the Breit-Pauli Hamiltonian in addition to the usual non-relativistic Hamiltonian, both directly and by means of a model potential, following the procedure of Cowan and Griffin [2]. The optimised orbitals were very similar in these two approaches, but their mean radii were smaller than those of a purely non-relativistic optimisation, thus displaying the relativistic contraction of the outer orbitals.

The states with occupations including  $3d^9$  are strongly mixed, so it is important to obtain accurate values for their separations. This is especially true for the  $J = 1$  odd parity as these levels have a direct E1 transition to the  $^1S_0$  ground state. Particularly important are the very strong transitions from the  $3d^9 4s^2 4f$  levels, for which the dipole matrix element is non-zero. These levels mix strongly with those of  $3d^9 4s 4p 4d$ , but only the  $3d^9 4s^2 4f$  configurations contribute directly to the dipole matrix, being just one orbital different from that of the ground state. It is therefore crucial that this mixing is determined accurately.

The results of oscillator strengths for these and other transitions will be presented at the conference. It is our intention to use the wavefunctions as target state wavefunctions in an electron-impact calculation, to compute collision cross sections and excitation rates. For this aspect of the work, we will use parallel R-matrix codes.

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# Absolute Recombination Rate Coefficients of Highly Charged Tungsten Ions

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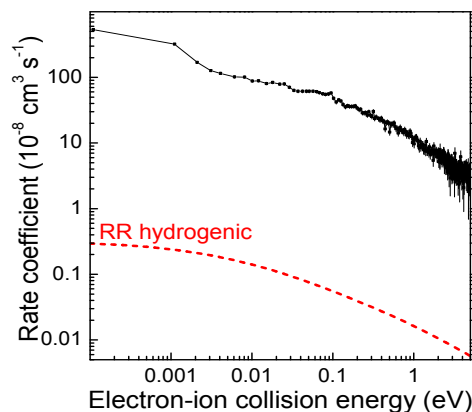
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**Abstract.** Ionization and recombination processes involving tungsten ions are of major interest for the fusion community. Since tungsten is used for plasma facing walls in nuclear fusion reactors, impurities of highly charged tungsten ions in the fusion plasma are inevitable. Radiation from these excited tungsten ions leads to plasma cooling. In order to control the plasma conditions, detailed knowledge of the atomic processes and atomic structures of tungsten ions are required. To date, most of the needed atomic data come from theory and only a small fraction is contributed by experimental measurements.

Here, we report on electron-ion recombination experiments of highly charged tungsten ions performed at the TSR storage ring in Heidelberg, Germany. Absolute experimental rate coefficients of several  $W^{q+}$  ions with  $18 \leq q \leq 21$  were measured. As an example, the merged-beam recombination rate coefficient of  $W^{20+}$  [1] is shown below. The impact of the measured rate coefficients on the modeling of fusion plasmas will be discussed.



Measured merged-beams rate coefficient for electron-ion recombination of  $W^{20+}$  at low relative collision energies [1]. The dash-dotted curve is the calculated merged-beams rate coefficient for radiative recombination (RR) using a hydrogenic approximation. Note that the measured rate coefficient is three orders of magnitude larger.

## References

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## Revised and extended analysis of doubly ionized bromine: Br III

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### **Abstract:**

The spectrum of doubly ionized bromine (Br III) has been investigated in vacuum ultraviolet wavelength region. Br III is As I –like ion with ground configuration  $4s^2 4p^3$ . This is a 3-electron system and possessing a complex structure. Its theoretical structure was predicted using Cowan's Configuration Interaction code, involving  $4s^2 4p^3$ ,  $4s^2 4p^2 (5p + 6p + 4f + 5f)$  configurations for odd parity matrix and  $4s 4p^4$ ,  $4s^2 4p^2 (4d + 5d + 6d + 5s + 6s + 7s + 5g)$ ,  $4s 5p^3 (5p + 4f)$ ,  $4p^4 (4d + 5s)$ ,  $4s 4p^2 (4d^2 + 5s^2)$  configurations for even parity system. The  $4s^2 4p^3 - [4s 4p^4 + 4s^2 4p^2 (4d + 5d + 6d + 5s + 6s + 7s)]$  transition array has been studied. Several reported levels of Br III were found to be erroneous and have been revised and new configurations have been added to the analysis. The spectrum used for this work was recorded on a 3-m normal incidence vacuum spectrograph in the wavelength region 300 - 2000Å using a triggered spark source. About 100 energy levels have been established out of which sixty are new. More than 220 lines have been identified in this spectrum. The accuracy of our wavelength measurements for sharp and unblended lines is  $\pm 0.005\text{Å}$ . The Ionization Potential of Br III is estimated to be at  $280700 \pm 300 \text{ cm}^{-1}$  ( $34.80 \pm 0.04 \text{ eV}$ ).

# Using (e, 2e) technique for ionization of Argon by electron impact

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The ionization of electrons from 3p levels of argon has been extensively studied either theoretically or experimentally. However, most of the previous TDCS measurements are reported as a function of scattering angle at small scattering angles and small momentum transfer at low and intermediate electron energy region (Stevenson et al., 2005; Ren et al, 2010).

In this study, we used a modified traditional electron spectrometer with electron gun (0-350 eV) and two 180° electron energy analyzers. We measured TDCS at 200 eV incident electron energy and ejected electron energies of 15, 20, 25 eV and scattered electron angles of 10° and 15°, at the coplanar asymmetric geometry. TDCS of the ejected electron energy of 15 eV at scattered electron angle of 15° with the comparison of the experimental data of Ren et al, 2010 is given. Also, present results accordance with the expectations in terms of binary to recoil ratio and momentum transfer direction.

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# A Partitioned Correlation Function Approach for Atomic Properties

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**Abstract.** Variational methods are used for targeting specific correlation effects by tailoring the configuration space. Independent sets of correlation orbitals, embedded in partitioned correlation functions (PCFs), are produced from multiconfiguration Hartree-Fock (MCHF) and Dirac-Hartree-Fock (MCDHF) calculations. These non-orthogonal functions span configuration state function (CSF) spaces that are coupled to each other by solving the associated generalized eigenvalue problem. The Hamiltonian and overlap matrix elements are evaluated using the biorthonormal orbital transformations and efficient counter-transformations of the configuration interaction eigenvectors [1]. This method was successfully applied for describing the total energy of the ground state of beryllium [2]. Using this approach, we demonstrated the fast energy convergence in comparison with the conventional SD-MCHF method optimizing a single set of orthonormal one-electron orbitals for the complete configuration space.

In the present work, we investigate the Partitioned Correlation Function Interaction (PCFI) approach for the two lowest states of neutral lithium, i.e.  $1s^2 2s^2 S$  and  $1s^2 2p^2 P^o$ . For both states, we evaluate the total energy, as well as the expectation values of the specific mass shift operator, the hyperfine structure parameters and the transition probabilities using different models for tailoring the configuration space. We quantify the “constraint effect” due to the use of fixed PCF eigenvector compositions and illustrate the possibility of a progressive deconstraint, up to the non-orthogonal configuration interaction limit case. The PCFI estimation of the position of the quartet system relative to the ground state of B I will also be presented.

The PCFI method leads to an impressive improvement in the convergence pattern of all the spectroscopic properties. As such, Li I, Be I and B I constitute perfect benchmarks for the PCFI method. For larger systems, it becomes hopeless to saturate a single common set of orthonormal orbitals and the PCFI method is a promising approach for getting high quality correlated wave functions. The present study constitutes a major step in the current developments of both *atasp2K* and *grasp2K* packages that adopt the biorthonormal treatment for estimating energies, isotope shifts, hyperfine structures and transition probabilities.

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# EUV FeXVII emission line branching ratio

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## ABSTRACT

Ne-sequence iron ions, FeXVII, are formed around the temperature of  $\log T_e \sim 6.7$ , which nearly corresponds to the maximum temperature reached in solar active regions. The EIS instrument on board the Hinode mission [1] has detected several weak FeXVII emission lines appearing in its observing wavelengths (170 - 210 Å, 250 - 290 Å), and they are identified as those from the transitions between  $2p^5 3s/3p - 2p^5 3p/3d$ .

Warren et al. (2008) [2] found that the observed intensity branching ratio of the transitions from the  $2p^5 3p (^1S_0)$  level to the  $2p^5 3s (^1,^3P_0)$  levels contradicted with theoretical predictions by a factor of  $\sim 2$  and Del Zanna and Ishikawa (2009) [3] noticed that FeXVII  $\lambda 204.6$  line was blended by emission lines originating from the transition regions.

Intensity ratios of these lines having a common upper level are successfully measured in the Large Helical Device (LHD) at NIFS, and the experimental value is derived to be  $\sim 1.1$ , by separating the contributions of blending FeXII and FeXIII lines [4, 5].

Re-analysis of an AR core and a small flaring event on 2007 June 2 reveals that the intensity ratio reduces significantly to  $\sim 1.5$ , by considering TR line blending, but it is still systematically higher than the experimental value.

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# Theoretical Study of Molecular Collisional Excitation for Modeling FIR/Submm Observations

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## Abstract.

Molecular collisional rate coefficients are required, for a range of temperatures, to interpret spectra of molecular gas not in local thermodynamic equilibrium (LTE). While the rate coefficients describing such processes can often be calculated, enhancements in the spectral line resolution and sensitivity expected from ALMA, SOFIA, Herschel, and other FIR/submm telescopes, place unquenchable demands on the collisional data. Further, collisional rate coefficients usually pose the largest source of uncertainty of the molecular data input to a radiative transfer analysis, in most cases simply due to the lack of such data. Despite some progress in state-to-state collision rate coefficient measurements over the last decade, limited results have been obtained for systems of astrophysical interest. Astrophysical models therefore rely heavily on theoretical estimates due to the difficulty of direct measurements of collisional rate coefficients. Theoretical predictions of rate coefficients involve both molecular structure and scattering components. State of the art calculations typically utilize *ab initio* electronic potential energy surface (PES) calculations and the close-coupled solution of the nuclear scattering equations on these surfaces. Both of these components involve significant computational effort. We review these issues and present recent work on computations of PESs and rotational and vibrational excitation of H<sub>2</sub>, HF, HCl, CO, CO<sub>2</sub> due to He and H<sub>2</sub> collisions. The role of collisional excitation in the modeling of various astrophysical environments as well as on-going and future work will be discussed.

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**Keywords:** Molecular collisional excitation, rate coefficients

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# The CHIANTI Atomic Database: New Improvements For Solar Physics Applications

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**Abstract.** Solar observations at EUV wavelengths obtained with Hinode and the Solar Dynamics Observatory (SDO) have presented new challenges for atomic physics. The EUV Imaging Spectrometer (EIS) on Hinode has returned high resolution spectra of the coronal iron ions (Fe VIII-XVII) for several years, allowing new line identifications to be made and enabling density diagnostics to be studied in unprecedented detail. Several new atomic calculations have been performed to better model the coronal iron ions, and important new results will be summarized. SDO has presented different challenges: the EUV Variability Experiment (EVE) obtains low resolution spectra averaged over the full solar disk over the range 50-1050 Å, while the Active Imaging Assembly (AIA) takes high resolution images in several narrow EUV passbands. For EVE there is a need for complete atomic models for large numbers of ions in order to better model the Sun's EUV irradiance. For CHIANTI, new atomic models under preparation include 1000's of levels, compared to current models with 10's or 100's of levels. Large, extended atomic models are also required to completely model the passbands of AIA, but the narrow size of these passbands also means that accurate wavelengths are essential. Efforts to produce accurate theoretical wavelengths for previously unobserved transitions have been performed by the CHIANTI team, but ultimately new high resolution solar or laboratory spectra are required, particularly in the soft X-ray region. A new release of CHIANTI containing the described improvements is scheduled for release this fall.

# Fe VII: A Problem Ion For Solar Physics

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**Abstract.** Fe VII is formed at temperatures of around 300,000 K in the solar atmosphere, and gives rise to a large number of emission lines in the range 150-300 angstroms, mainly from 3p-3d transitions. As the lines are rather weak, Fe VII was somewhat neglected in the past but high resolution EUV solar spectra from Hinode coupled with recent, comprehensive atomic data have enabled the solar Fe VII spectrum to be studied in detail for the first time. However the comparison between theory and observation is rather poor with many discrepancies of a factor 2 or more. In addition, some of the key transitions appear to have been misidentified by J.O. Ekberg in his laboratory reference work of 1981. A summary of the current state of Fe VII modeling is presented, and a recommendation is made for new laboratory studies and collision calculations.

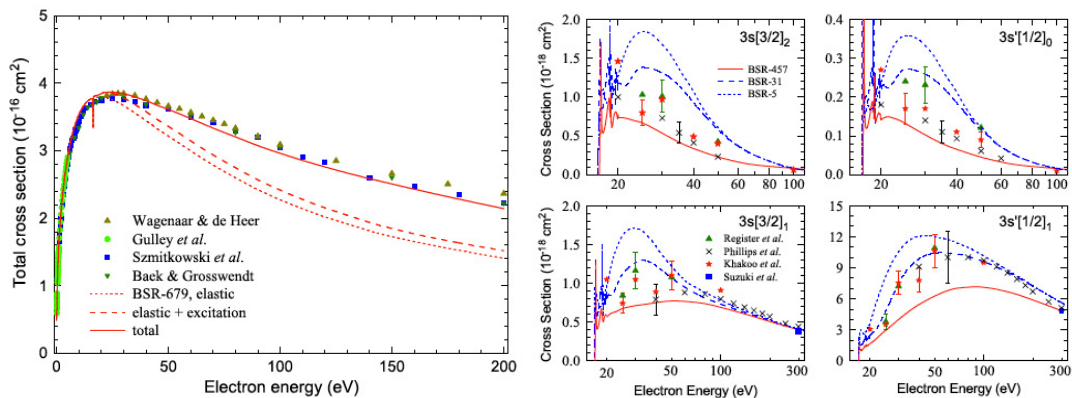
# B-Spline R-Matrix with Pseudo-States Treatment of Electron Collisions with Neon

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**Abstract.** Calculated cross sections for elastic scattering, excitation, and ionization of Ne atoms by electron impact are presented and compared with experiment.

We report large-scale B-spline R-matrix with pseudo-states calculations for electron scattering from Ne atoms. Combining a highly sophisticated structure description with a convergent multi-channel collision model, including coupling to the ionization continuum, we provide accurate and effectively complete datasets for many applications.



The figures show results for the angle-integrated total (elastic plus excitation plus ionization) and the individual cross sections for excitation of the four states in the  $2p^5 3s$  manifold over a wide range of incident energies. For the latter case, note the importance of coupling to the ionization continuum in the 457-state model compared to the 31-state and 5-state models, which only contain discrete states in the close-coupling expansion. While we obtain excellent agreement with experiment for the total cross section, the scatter in the state-selected experimental data indicates the difficulty of the measurements. Based on detailed convergence studies and other observables, such as angle-differential cross sections and light polarizations (to be shown at the conference), we believe that the 457-state results are the most reliable and should be used in modeling applications. Our predictions are available on the LXCAT database.

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# Long-range Interactions of Excited Helium Atoms with Alkali and Alkaline Earth Atoms

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**Abstract.** The long-range interaction plays an important role in determining the dynamics of cold or ultracold atoms. The long-range interaction coefficients  $C_5$ ,  $C_6$ ,  $C_7$ ,  $C_8$  and  $C_{10}$  for the first four excited states of helium atoms (i.e.  $\text{He}(2^3\text{S})$ ,  $\text{He}(2^1\text{S})$ ,  $\text{He}(2^3\text{P})$  and  $\text{He}(2^1\text{P})$ ) with the ground and low-lying excited states of the alkali metal (Li, Na, K and Rb) and alkaline earth metal (Be, Mg, Ca and Sr) atoms are computed from the oscillator strength sum rules. The oscillator strengths of the helium and lithium atoms are calculated using Hylleraas basis functions. The oscillator strengths of the alkali metal (including Li) and alkaline earth metal atoms are calculated with a semiempirical method that treats the valence particles in an *ab initio* manner and uses a model potential to describe the core-valence interaction. For the long range interaction between helium and lithium atoms, the coefficients calculated with Hylleraas basis functions agree with those obtained by the semiempirical method at the 0.1% level of accuracy. For the long-range interaction between helium and other atoms, the uncertainties of the coefficients  $C_5$ ,  $C_6$  and  $C_7$  are about 1~5% while the uncertainties of the coefficients  $C_8$  and  $C_{10}$  are about 5~10%.

# Elastic scattering of positronium: Application of the confined variational method

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**Abstract.** We demonstrate that the phase shift in elastic S-wave positronium (Ps)-atom scattering can be precisely determined by the confined variational method, in spite of the fact that the Hamiltonian includes an unphysical confining potential acting on the center-of-mass of the positron and one of the atomic electrons. The calculated phase shifts are precise mainly because the unphysical effect of the potential can be eliminated by adjusting the confining potential. Using the stochastic variational method, explicitly correlated Gaussian-type basis functions are optimized and the energies of confined Ps-atom systems are determined. Then the discrete energies are taken as a reference for tuning auxiliary one-dimensional potentials. The phase shifts calculated for the one-dimensional potential scattering are the same as the phase shifts of the Ps-atom scattering. For the Ps-hydrogen scattering, the present calculations are in very good agreement with the Kohn variational calculations. Therefore, the 2~4% discrepancy between the Kohn variational and R-matrix calculations is resolved. For Ps-helium scattering, our calculations achieve a higher precision than reported in any previous publication.





starts	Sunday	Monday (Oct 1)	Tuesday (Oct 2)	Wednesday (Oct 3)	Thursday (Oct 4)
8:15		Bus departs from hotel*	Bus departs from hotel*	Bus departs from hotel*	Bus departs from hotel*
8:50		Welcome (Gillaspy & May)	Announcements	Announcements	Announcements
		Chair: Wiese	Chair: Podder	Chair: Brickhouse	Chair: Gillaspay
9:00		Schippers	Lisgo	Kallman	Koike
9:30		Colgan	Pütterich	Behar	Kaganovich
10:00		Pickering	Morita	Kaastra	Hamaguchi
10:30		Coffee break	Coffee break	Coffee break	Coffee Break
		Chair: Sansonetti	Chair: A. Müller	Chair: Crisp	Chair: Braams
11:00		Drake	Nakamura	Marchuk	Chung
11:30		Nörtershäuser	Phaneuf	Tanuma	Panel 2: Data Assessment
12:00			<i>group photo</i>		
12:30		Lunch	Lunch	Lunch	Business meeting (Green Auditorium)
1:00					
		Chair: Dubernet	Chair: Schultz	Chair: Wahlgren	Bus to hotel* and subway (Escort to DC via subway)
1:30		Tiemann	Rothman	Savin	
2:00		H. S. P. Müller	Qu	Campbell	
2:30		Wolf	Loch	Tennyson	
3:00		Petrovic	Foster	Coffee break	
				Chair: Curry	
3:30		Coffee break	Coffee break	Jönsson	
4:00	Registration*	Poster Session A	Panel 1: Future Opportunities	Leckrone	
4:30			Database Demo	Poster Session B	
5:00					
5:30					
6:00	Reception*	Bus to hotel*	Bus to hotel*	Bus to hotel*	
6:30	(ends 8:00)			Cash bar*	
7:00				Banquet*	

\*Marriott Washingtonian Center, 9751 Washingtonian Boulevard (Gaithersburg, MD). If you are staying at the Courtyard Marriott, it is a short walk to the Marriott Washingtonian Center.