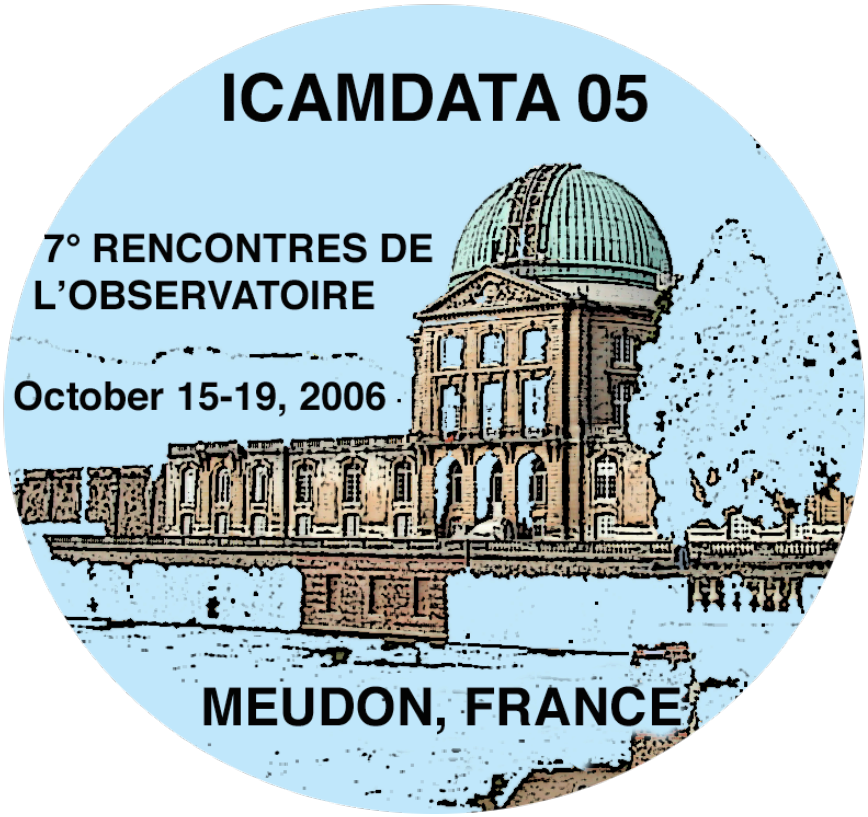

The participant's vademecum

Scientific Program

Book of Abstracts

Editors

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Evelyne Roueff

ICAMDATA 05

7° Rencontres de l'Observatoire - Meudon

16 – 19 October 2006

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CONTENTS

How to reach the conference location from Paris?

Highly Recommended : A bus transportation from Paris to Meudon will be organized every day.

Departure 8:15 am: Place Raoul Dautry, between Montparnasse train station and Montparnasse tower.

Métro : Lines : 4, 6, 12, 13 Station : Montparnasse Bienvenue

RATP Buses : Lines : 28, 48, 89, 91, Station : Gare Montparnasse

Return : Every day after the conference,

BUS DEPARTURE

How to come to the Observatory of Meudon from Paris by train ?

You can reach the Observatory by yourself if you are unable to catch the special buses :

2 possibilities by train :

- ◊ Train from Montparnasse station
- ◊ RER line C

By Train from Montparnasse station _____

At Montparnasse station, take a train going to Sèvres Rive Gauche or to Versailles-Chantiers, Rambouillet, Chartes, etc...

Make sure the train stops at the Meudon or Bellevue stations !

Get out at the 3rd station: Meudon (after Vanves-Malakoff and Clamart). Outside station, turn to the right, after 200 m turn again to the right then straight ahead up to the top of the hill along an avenue lined with stately chestnut trees.

Or get out at the 4th station: Meudon-Bellevue. Outside station, turn left on the avenue du Château: the entrance of the Observatory is on the top of the hill.

By RER line C _____

This train cross Paris from east to west. Take it in the direction of Versailles Rive Gauche

Make sure the train stops at Meudon-Val Fleury !

Conference diner at La Coupole

The Conference diner will take place on *wednesday 18th October from 19h at La Coupole*.

Address : 102 boulevard Montparnasse - 75014 Paris *Metro*: Vavin

Phone : 01 43 20 14 20

For years, la Coupole has boasted the most famous lamb curry in Paris, simmered to perfection under the direction of chef Paul Delbard in the ultra modern kitchens that were revamped when it was acquired by Jean-Paul Bucher in 1988.

Much of the legend of Montparnasse was forged in this former wood and coal store, bought in 1927 by Messrs. René Lafon and Ernest Fraux – managers of the Dôme café - to create the largest brasserie in Paris - 1000m² which were to grace the presence of all the rive gauche's artists of all nationalities.

The visitor's book is a veritable catalogue of modern artists and the vast bar has welcomed great personalities such as Kessel and Hemingway.

The 33 pillars and columns that mark out the immense dining room are still faithful to their post, and for the vast celebration organised for its 70th anniversary, la Coupole paid tribute to the artists of these pillars, students of Matisse and Fernand Léger.

Public transports in Paris are very efficient

Metro & RER

Both are underground trains inside Paris. The same tickets can be used for metro and RER. The main difference is that the RER goes goes in the suburb cities around Paris.

The same tickets can be used for buses, metro and RER in Paris intra-muros.They are sold by 10 (10.90 euros) or individually (1.40 euros).

If you use the RER to go outside from Paris, you have to buy a special ticket whose price depends on the travel distance.

RER C goes to Meudon (Versailles)

RER B goes to the airports Charles de Gaule and Orly.

Bus

There are a variety of directions available with buses. The tickets are identical to those of metros. You may also buy them to the driver.

How to get connected to internet ?

For this, you just need to configure your computer on the web adjustments, DHCP mode.

If you have a Macintosh with MacOS X, it should be automatic. If needed, go in Menu Apple/ System preferences/ Web / Airport Card/ Configuration via DHCP/

If you have a PC with Windows, go in Start/ Parameters/ Configuration Panel / Web connexion and far access / Properties / TCP Properties / IP / Automatically get an IP address

Then you just need to get to any web page http://www.google.fr, for instance. The user will thus be automatically sent to a given page (hence the expression “captive gate”) on which he (she) will have to provide his (her) identifier (data and password) on the following page.

Caution : The navigator window in which the authentification was done must in no way be closed as long as the user wishes to be connected.

Some advices to make it easier

Use the mitres in Mozilla or Firefox, to websurf elsewhere.
In case of error when identifying, just close and re-start your web navigator.

Program

Buses will leave each morning from Gare Montparnasse, Place Raoul Dautry at 8 :15 am

Monday 16th October

9 :00	*Coffee and Registration*	*Installation of the posters*
10 : 00	**Vice-President of the Observatoire de Paris**	*Welcome address*
10 : 15	**Marie-Lise Dubernet *** LERMA, France	*The Virtual Observatory: its goals and the relevance of atomic and molecular data*
11: 00	Michael Brunger Flinders University, Australia	*Data needs and modeling of the upper atmosphere*
11:30	Peter Ventzek, Tokyo Elecron, USA	*Modeling and data needs for plasma processing in semiconductor manufacturing*
12 : 00	Rosine Lallement, Verrières le Buisson, France	*Charge Exchange X-ray emission*
12 :30	*Lunch*	
14 : 15	**Klaus Bartschat *,** Drake University, USA	*High-Precision Cross Sections for Low-Energy Electron-Atom Collisions*
15 : 00	Torsten Markus, Juelich, Germany	*Thermodynamic data for modeling of LTE plasmas*
15 : 30	Yuri Ralchenko NIST, USA	*Data Base demonstration I*
16 :30	*Coffee break*	
17: 00	Poster Session I	
18 :10	*Bus departure*	

** Keynote speaker*

Tuesday 17th October

9 :15	**Daren Stotler *** PPPL, USA	*Atomic Physics in ITER. The Foundation for the Next Step to Fusion power*
10 : 00	Edouard Audit CEA Saclay, France	*Numerical modeling for intense laser physics*
10 : 30	Hugh Summers, University Strachlyde, UK	*ADAS: atomic data, modelling and analysis for fusion*
11: 00	*Coffee break*	
11:30	Jose Cernicharo, Madrid, Spain	*Terahertz spectroscopy in space with the future instruments Herschel and ALMA*
12 : 00	Tetsuya Watanabe, NAO, Japan	*Solar and LHD plasma Diagnostics in EUV*
12 : 30	Boris Potapkin, Moskow, Russia	*First principle based development of the kinetic mechanisms in chemically active light emitting Nonthermal Plasmas and Gases*
13 :00	*Lunch*	
14 : 15	**Nigel Mason *** Open University, UK	*Electron induced processing; Applications and data needs*
15 : 00	Michael Allan, Friburg University, Suisse	*Improved techniques of measuring accurate electron - molecule cross sections near threshold and over*
15 : 30	Ann Orel, UCD, USA	*Resonant dissociative attachment, vibrational excitation and recombination of molecules and molecular ions*
16 : 00	Jiri Horacek, Prague, Czech republic	*Long-lived states of molecular hydrogen anion*
16 :30	Christophe Laux, Ecole Centrale Paris, France	*Challenges in the spectroscopic modeling of air plasma radiation for aerospace applications*
17 :00	*Coffee break*	
17: 30	Poster Session II	
18 :30	*Bus departure*	

Wednesday 18th October

9 :15	**Kate Kirby *** ITAMP, USA	*Atomic and molecular physics for forefront astronomy*
10 : 00	Michael Finkenthal JHU, USA	*Atomic data needs for laboratory and astrophysical plasma physics research*
10 : 30	Kelly Chance, CFA, USA	*Spectroscopic needs for atmospheric pollution measurements*
11: 00	*Coffee break*	
11:30	Walter Lapatovich, OSRAM, USA	*The Role of Molecules in Low Temperature Plasmas for Lighting*
12 : 00	David Schultz	*Data Base Demonstration II*
13 :00	*Lunch*	
Afternoon		*FREE*
19 :00		*Conference dinner at La Coupole, Paris*

Thursday 19th October

9 :15	**Bernd Schweer *** Juelich, Germany	*Plasma-wall interactions in fusion devices and plasma processing technology*
10 : 00	Rudolf Neu MPI, Germany	*Tungsten spectroscopy for fusion plasmas*
10 : 30	Thomas Kruecken, Philips lab, germany	*Plasma and radiation modeling of EUV sources for micro lithography*
11: 00	*Coffee break*	
11:30	Motoshi Goto, NIFS, Japan	*Plasma spectroscopy for magnetically confined fusion plasma*
12 : 00	Amiel Sternberg, Tel Aviv, Israel	*Atoms, Molecules, and Radiation in the Interstellar Medium*
12 : 30	Verena Grill, Innsbrück, Austria	*Molecular data for biological applications*
13 :00	*Lunch*	
14 : 15	Jianmin Yuan, Changsha, China	*Atomic data for opacity calculations*
14 : 45	Andreii Starostin, Troitsk, Russia	*Kinetic coefficients in dense media*
15 : 15		*BUSINESS MEETING*
16 :15		*END OF THE CONFERENCE and BUS DEPARTURE*

Keynote and invited talks

The Virtual Observatory: its goals and the relevance of atomic and molecular data

Marie Lise Dubernet,[1]

[1] *LERMA, Observatoire de Paris, 5, Place Jules Janssen, 92195 Meudon Cedex, France*

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Domain : Astrophysics, Atomic and Molecular Databases

'The International Virtual Observatory Alliance" [1] promotes the *"development of tools, protocols and collaborations necessary to realize the full scientific potential of astronomical databases in the coming decade"*. The alliance consists of representatives from all funded international Virtual Observatory projects who meet on a regular basis to refine the roadmap and reach consensus on choices for the "common ground issues". These issues concern standardisation of astronomical data exchanges (format of data, query langages), as well as the ability to locate and make use of any ressource located anywhere in the IVOA space. Databases in Atomic and Molecular Physics are part of these efforts because their data are essential both for the interpretation of astrophysical spectra provided by ground or space-based telescopes and for the modeling of various astrophysical media.

We report here our latest developments concerning access to Atomic and Molecular Linelists Databases within the Virtual Observatories, addressing the definition of standards through a proposed Data Model [2], an access protocol to linelists [3], and their implementation on customized spectroscopic data from the CDMS [4]/JPL [5] databases. We will present how these new standards allow interoperability between the CDMS/JPL and the BASECOL [6] databases, and between these databases and both a numerical code (PDR code [7] from Meudon) and a spectral analysis software (DALIA) [8].

[1] http://www.ivoa.net

[2] M.L. Dubernet, P. Osuna, M. Guainazzi, E. Roueff, J. Salgado, IVOA, **Version 0.5, January 2006**, "Atomic and Molecular Lines Data Model"

[3] J. Salgado, P. Osuna, M. Guainazzi, M.L. Dubernet, IVOA, **Version 0.2, August 2005**, "Simple Line Access Protocol".

[4] http://www.ph1.uni-koeln.de/vorhersagen/

[5] http://spec.jpl.nasa.gov/

[6] http://www.obspm.fr/basecol

[7] http://aristote.obspm.fr/MIS/

[8] http://lerma40.obspm.fr/ dalia/

Data Needs and Modeling of the Upper Atmosphere.

Michael J. Brunger,[1] L. Campbell,[1] M. A. Bolorizadeh[2]

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[2] *Physics Dept., Shahid Bahonar University of Kerman, Kerman, Iran*

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Domain : Atmospheric Physics and Chemistry

Accurate atomic and molecular data is essential in modeling of the upper atmosphere. Feedback processes between many different species determine that successful modelling requires accurate values for reaction rates and electron impact cross sections. This is particularly the case when atmospheric processes, such as diffusion, also need to be considered. An example where basic data are essential is the combination of electron impact excitation rates of molecular nitrogen [1] and the rate of reaction of vibrationally excited nitrogen with O^+ ions. This combination, along with ambipolar and molecular diffusion, is important in calculating the electron density in the ionosphere. Another example is infrared emission during an aurora. It was originally assumed that a chemiluminescent reaction was the only significant source of the (1,0) emission from the ground state of nitric oxide, but recent measurements [2] of the low-energy electron-impact excitation of NO have allowed calculations to show that the electron-impact component is significant [3]. Accurate electron cross sections for the excited states of N_2 are required in the calculation of auroral emissions [4]. These and other examples will be described and the need for more accurate data discussed.

[1] L. Campbell, M. J. Brunger, D. C. Cartwright and P. J. O. Teubner, Planet. Space Sci. 52, 815–822 (2004).
[2] M. Jelisavcic, R. Panajotovic and S. J. Buckman, Phys. Rev. Lett., 90, 203201 (2003).
[3] L. Campbell, M. J. Brunger, Z. Lj. Petrovic, M. Jelisavcic, R. Panajotovic and S. J. Buckman, Geophys. Res. Lett. 31, L10103 (2004)
[4] L. Campbell, M. J. Brunger, P. J. O. Teubner and D. C. Cartwright, J. Electron Spectr. Rel. Phenom. 144–147, 119–122 (2005).

Modeling and Data Needs for Plasma Processing in semiconductor Manufacturing.

Peter Ventzek,[1]

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peter.ventzek@tel.com

Domain : Low Temperature Laboratory Plasmas

Plasma processing for semiconductor device fabrication increasingly relies on theory, modeling and simulation for concurrent engineering in process equipment development, process integration and manufacturing optimization. Plasma chemistry and plasma?surface interaction data are the foundation of engineering-class process equipment and integration models. The rapid introduction of novel materials and films in semiconductor devices beyond the 45 nm technology node make increasingly urgent the development of methods for the rapid generation of plasma chemistry and plasma surface interaction data. This presentation will describe the state-of-the-art in methodology used for the generation of plasma chemistry and plasma surface interaction data, provide and overview of data needs and illustrate the application of data in the semiconductor manufacturing industry.

Charge-exchange X-ray emission

Rosine Lallement,[1]

[1] *Service d'Aéronomie, Verrières-le-Buisson, France*

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Domain : Astrophysics

X-ray and EUV emission due to charge exchange (CX) between highly charged ions and neutrals has recently been recognized to occur in a number of astrophysical objects. In particular, comets and planets have been observed to be the source of such an emission due to the interaction between atoms and molecules from their atmospheres and impacting solar wind high ions. I will review measurements and modelling, with special emphasis on the diffuse soft X-ray emission from the heliosphere, the cavity carved by the solar wind in the interstellar medium. This omni-directionnel emission is due to the interaction between solar wind ions and interstellar neutrals flowing within the heliosphere. It is found today to be responsible for a large fraction of (if not all) the emission previously attributed to the Local Interstellar Hot Bubble (a 100 parsecs cavity around the Sun supposed to be filled with one million K gas). I will also discuss a number of potential CX X-ray emitters in galaxies.

Because new X-ray satellites have enough sensitivity and spectral resolution to detect the signatures of the CX lines, these findings have stimulated experimental work on the cascading photon spectra for individual ions, and there is now a strong need for theoretical work on state-selective population cross-sections for CX collisions and ion radiative transition probabilities.

High-Precision Cross Sections for Low-Energy Electron−Atom Collisions.

Klaus Bartschat, Oleg Zatsarinny

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Domain : Low-Energy Electron−Atom Interactions

In recent years, much progress has been achieved in calculating reliable cross-section data for electron scattering from atoms and ions. In particular, the "convergent close-coupling" (CCC) [1] and "*R*-matrix with pseudo-states" (RMPS) [2] methods have been extremely successful in describing elastic scattering as well as electron-impact excitation and ionization of light quasi-one and quasi-two electron targets, such as atomic hydrogen, helium, the alkalis, and the alkali-earth elements. However, accurate calculations of electron collisions with more complex targets, notably the heavy noble gases Ne−Xe, heavy quasi-one electron targets such as Zn, Ba, or Hg, and transition metals such as Fe or Mo [3], continue to be a major challenge.

We have further developed a new version of the *R*-matrix (close-coupling) method, using a *B*-spline basis with non-orthogonal sets of term-dependent orbitals [4-6]. This method allows us to generate target descriptions of unprecedented accuracy in collision calculations. Example results for some of the systems mentioned above illustrate that the flexibility of the *B*-spline *R*-matrix (BSR) method to describe both the N-electron target and the $(N+1)$-electron collision problems is of crucial importance for obtaining highly accurate cross sections, particularly in the low-energy near-threshold regime, which is often dominated by resonance structure.

[1] I. Bray, D.V. Fursa, A.S. Kheifets, and A.T. Stelbovics, J. Phys. B **35** (2002) R117.

[2] K. Bartschat, Comp. Phys. Commun. **114** (1998) 168.

[3] K. Bartschat, in *Atomic and Molecular Data and Their Applications*, D.R. Schultz, P.R. Krstic, and F. Owbny (eds.), AIP Conf. Proc. #636 (2002) 192.

[4] O. Zatsarinny and C. Froese Fischer, J. Phys. B **33** (2000) 313.

[5] O. Zatsarinny and K. Bartschat, J. Phys. B **37** (2004), 2173

[6] O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273.

Thermodynamic Data for Modeling of LTE Plasmas

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Domain : Plasma

The Modeling of LTE Plasmas plays an increasing role for the understanding of the plasma behavior and it?s properties. The thermochemical analysis and modeling is a basis for a continuous improvement of the plasma performance. Physical and chemical properties are strongly related to the overall energy balance. One aim of the modeling is to gain a detailed knowledge about radiation emission and energy loss mechanisms Here the interaction of the plasma with the surrounding atmosphere and materials is a major topic. Complex chemical reactions such as corrosion and transport properties between the components need to be studied in order to realize stable performance. The contribution will focus on the determination of key thermodynamic data that are the basis for the description of particle densities in a plasma and also gives an overview of modeling software and techniques. As example the plasma in discharge light sources will be highlighted.

Atomic Physics in ITER – The Foundation for the Next Step to Fusion Power

D. P. Stotler[1]

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Domain : Fusion

ITER represents the next step towards practical magnetic confinement fusion power [1]. Its primary physics objective is to study plasmas in which the fusion power exceeds the external heating power by a factor of 5 to 10. Among its technological objectives are the use of superconducting magnets and remote maintenance, the handling of high heat fluxes, and the testing of tritium breeding concepts. Atomic physics processes will play a fundamental role in facilitating the achievement of these objectives [2]. First, atoms and molecules generated by the interaction of the ITER plasma with surrounding material surfaces will impact and, in some respects, dominate the particle, momentum, and energy balances in both the adjacent and confined, core plasmas. High quality atomic physics data for the relevant species (including hydrogen atoms and molecules, as well as intrinsic impurities beryllium, tungsten, and carbon) will be required to interpret and predict their behavior as they travel into the plasma. Second, extrinsic impurity gases, such as neon and argon, will be introduced into the edge plasma so that their radiation will spread heat coming out from the core more uniformly over the surrounding material surfaces than it would otherwise. Third, many of the diagnostics used to monitor the dense ($n_e \sim 10^{20}$ m^{-3}), hot ($\sim 1 \times 10^8$ K) core plasma leverage off of atomic physics effects. Beam emission and charge exchange recombination spectroscopy based on a dedicated diagnostic neutral atom beam will yield ion temperatures and rotation velocities as well as local impurity ion densities, including that of the helium ash generated by the fusion reactions. X-ray crystal spectrometers will provide independent and complementary measurements of the impurity ion temperatures and rotation velocities. A diagnostic based on the motional Stark effect will measure the local orientation of the magnetic field.

[1] ITER Technical Basis, ITER EDA Documentation Series No. 24, IAEA, Vienna (2002).

[2] ITER Physics Basis Editors, Nucl. Fusion 39, 2137 (1999).

Numerical modelling for intense laser physics.

Edouard AUDIT [1] and Guy Schurtz[2]

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Domain : Astrophysics

The recent start-up of large intense laser facilities such as the Ligne d'Intégration Laser (LIL) or the LULI2000 and the arrival in the near future of the Laser Megajoule (LMJ) gives a great perspective for laboratory astrophysics, dense matter studies and inertial fusion. To make the most of these opportunities, several teams have set up a program which aims at satisfying simulation needs in the fields of Astrophysics, Hot Dense Matter and Inertial Confinement Fusion. A large part of the scientific production in these fields relies upon simulations of complex unsteady hydro flows, coupled to non equilibrium transport and chemical kinetics. As the characteristic time scales of transport may be much shorter than the fluid time scale, implicit numerical methods are often required. Atomics physics data, and in particular equation of states and opacities, are a key and critical ingredients for the simulations done in stellar physics, laboratory astrophysics and in many other fields of astrophysics. We will show the different codes used in the various fields of the project and the different methods used to capture the desired physics. We will also present ODALISC, a new opacity database aiming at providing the community with spectral opacities and numerical tools to use them efficiently in radiation-hydrodynamics codes.

ADAS: Atomic data, modelling and analysis for fusion

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Domain : Fusion, Spectroscopic diagnostics

The Atomic Data and Analysis Structure, ADAS, comprises extensive fundamental and derived atomic data collections, interactive codes for manipulation and generation of collisional-radiative data and models, off-line codes for large scale fundamental atomic data production and codes for diagnostic analysis in the fusion and astrophysical environments. ADAS data are organized according to precise specifications, tuned to application and are assigned to numbered ADAS data formats. Some of these formats contain very large quantities of data and/or have achieved fairly wide-scale adoption in the fusion community.

The talk will focus on recent extensions of ADAS designed to orient ADAS to the needs of ITER. The issue of heavy atomic species, expected to be present as ITER wall materials, dopants or control species, will be addressed with a view to the economized handling of the emission and ionization state data needed for diagnostic spectral analysis. Charge exchange and beam emission spectroscopic capabilities and developments in ADAS will be reviewed from an ITER perspective and in the context of a shared analysis between fusion laboratories. Finally an overview and summary of current large scale fundamental data production in the framework of the ADAS project will be given and its intended availability in both fusion and astrophysics noted.

Terahertz spectroscopy in space with the future instruments Herschel and ALMA

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I will present the capacities of Herschel and ALMA for molecular spectroscopy in the space in the far-infrared and submillimeter domains. These new facilities will certainly open a new view of the Universe. However, the interpretation of the data will require an important effort in the domain of laboratory spectroscopy and of ab initio calculations. The sensitivity of these instruments will bring spectroscopic observations to the spectral confusion limit. Special procedures will have to be used in order to identify spectral features from well known species before new molecules could be found.

Solar and LHD Plasma Diagnostics

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I. Murakami,[2]
M. Yamamoto[3]

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Domain : Astrophysics

Japanese sun observing mission; Solar-B is to be launched on 23-Sep-06. The EUV Imaging Spectrometer (EIS) on board Solar-B [1] will be able to observe, for the first time in Solar EUV observations, spectra and monochromatic images of non-ionization-equilibrium plasmas in the solar transition-region and corona at two-wavelength bands of 170 - 210Å and 250 - 290Å, with typical time-resolutions of 1 - 10 seconds. Time-dependent collisonal-radiative model has been developed to diagnose temperatures and densities of those plasmas in the outer atmospheres of the Sun. No systematic models yet exist for iron ions of L- and M-shells, which are very important for coronal plasma diagnostics. Atomic data of FeX to FeXV are surveyed and evaluated, and most recommended data are determined[2]. Obtaining of the experimental data is recommended: Possibility of getting the experimental data of ionization and recombination cross sections for iron ions with an EBIS instrument called NICE (Naked Ion Collision Experiment) and a new EBIT (Electron Beam Ion Trap) for EUV lines is in consideration. EUV spectra in the wavelengths of 170 - 190Å were also taken by Large Helical Device (LHD) of NIFS, injecting iron TESPEL (tracer-encapsulated solid pellet).

[1] Culhane, J. L. et al.: 2005, Ad. Sp. Res., 36, 1491.
[2] NIFS-DATA95, 2006, in press.

First-Principles-Based Development of Kinetic Mechanisms in Chemically Active Light-Emitting Nonthermal Plasmas and Gases

Valerie Astapenko[4], Alexander Bagatur'yants[4], Maxim Deminsky[1,4], Alexander Eletskii[1,4], Igor Kirillov[1], Andrei Knizhnik[1,4], Boris Potapkin [1,4] , Elena Rykova[4], Stanislav Umanskii[4], Andrei Zaitsevskii[1,4], Marina Strelkova[1], Leonid Sukhanov[1], Andrei Safonov[4], George M. Cotzas[2], Tony Dean[2], J. Darryl Michael[2], Vikas Midha[2], David J. Smith[2], Timothy J. Sommerer[2], Bala Varatharajan[2], Adrian Tentner[3]

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Domain : Low Temperature Laboratory Plasma

Recent progress in several related research areas such as first-principles electronic-structure calculations of atoms and diatomic molecules, theory of elementary processes, kinetics, and numerical engineering, and also continuing exponential growth in computational resources enhanced by recent advances in massively parallel computing have opened the possibility of directly designing kinetics mechanisms to describe chemical processes and light emission in such complex media as nonequilibrium plasmas and reacting gases. It is important that plasma and combustion kinetics can be described in the framework of this direct approach to a sufficiently high accuracy, which makes it an independent predictive research tool additional to experimental techniques. This paper is devoted to an overview of the key events in electronic structure theory, theory of elementary processes, kinetic theory, and computing engineering that provide a basis for this development. Two examples of the development of first-principles-based mechanisms devoted to mechanism of hydrocarbon fuel combustion at high temperatures and light emission in non-thermal glow discharge plasma of metal halides are discussed in detail with special attention paid to a comparison of the results obtained at every level of system description with the appropriate experimental data. Software tools that can be used in such multilevel theoretical works are discussed as well.

Electron Induced Processing; Applications and data needs

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Domain : Low Energy Electron Molecule Interactions

Electron induced reactions in both gaseous and condensed phases initiate and drive many of the basic physical and chemical processes in science and technology. For example, it has recently been demonstrated that low energy electrons may play a key role in radiation damage of the DNA of living systems[1] while electron processing plays a key role in aeronomy and atmospheric chemistry[2]. In the technological field electron induced reactions underpin most of the multibillion dollar modern semiconductor industry since it is those reactive fragments produced by electron impact of etchant gases that react directly with the silicon substrate[3].

Electron induced processes are also of extraordinary importance for determination of structure and chemical reactivity of species adsorbed on surfaces[4], indeed recently it has been demonstrated that, using STM based technology, discrete electron reactions may be performed at the individual molecular level thus introducing the prospect of designer synthesis on the nanoscale[5]. Electron induced chemistry in ice films plays a key role in molecular formation in both the interstellar chemistry and on planetary surfaces, underpinning much of modern astrochemistry.[6]

However the data base for electron-molecule interactions remains woefully inadequate[7,8] providing a major impediment to development of many of these fields. In this talk I will review the many applications of electron induced processes, review the current state of our knowledge and suggest a strategy by which we might improve the data base.

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Improved techniques of measuring accurate electron - molecule cross sections near threshold and over the entire angular range

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Domain : Low Energy Electron Molecule Interactions

Elastic and vibrational excitation cross sections were measured in N_2 at energies at and below the $^2\Pi_g$ resonance region, and over a large angular range using the Magnetic Angle Changer (MAC) with particular attention to the determination of the instrumental response both as a function of energy and as a function of scattering angle [1]. In the intermediate angular range, about $40^\circ - 130^\circ$, the new results agree well with many published cross sections, but larger discrepancies are found at angles below and above this range. The new results agree very well with the calculations of Morrison and coworkers [2,3] and of Telega and Gianturco [4,5]. The method was also applied to near threshold electronic excitation of neon [6] and (at a fixed scattering angle) of argon and xenon [7], where a very good agreement with the Breit-Pauli *B*-spline *R*-matrix calculation was obtained [6,7]. Fixed angle measurements were then performed for formic acid [8] and its dimer. The most remarkable finding here was a very strong 'unspecific' vibrational excitation in the dimer.

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Resonant Dissociative Attachment, Vibrational Excitation and Recombination of Molecules and Molecular Ions

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Domain : Low Energy Electron Molecule Interactions

Electron collisions with molecules and molecular ions that lead to excitation and dissociation play a key role in a number of environments, since they produce the radicals and molecular fragments that initiate and drive the relevant chemistries. Examples range from the technologically important plasmas used in plasma enhanced chemical vapor deposition, to planetary atmospheres and interstellar clouds, to DNA damage driven by secondary electron cascades produced by radiation. In general due to the large mass difference between the electron and target, the cross section is dominated by resonant processes. where the electron can temporarily attach to the molecule and change the forces felt between its atoms for a period of time comparable to a vibrational period. This can lead to resonant vibrational excitation and dissociative attachment, for neutral targets, or dissociative recombination in the case of ions. In this talk, I will outline the basic theory that underlies these processes, and our approach to study them. I will illustrate the method with the study of dissociative recombination for the He_2^+, Ne_2^+, and Ar_2^+ molecular ions, vibrational excitation and dissociative attachment to CF, and dissociative recombination in the CF^+ leading possibly to F^-.

Long-lived states of molecular hydrogen anion.

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Domain : Astrophysics

The hydrogen molecule is the most abundant and most important molecule in the Universe. In its neutral form it is well understood but the structure of the molecular anion H_2^- is much less known. According to most theoretical estimates the molecular hydrogen anion is highly unstable with the very short lifetime of the order of 10^{-15} s. The lowest hydrogen anion $^2\Sigma_u^+$ state is well known both from theoretical as well as experimental studies. Some experiments however claim to observe a long-lived metastable states of the hydrogen anion with the lifetime of the order of microseconds [1, 2] exceeding by many orders the theoretical lifetime. A more recent and elaborated experiment [3] failed however to see any hydrogen anions with the lifetime longer than 10^{-11} s. This conundrum was unambiguously solved recently by the use of the accelerator mass spectrometry [4] and the existence of metastable states with the lifetimes of microseconds was confirmed. Later the hydrogen anions were observed in high resolution mass analysis [5] and their lifetime measured [6]. The nature of the metastable states will be explained and discussed in terms of the nonlocal resonance model [4, 7]. The necessary prerequisite for these states to exist is the high rotational excitation of the hydrogen molecule.

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Challenges in the spectroscopic modeling of air plasma radiation for aerospace applications

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Atomic and Molecular Physics for Forefront Astronomy

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Domain : Astrophysics

Across a wide range of wavelengths and encompassing a rich menagerie of astrophysical objects and environments, the need for atomic and molecular data to advance forefront astrophysical research has never been greater. Over the last decade, astronomical discoveries, such as the detection of brown dwarfs and extra- solar planets, and the observation of new phenomena, such as x-rays from comets, have created a demand for more and different kinds of data. The next generation of ground- and space-based instruments with greater sensitivities and higher spectroscopic resolution will expand our windows on the Universe, increasing the pressure for atomic and molecular data of higher accuracy and greater completeness. Examples of recent successes as well as future opportunities for research in this area will be discussed.

Atomic data needs for laboratory and astrophysical plasma physics research

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The talk will adress the problems related to the data needs in the area of modeling XUV spectra emitted by laboratory as well as astrophysical plasmas. We will limit the discussion to optically thin plasmas in order to be able to focus on the basic ingredients without need to worry about opacity effects. Based on examples taken from the world of the magnetically confined nuclear fusion plasma experiments or X-ray observations recorded from missions such as Chandra, XMM, we will first identify the problems related to the data analysis and the extraction of physical meaning from it. Then, we will discuss the state of the art of the atomic data, both in the area of energy structure/transition rates for the atoms and the charge states of interest as well as that of the radiative and collisional processes involved in the excitation, ionization and recombination mechanisms considered in the CR modeling of the spectra. The essential question of the 'benchmarking' of the theoretical computations will also be adressed.

Spectroscopic Needs for Atmospheric Pollution Measurements

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Domain : Atmospheric Physics and Chemistry

This article provides an overview of current results and capabilities for spectroscopic measurements of atmospheric pollution, particularly from Earth satellites. This is now a sizable field of research, with some dozen satellites now performing measurements or being planned or prepared for launch. Measurements of tropospheric chemical constituents, their sources, sinks, transport, and transformation, provide crucial information on tropospheric oxidation chemistry and pollution of the lower atmosphere, and are now being employed to improve global emission inventories of odd nitrogen (NO_x) and volatile organic compounds (VOCs).

The presentation gives an overview of research in the field and gives a number of examples, primarily taken from research done at the Harvard-Smithsonian Center for Astrophysics, with additional input from our collaborators and colleagues. Examples include measurements of: formaldehyde (HCHO), the major proxy for VOCs; glyoxal (CHOCHO) a recent additional proxy for VOC emissions, NO_2, the major proxy for NO_x; global distributions of tropospheric ozone and carbon monoxide, SO_2 from volcanoes and from anthropogenic pollution, and the formation of enhanced BrO over the polar ice shelves. The needs for improved laboratory spectroscopic measurements for the various pollutants will be presented.

The Role of Molecules in Low Temperature Plasmas for Lighting

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Domain : Lamps and Lasers

High intensity discharge (HID) lamps are low temperature (0.5eV), weakly ionized plasmas sustained in a refractory but light transmissive envelope for the purpose of converting electrical power into visible radiation [1]. For commercial applications this conversion must occur with good efficiency and with sufficient spectral content throughout the visible (380-780nm) to permit the light so generated to render colors in a fashion comparable to natural sunlight. These goals are often achieved by adding multiple metals to a basic mercury discharge. Because the vapor pressure of most metals is very much lower than mercury itself, chemical compounds containing the desired metals, and having higher vapor pressures are used to introduce the material into the basic discharge [2]. Complexing agents which further improve the vapor pressure are used to enhance the amount of metals in the discharge [3,4]. The metal compound and complexes are usually polyatomic species which vaporize and subsequently dissociate as they diffuse into the bulk plasma. Under the approximation of local thermodynamic equilibrium (LTE) the particles are in equilibrium, but not with the radiation field. Strong thermal (106K/m) and density gradients are sustained in the discharge. Atomic and molecular radiation produced in the high temperature core transits through colder gas regions before exiting the lamp. In these regions where the complex molecular species exists in an undissociated state, bound-free transitions can result in energy being effectively converted from light radiation into heat in the mantle. Bound-bound transitions in identifiable molecules can result in modification of the spectral output in unpredictable and counter-intuitive ways. Examples of complexing agents [5] and their effect on the spectral output of typical rare-earth containing HID lamps will be given. The melt composition and the complexing agents themselves may change with time, as chemical reactions in the lamp occur, and their benefit is accordingly altered. Optical absorption and emission data, molecular structure and electron impact and attachment cross section data on these molecular components is sparse [6] but necessary to understand lamp performance in the lamps re-ignition phase and during steady state operation. More data is needed.

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Plasma-wall interactions in fusion devices and plasma processing technology

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Domain : Fusion

The international project ITER in Caderache, France, should achieve a positive energy balance in magnetically confined plasmas for the first time. A key question for the performance will be the influence of the fusion plasma on plasma facing components. The main emphasis of the actual research programs is on the investigation of the processes of plasma wall interaction, erosion, transport and deposition of material especially for long time operation in order to find technological solutions for an economical operation of fusion reactors. In the past significant improvements of plasma operation in fusion experiments were obtained with carbon walls. But the application of carbon might be avoided due to activation aspects. A review about the actual research on plasma wall interaction and the application of technical plasmas for treatment of plasma facing components will be presented. Special attention will be given on spectroscopic methods for the diagnostic of plasma edge and technical plasmas.

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Tungsten Spectroscopy for Fusion Plasmas

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Domain :Fusion

Tungsten is one of very few candidate materials for plasma facing components in future fusion devices. Until recently, it has received only little attention in fusion experiments because of its deleterious effect on the plasma performance experienced in early fusion devices. However, due to this potential hazard a thorough diagnostic of the W influx into the plasma and the W content in the plasma is of outmost importance. Therefore, investigations have been started at tokamaks and EBITs to provide atomic data for W in high temperature plasmas. Usually the influx of impurities is deduced from the intensity of spectral lines from neutrals or ions in a low ionisation state. For this purpose the appropriate ionisation rates and excitation rates have to be known. At the moment, a WI transition ($^7S - ^7P$) at 400.8 nm is used, but an extension of the method to other lines is under investigation. In the core of present day plasmas ionisation states up to W^{56+} can be reached and in a reactor states up to around W^{68+} will be present. In order to extract information on the local W concentrations over the whole plasma radius atomic data (excitation, ionisation, recombination) for all the charge states up to the maximum ionisation state are necessary. Similarly a high sensitivity has to be achieved since the central W concentrations should stay below 10^{-4}. For an unambiguous identification of the transitions EBIT measurements are of great advantage, but due to the lower electron density compared to fusion plasmas, investigations there are indispensable. The talk will highlight recent experimental and theoretical advances and indicate the needs for further investigations.

Plasma and Radiation Modelling of EUV Sources for Micro Lithograpy

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Domain : Low Temperature Laboratory Plasmas

Future extreme ultraviolet (EUV) lithography will require very high radiation intensities in a narrow wavelength range around 13.5 nm, which is most efficiently emitted as line radiation by highly ionised heavy particles. Currently the most intense EUV sources are based on Xenon or Tin discharges. After having investigated the limits of a hollow cathode triggered Xenon pinch discharge a Laser triggered Tin vacuum spark discharge is favored by Philips Extreme UV.

Plasma and radiation properties of these highly transient discharges will be compared. Besides simple MHD-models the ADAS software package [1] has been used to generate important atomic and spectral data of the relevant ion stages. To compute excitation and radiation properties, collisional radiative equilibria of individual ion stages are computed. For many lines opacity effects cannot be neglected. The optical depths, however, allow for a treatment based on escape factors. Due to the rapid change of plasma parameters the abundancies of the different ionisation stages must be computed dynamically. This requires effective ionisation and recombination rates, which can also be supplied by ADAS.

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Plasma spectroscopy for magnetically confined fusion plasma

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Domain : Fusion

The spectroscopic diagnostics for fusion plasmas can be categorised into two groups according to its purposes. One is based on the measurement with high wavelength resolution aiming at obtaining various properties of emission line profile such as the width, shift, and so on. In many cases these quantities are directly connected to the specific plasma parameters, and they have been used as the standard diagnostic methods. The other is based on the observation in a wide wavelength range which gives us the population distribution over excited levels of various atoms and ions. From the results and the colliaional-radiative model calculation, plasma parameters such as the electron temperature and density are estimated. The reliability of the obtained parameters inevitably depends on the accuracy of the atomic data, and this kind of measurement has not been regarded as an established diagnostic method. The situation is, however, changing owing to the accurate atomic data recently being produced. The talk will introduce several spectroscopic measurements based on both the categories for LHD, the heliotron-type fusion device. The Zeeman spectroscopy gives us the precise line emission locations in conjunction with the magnetic field structure in the plasma [1, 2]. The Balmer series lines of neutral hydrogen are exploited to estimate the plasma parameters for the Serpens mode [3] recently found in LHD. The formation of complete LTE plasma is confirmed in a comprehensive analysis of the spectrum observed for the relatively high density plasma formed around the hydrogen and impurity pellets.

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Atoms, Molecules, and Radiation in the Interstellar Medium

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Domain : Astrophysics

I will present an overview of interstellar photon-dominated regions (PDRs), and X-ray dominated regions (XDRs), with emphasis on recent observations, and basic atomic and molecular processes.

Molecular data for biological applications

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Electron attachment as well as electron impact experiments have been performed on molecules of biological relevance, like several nucleobases.[1-2] The experiments have been carried out using an hemispherical electron monochromator with high electron energy resolution in combination with a quadrupole mass spectrometer. Additional experiments on life-times of special anionic states have been undertaken using a Nier-type ionization source in combination with a double focussing sector field mass spectrometer. The focus of the electron attachment studies was the bond- as well as site-selective loss of H atoms from isotopically labelled nucleobases, which could be observed at very low electron energies. Threshold electron impact ionization data have been recorded for several biomolecules, and the appearance energies of each parent and the most abundant fragment ions were determined using fitting procedures based on the Wannier threshold law.

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[2] S. Denifl, B. Sonnweber, G. Hanel, P. Scheier and T.D. Mrk, Int. J. Mass Spectrom. 238 (2004) 47-53

Atomic data for opacity calculations

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Domain : Low Energy Electron Molecule Interactions

Opacity calculation concerns a huge number of atomic data, including energy levels, oscillator strength, spectral line profile parameters, and photoionization cross sections. Theoretical methods, emphasizing on various physical effects with a variety of accuracy, have been employed to obtain the data. For atomic energy levels and the oscillator strength, one- and multi- configurational self-consistent schemes in both full relativistic and non-relativistic forms have been used to show how the detailed treatment of the physics, such as the electronic correlations and the relativistic effects, affects the finally calculated opacity. Quantum mechanical and semi-classical approaches have been used to deal with the electron impact broadening of the spectral lines. Efforts have been given to clarify the environmental (density and temperature) dependence of the influence of the detailed line profiles on the opacity. One channel and multi-channel close-coupling approaches have been applied in the calculations of the photoionization cross sections. With the channel coupling, we have shown the importance of the autoionizing effects for the transmission spectra. Density, temperature, and chemical components have direct influence on the atomic structure and atomic processes. Efforts have been given to display this kind of influence via a simplified way of average atom model. As examples, x-ray transmission spectra and the spectra-resolved opacities of Al, Fe, O, C, and Mg, which one often encounters when dealing with astrophysical problems, have been obtained independently based on the so-called detailed-term (or level)-accounting treatments for the atomic data.

Kinetic coefficients in dense media

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Equilibrium rate constants of inelastic processes in dense media have been studied with taking account the quantum corrections to the particle momentum distribution function (PMDF). The main problem in evaluation of the rate constants of inelastic processes as well as PMDF relates to finding the scattering amplitude out of the energy shell. This problem is resolved within the frame of the approach developed based on the asymptotic representation of the wave function of scattering particles. The explicit solution has been obtained for the problem of vibrational relaxation of diatomic molecules. The specific calculations performed for low temperature atmospheric pressure relaxation.

Posters

P1

Study of the K-H2 quasi-molecular line satellite astrophysical applications

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Domain : Astrophysics

We present new theoretical calculations of the line profile of potassium perturbed by molecular hydrogen with an emphasis on properties of the quasi-molecular line satellite.

P2

Experimental and theoretical study of alkali lines broadening for astrophysical applications

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Domain : Astrophysics

The visible and near infrared spectra of L and T-type brown dwarfs exhibit prominent features corresponding to atom resonance lines of alkali-metal atoms [1]. Similar features are expected to appear in the spectra of extraterrestrial giant planets (EGPs) [2,3]. The spectra of cool brown dwarfs are dominated by the resonance lines of Na at 590 nm and of K at 760 nm. Because of the large concentrations in these objects of gaseous H_2 and He at temperatures around 1000 K, the profiles of Na and K lines are strongly broadened by collisions up to 100 nm on each side of the line core. This broadening is pressure and temperature sensitive and consequently the ability to model precisely those alkali lines is a powerful tool to retrieve the atmospheric conditions of cool brown dwarfs and EGPs.

To improve the data available for modeling, we have designed a spectroscopic experiment to measure absolute absorption coefficients of alkali vapors colliding with H_2 and He at astrophysically relevant temperatures. The atomic densities are measured precisely using the anomalous dispersion ("hook") method. Investigating the spectral range 380-920 nm, we observed the broadening of the K 770 nm lines and we find the K 404 nm doublet exhibits a putative satellite feature on its blue wing. The theoretical calculations utilize accurate molecular potential energies and transition dipole moments and fully quantum-mechanical methods. Supported in part by NASA grant NNG06GF06G.

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P3

M_F-Dependent Lifetimes Due to Hyperfine Induced Interference Effects

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Domain : other

We report on a theoretical investigation of M_F-dependent lifetimes due to interference between different types of multipole transitions, and in particular the $3d^{10}\ ^1S_0 - 3d^9 4s\ ^3D_3$ transition in Nickel-like ions. For pure states this decay is only allowed through a magnetic octupole (M3) transition, but in the presence of a nuclear spin an electric quadrupole (E2) transition is induced by the hyperfine interaction, and the interference between the two types of multipoles makes the lifetimes of the hyperfine levels M_F-dependent.
Extensive Multiconfiguration Dirac-Fock calculations were performed to calculate the $3d^{10}\ ^1S_0 - 3d^9 4s\ ^3D_3$ M3 transition element, the $3d^{10}\ ^1S_0 - 3d^9 4s\ ^3D_2$ E2 transition element and the hyperfine interaction matrix elements between $^3D_3$ and $^3D_2$. First order perturbation calculation were used to calculate the hyperfine induced E2 transition element and the M_F-dependent lifetimes.
Detailed results for Ni-like Xenon is presented. Xe consists of 9 different isotopes of which two have a nuclear spin (one with $I = 1/2$ and one with $I = 3/2$) resulting in 25 different lifetimes depending on isotope, F-value and M_F-value. [1] used a single exponential fit to experimentally determine the lifetime of the $3d^9 4s\ ^3D_3$ state in Ni-like Xe. It is shown that a single exponential could be fitted to a theoretical decay curve, where each lifetime was weighted according to a gas of natural mixing of isotopes, with good accuracy. Depending on which interval the single exponential was fitted to, different lifetimes was obtained.

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P4

Importance of the molecular photo-destruction cross sections to model the ISM

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Domain : Astrophysics

To better understand how stars could form, it is crucial to model accurately the physical and the chemical properties of the galactic interstellar medium (See [1], [2] and [3]). To perform it, I used the Photo-Dissociation Region (PDR) code developed in Meudon (see [4] and [5]). Moreover, the knowledge of the molecular features as their photo-destruction cross sections values is also required to make trustworthy predictions not only in term of molecular abundances but also to correctly estimate their photo-destruction rates. I focussed my study on the photo-dissociation and the photo-ionisation of the following species : C_2, C_3, CO, CH, OH, NH and CN for which I gathered from the literature new values.
I will present here the results I obtained and the implication of these updated photo-destruction cross sections values in term of PDR predictions.

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[5] Le Petit et al., 2002, A&A, 390, 369

P5

The database DESIRE

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Domain : Spectroscopy, Astrophysics

We have started a systematic investigation of the radiative properties of the elements of the sixth row of the periodic table. Using a combination of experimental radiative lifetimes obtained with the time-resolved laser-induced fluorescence (LIF) technique and of theoretical branching fractions (BF) calculated with a relativistic Hartree-Fock (HFR) approach, taking configuration interaction and core-polarization effects into account, transition probabilities have been deduced for a number of transitions of astrophysical interest. So far results have been obtained for the elements Ta [1], Re [2-3], Os [4], Ir [5], Tl [6] or Au [7] or their ions. The results obtained are stored in the database **DESIRE** (**D**atabas**E** for the **SI**xth **R**ow **E**lements), an extension of the database **DREAM** (**D**atabase on **R**are **EA**rths at **M**ons University), which will be progressively created on a web site of the University of Mons-Hainaut in Belgium (See e.g. [8]). In the present contribution, the procedures followed to obtain the new results but also on the difficulties associated with their determination will be discussed.

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P6

Isotopic and Symmetry Effects in the Study of Cold Monatomic ^{85}Rb and ^{87}Rb Gases

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Domain : Other

The isotopic and quantum effects in the study of a low-temperature monatomic rubidium gas are considered in this work. By adopting the Chapman-Enskog model for temperatures ranging from 1K up to 100K, the diffusion coefficients with the symmetry effects, due to the identity of the colliding atoms, are calculated quantum mechanically. By including the exchange interactions, the ground *gerade* and *ungerade* potentials are constructed. The investigation is further extended to analyze the resonance structures in the diffusion cross sections and to compute the scattering lengths.

P7

Interference effects on lifetimes in low-Z Ni-like ions.

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Domain : Other

We report in Multi-configuration Dirac-Hartree-Fock calculations for forbidden lines in Ni-like ions. As reported elsewhere(see poster by M.Andersson et al at this conference), some systems in this isoelectronic sequence show an interference effect between M3 and hyperfine induced E2-transitions, resulting in lifetimes depending on the magnetic quantum number M_F. In this poster we investigate the lower-end of the sequence, where correlation is important, but the relativistic effect smaller.

P8

High precision electron-ion collision experiments at the Heidelberg Storage Ring TSR

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Domain : Low Energy Electron Molecule Interactions

Merged beam setups like at the heavy-ion storage ring TSR in Heidelberg are very powerful tools to measure cross sections of electron-ion collision processes such as dissociative recombination in molecular ions or di-electronic recombination in atomic ions as function of the collision energy. Ions at energies of $\sim$ 1MeV/amu are stored in the ring by magnetic fields for times of up to 100s. Extending the known technique [1], a new electron target [2], working together with the electron cooler, is used since two years to improve the electron energy resolution, now reaching down to $kT_{\perp} \approx 0.5$meV. It was used to measure low-energy cross sections for molecular and atomic ions with very high, unprecedented resolution. In addition, negative product ions were observed with a scintillation detector.

We will give examples on recent measurements on dissociative recombination. In particular, the cross section of HD^+ dissociative recombination was remeasured and previously unresolved structures were found in the range of $E_d = 0 - 200$meV. These allow a detailed comparison with theoretical model calculations (MQDT) [3] with the further goal of assigning the measured structures in the cross section to resonances due to the involved intermediate states in the indirect dissociative recombination process.

We will also give examples of recent results on dielectronic recombination of multiply-charged iron ions relevant for both low and high temperature astrophysical plasma [4,5].

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P9

Recent advances in atomic physics codes for astrophysics studies

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Domain : Astrophysics

Atomic structure codes are used to provide data for detailed spectroscopy, in view of diagnostic as well as radiative transfer in stellar and solar atmospheres. They are also used for gross spectra and average quantities such as mean charge state, Planck and Rosseland mean, non-LTE emissivity,... In the last decade, substantial improvement has been made in this domain, new theories and methods to deal with the statistics of zillion of levels and lines has been formulated. Robust, fast and user friendly codes for "extensive data production",... We shall present the codes we have initially set for laser produced plasma (and isolated ions), but which will also be used also for Astrophysical studies, with emphasis on - detailed spectroscopy (HULLAC [1]) - LTE average quantities and gross spectrum (STA[2]) - non-LTE properties (HULLAC-v9 [3], SCROLL [4]) and will propose potential applications of these codes.

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P10

Comparison of two major sources of uncertainty in Titan ionospheric chemistry model

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Domain : Other

Discrepancies between the outputs of different models and available data are difficult to assess in the absence of quantified uncertainties. In particular, modelling the chemistry of planetary ionospheres involves numerous physical and chemical parameters, which values are known from laboratory measurements with experimental uncertainty factors. These uncertainty sources should be accounted for in the modelling. In a previous study about Titan ionospheric chemistry [1] we reported the first detailed uncertainty analysis concerning the kinetics parameters of the ion-molecule reactions. We showed that uncertainties on branching ratios contribute significantly to the estimated uncertainties on ion densities. Neutral species were considered as a fixed bath in Titan's ionosphere. Considering that ion densities closely depend on the neutral atmosphere ([2],[3]), we expect an important impact of densities of neutral species on the uncertainties of ion densities.
In this work, we take into account both uncertainty sources, quantifying their respective contribution to the ion density uncertainties. Uncertainty propagation is performed by Monte Carlo sampling. In addition, we assess the sensitivity to three turbulent diffusion profiles for the neutral species, corresponding to the extreme profiles at high altitudes described in the litterature.

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P11

14 eV Resonant Processes in e-H_2 scattering

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Domain : Low Energy Electron Molecule Interactions

Extensive cross section calculations and measurements have been devoted in the past decades to the study of the dissociative electron attachment (DEA) and resonant vibrational excitations (RVE) occurring through the formation of the intermediate H_2^- ion in its ground $^2\Sigma_u^+$ or first excited $^2\Sigma_g^+$ state. These two states give rise to the well known 3.75 eV and 10 eV resonance peaks in the measured DEA cross sections. The underlying processes have been well described and the experimental data successfully reproduced by many different models. Quite different is the situation for the so-called 14 eV peak appearing in the experimental observations [1]. The origin of this peak is, to date, not yet understood, and has been attributed to the $H_2^{-*}\,^2\Sigma_g^+$ excited ion state correlating with $H^-(1s^2)$ and $H(n=2)$ atomic states [1]. In order to contribute to the clarification of the 14 eV process, but also to provide information on resonant processes involving H_2^{-*} ion, which may have some role in plasma systems, we present in this communication local potential cross section calculations for the processes

$$H_2(X^1\Sigma_g^+, v_i=0, j=0)+e \rightarrow H_2^{-*}(^2\Sigma_g^+) \rightarrow H^-(1s^2)+H^*(n=2) \qquad DEA$$
$$H_2(X^1\Sigma_g^+, v_i=0, j=0)+e \rightarrow H_2^{-*}(^2\Sigma_g^+) \rightarrow H_2(X^1\Sigma_g^+, v_f, j=0)+e \qquad RVE$$

Comparison with the experimental data for both processes will be discussed.

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P12

Collisional-Radiative Models of Low Ionized Rare Gas Plasmas

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Domain : Astrophysics

We have recently developed a time-independent Collisional Radiative (C-R) model which is necessary to perform spectroscopic diagnostics of relatively cool Ar and Xe plasmas [1]. The higher electronic temperature (Te) limit of the present model corresponds to situations where the available energy is sufficient to remove all six of the outer (3p or 6p) electrons of the atom.
Comparisons of the theoretical spectra generated from this model with those obtained experimentally from various Ar and Xe plasmas have been used for validation of the theoretical approach [2]. Our results are also compared to those derived from the well known set of codes developed at LANL [3].
Non-intrusive emission spectroscopy p lasma diagnostics allows for the evaluation of the local temperature and density; it also provides information on the constituents and on the most important processes encountered in the plasma. For a satisfactory application of such diagnostics a full C-R model is needed, taking into account all of the species present, both neutral and ionized, together with their excited state level structure and transition probabilities between the levels; all contributing processes are taken into account through their respective reaction rates.
Our C-R model has been used to analyze various Ar and Xe spectra. A version specific to lower temperatures was previously used to diagnose and model two prototype Stationary Plasma Thrusters (SPT-50) made available to us at the Ecole Polytechnique and the ONERA Laboratories, both located in Palaiseau, fed with Ar and Xe, a coaxial microwave Ar plasma reactor (RCM) functioning in our Laboratory and a direct current Ar discharge device with carbon cathode operating at the LPIIM laboratory of Universit?de Provence [4]. It is now used to study the spectrum of a low temperature Xe plasma contained in a hollow cathode with dielectric barrier available at the LPGP Laboratory and the radiation emission of the WEGA Stellarator operated at IPP Greifswald, when fed with Ar [5]. According to measurements made at IPP, a Te of about 10 eV is typical in WEGA for Ar discharges, with an electron density, ne of about 1012 cm3. Our calculations based on a coronal model show the full Ar I to Ar V spectra, plus some radiation from Ar5+ [6]. Of course, all of these spectra are not expected to be simultaneously present in an homogeneous plasma with a single Te , but in the case of the separatrix- and/or limiter-plasma of WEGA a mixture of temperatures may explain the simultaneous detection of signatures of all of the ionized Ar species on top of the neutral, possibly altering the total radiated energy. Therefore a superposition of Maxwellian distributions may be necessary for some or all of the present species. Typical Ar I-III spectral lines have been identified in the present work in various WEGA discharges. The main features of the relevant spectra will be shown and discussed during the Conference. They will also be compared to our theoretical spectra, in order to investigate the relative populations of each ionized species and judge about the form of Te in connection with departure from a unique Maxwellian distribution.

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P13

Atomic data for Ar ions

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Domain : Astrophysics

Transition probabilities (Aij) and electron impact excitation cross sections (se) of singly and higher ionized species of Ar have been evaluated, in order to extend our Collisional - Radiative (C-R) code to Argon plasmas with up to six times ionized species [1]. All argon spectra from Ar I through Ar VI are now included in calculations of Ar plasmas with all outer shell 3p6 electrons taken into account, depending on the electron temperature of interest. Comparison of atomic structure and radiative properties from the following codes have been made: (a) our CbA Coulomb Approximation code, based in the approximation introduced in [2], (b) the code contained within the SUPERSTRUCTURE package developed at University College [3] and (c) the Los Alamos National Laboratory (LANL) codes [4] available through the Internet [5].

Data obtained from other theoretical calculations or measured experimentally, including data from existing databases, whenever available, have also been taken into account. Existing data are known to be very scarce, while a large number of transitions must be taken into account in modelling the spectra from each multiplet. Such modeling requires ab initio calculations for transitions involving levels for which the corresponding energies have not been measured. The available evaluated energy levels (and transition probabilities, whenever they exist) from the NIST site [6], although of very good quality, are not sufficiently complete for our task; therefore, we have carried out calculations to supplement the database for the C-R model.

Together with the spontaneous emission, electron impact excitation and de-excitation processes are required for modelling the plasma spectra. As is the case for radiative processes, the available tabulated data are not sufficiently complete for carrying out the C-R model. Therefore, calculations of se have also been carried out for transitions between the same multiplets considered for structure and transition probabilities. Due to the increased importance of the electron impact excitation in cases in which the lower level of the transition is significantly populated, the ground and metastable levels values are always included in the calculations. Once the excitation cross section is evaluated, the inverse process, collisional de-excitation, can be easily evaluated through detailed balance. We have made extensive use of the LANL codes [7] to obtain a consistent set of excitation cross sections for use in the C-R model. Some of the results obtained will be presented and discussed during the Conference.

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P14

Detailed versus statistical approachs for spectral opacity calculations: study of LTE iron plasmas

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Domain : Astrophysics

The opacity code SCAALP [1,2] allows detailed and statistical treatments of bound bound transitions where the detailed line term accounting is performed in pure jj coupling. This code is used here to calculate iron opacities assuming local thermodynamic equilibrium. Detailed and statistical calculations are performed for densities between 10^{-5} and 10^{-3} g cm^{-3} and for temperatures between 20 and 100 eV. In this thermodynamic regime, the *Rosseland* mean opacity is always significantly smaller when detailed line accounting approach is used in place of the statistical one. *Rosseland* and *Planck* mean opacities are presented and compared to other opacity codes. Spectral opacities are also presented. The impact of precise atomic data and the limits of statistical treatment are discussed.

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P15

Breit-Pauli calculation of Mg V transitions among $2s^2 2p^4$, $2s2p^5$, $2p^6$ and $2s^2 2p^3 3\ell$ levels

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Domain : Astrophysics

A full Breit-Pauli calculation of oxygen-like magnesium fine-structure levels belonging to $2s^2 2p^4$, $2s2p^5$, $2p^6$ and $2s^2 2p^3(^4S, {}^2D, {}^2P)3\ell$ configurations will be presented. We have used the CIV3 program of Hibbert [1,2] in this work. Atomic orbitals up to $8d$ are chosen carefully to account for important correlation effects among various configurations. The $3s$, $3p$ and $3d$ orbitals are optimised on the energies of real states and remaining orbitals are chosen either as a correction type or as correlation type. At the LS stage we have thus used 380,559 configurations including up to three-electron promotions from the ground configuration. At the LSJ stage we retained 120,736 of them whose eigenvector strengths are ≥ 0.001 for the calculation of 86 fine-structure levels belonging to the above configurations. We then apply our fine-tuning procedure to bring the energies in line with the observed values wherever available: we adjust by a small amount the diagonal elements of the Hamiltonian matrix. Oscillator strengths, radiative rates and line strengths for all the E1 transitions among these 86 levels are then calculated.

Results are compared with a similar energy adjusted calculation of Fischer [3], the most recent calculation of Bhatia *et al* [4] and the recommended data of NIST [5]. It is found that present results show excellent agreement with the MCDF calculation of Fischer [3] for most of the transitions. The results of Bhatia *et al* [4] are consistantly higher by 20 to 50%.

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P16

From accurate atomic data to ellaborate stellar modelling.

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Domain : Atomic Physic - Astrophysics

The Atomic physics field has served astronomy for a long time and it has also been stimulated by it. Despite the maturity of the field, the new requirements for accuracy and completeness from astronomers demand more challenging calculations. Current problems require the relaxation of approximations and a detailed study of different effects like relativistic effects, radiation damping and target expansions.
We present the latest results on the electron impact excitation collision strengths of He-like ions including all levels up to the complex with $n = 4$, relativistic and radiation damping effects. These data are important in X-Ray spectroscopy. As a second set of results, we present our work related to opacities. The effect of the inner-shell transitions for opacities at high temperature - high density regimes and how the new opacities from The Opacity Project (OP) are crucial for stellar physics. Despite the overall good agreement with another source of data (OPAL,LLNL), the differences are noticeable. This new set of data is used to determine constraints on the solar composition and to shed some light on the 'Solar Convection Problem'. While the discrepancies between the two sources are minor for the Rosseland mean opacities, they affect more severely the radiative accelerations. The comparison between the accelerations computed with OPAL data and those obtained with OP data outlines how sensitive they are to details in monochromatic opacities. The consequences for stellar models are presented.

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P17

Recent progress in absorption oscillator strengths and predissociation rates for CO in the 925-1076 Å range

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Domain : Molecular Astrophysics

Accurate modelling of the abundance and excitation of CO in interstellar clouds, circumstellar matter and planetary atmospheres requires basic quantitative spectroscopic data, especially oscillator strengths and predissociation probabilities. It has been almost 20 years since the Meudon group started combining such high resolution and synchrotron radiation techniques below 1200 Å. More recently we published a coherent set of f-values of the A-X bands [1] and a line by line atlas of the singlet-triplet intersystem bands [2].

Here we report on the recent efforts of the Meudon and Toledo teams to measure a consistent set of f-values and predissociation rates for Rydberg bands in the 925-1076 Å range. Modern techniques have been used in order to improve our earlier results. High resolution spectra have been obtained at the SuperACO Synchrotron facility using the SU5 beam line. The absorption spectra were analyzed with simulation-fitting codes leaving the band oscillator strengths and predissociation line widths as free parameters. The necessary simulated spectra were calculated with models taking into account the interactions between the different Rydberg or valence states using the tabulated line positions and the results of classic deperturbation studies [3], [4]. Oscillator strengths have been obtained for the 9 strongest Rydberg bands for $^{12}C^{16}O$, $^{13}C^{16}O$, $^{13}C^{18}O$ as well as predissociation rates for lines whose widths were big enough to be treated as free parameters. Combining the band ocillator strengths and the calculated synthetic spectra provides line oscillator strengths which can be used to calculate spectra at any temperature of interest.

These earlier data have been compiled in the MOLAT data base. The more recent results will be added in the form of lists of line positions and intensities useful for the calculation of synthetic spectra.

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P18

An Atomic Database at Queen's University Belfast

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Domain : Storage, retrieval and manipulation of atomic data

We are developing an open-source, interactive atomic physics database system, called the Queen's University Interactive Database (QUID). Data covered by QUID will include energy levels, line wavelengths, radiative rates (and hence corresponding oscillator strengths and line strengths), excitation cross sections and excitation rates. Users will be able to search for data over a wide range of parameters, including element and ionisation stage, atomic configuration, energy range, wavelength range and isoelectronic sequence. Interpolation and extrapolation of data will also be available.

QUID has been designed to accept datasets from outside Queen's University via an online submission procedure. Additional features include a user forum in which members can discuss future developments, as well as the ability for users to leave comments and peer-review other users' work, thereby creating an 'eBay' style score for each submitted item. The software itself is to be made readily available, along with the development documentation, for all parties interested in deploying QUID at their institute.

P19

The MCHF/MCDHF Collection of transition data

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Domain : Astrophysics

The MCHF/MCDHF Collection (http://atoms.vuse.vanderbilt.edu) is an online database of energy levels, lifetimes, transition data, and some g_j factors. All results are derived from theory that includes relativistic effects. The types of transitions are E1, E2, M1, and occasionally higher multipoles. The labels for energy levels currently are designated only in LSJ coupling and are computer generated from the wave function composition. When conflicts arise, a detailed analysis is performed. Two views are supported in the database. In the first, results are presented in terms user selected tables, whereas in the second, the user may select energy levels and transitions between levels, according to nuclear charges along an isoelectronic sequence. In this view, energy levels are compared with tabulations found in ASD (http://physics.nist.gov/cgi-bin/AtData/main_asd) (Version 2) and the discrepancies between length and velocity forms of the transition probabilities are reported. This tool has been found to be extremely valuable for the over-all evaluation of theoretical data. Most results were computed with extensive correlation using Breit-Pauli theory that includes low-order relativistic effects. Calculations based on multiconfiguration Hartree Fock theory were for iso-electronic sequences with 3-18 electron and usually ten or more ions [1, 2]. For a few atoms non-orthogonal spline methods have been applied capable of determining many states of a Rydberg series [3]. For more highly ionized systems, some multiconfiguration Dirac-Hartree-Fock results have been performed. New results for the Al-like sequence will be described and data for Ar XII and Ar XIV will be evaluated.

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P20

Theory of Radiative-Stark Mixing at Ultra-Cold Energies*

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Domain : Low Temperature Laboratory Plasmas

Slow collisions of heavily charged ions with an excited atom at large impact parameters lead to ℓ-changing transitions within the degenerate states of a given energy shell n. An exact analytical (quantal and classical) treatment of this Stark mixing induced via the ion-dipole interaction in the slow collision between an ion and a hydrogenic target has already been provided [1,2]. Any excited atom is always coupled to zero-point fluctuations of the radiation field. Because the collisional timescales are comparable to time for radiative decay, it becomes important at ultralow energies to incorporate the radiative decay effect into the theory of Stark mixing. Collisional Stark mixing coupled with radiative decay, can be termed *Radiative-Stark mixing*. In this paper, we shall present the theory of Radiative-Stark mixing and shall illustrate the effects of the coupling.

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P21

Nuclear fusion rate for an ordinary $dd\mu$ ion

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Domain : other

A consistent theoretical approach, based on a new wave function to $dd\mu$ molecular ion is developed. The present method provides a calculation of nuclear fusion rate for $(J,v)=(1,1)$ level, a resonance state. The behavior of the wave function is important for the calculation of the element matrixes related to nuclear and photon fields [1,2,3]. In this work, we introduce the below wave function for the $dd\mu_{1,1}$ ordinary ion:

$$\psi(\vec{r},\vec{R}) = \zeta Lf(R)\chi^{1,1}(R) \sum_{m=1,0,-1} \sum_{i=1,2} Y_{1,m} c_i(\beta_i,\beta_i^{'}) \exp(-|\beta_i^{'}\vec{r}+\beta_i\vec{R}|).$$

Where $\vec{r}$ and $\vec{R}$ are the notations for the displaying of Jacobin coordinates of the muon and the nuclei. The radial wave function $\chi^{1,1}(R)$ is related to the moving of the nuclei in the effective potential. For the mentioned muonic ion, the constant parameters are variationaly optimized and then, used for the fusion rate of $(1,1)$ level. The calculated rate is in the orders of 10^9 s^{-1}, and close to precise data. As the limited function $Lf(R)$ is linear from $R=0$ to $2.2\times10^{-10}cm$ and then being constant(=0.7071), the numerical calculations are done with a short computation time.

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P22

Ion Chemistry Model for Methane Combustion

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Domain : Combustion

Ion chemistry models for combustion of hydrocarbon fuels are required in order to simulate the interaction of electric fields with flames e.g. in electric field combustion control and flame sensing by means of ionization probes. Therefore we compiled a reaction kinetic model describing chemo-ionization in methane combustion, charge transfer, and recombination. Starting point was the reaction mechanism of methane combustion of the Gas Research Institute GRImech 3.0 to be used in the Chemkin software package. This model was complemented by reactions describing the formation of HCO^+, H_3O^+, CH_3^+, $C_3H_3^+$, and electrons by chemo-ionization and charge transfer and the formation of O^- and O_2^- negative ions by electron attachment to O_2-molecules [1-2]. Implementation of this reaction mechanism into the PREMIX module of Chemkin 3.7 resulted in ionization degrees for premixed methane-air flames at atmospheric pressure having the correct order of magnitude. The concentration profiles of electrons and ions, however, were not realistic because Chemkin 3.7 did not take into account space charge induced electric field formation impeding diffusion induced charge separation on length scales exceeding the Debey length in the flame plasma [3]. Further we found that the chemistry solver has not the accuracy which would be required in order to simulate space charge densities correctly.

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P23

Imaging system by Microwave for Materials defects Characterisation

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Domain : Other

The simplicity of the technique and the non contact nature make this approach method very beneficial and interesting. The paper presents results of investigation of Near-filed microwave imaging system in detecting subsurface defects in composite materials. The quality of the experimental image captured with this system has demonstrated the potential of the technique for material characterisation. To this end, a micro-metrique system of displacement is used to displace a probe witch scans over different regions. Then proprieties of the reflected wave give the needed information about the specimen under test investigation.

P24

The importance of both electron correlations and relativistic effects for intermediate-Z elements

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Domain : Astrophysics

Using a modified R-matrix code, the fine-structure-resolved partial photoionization cross sections of ground and excited Na (Z=11) are calculated within the Breit-Pauli approximation, which involve bound and continuum state wavefunctions. Our calculated energy levels of Na^+ and Na agree well with the experimental values within 1%. The calculated branching ratios of the J-resolved partial cross sections of excited Na are in excellent agreement with the recent measurements[1]. Our calculated cross sections and minimum position of ground Na in the low photoelectron energy range (<9 eV) are in excellent agreement with the experimental results[2]. In the high energy range (>9 eV), there is an abnormal bump in the experimental measurements, which is a long-standing experimental puzzle[2]. It is interesting to note that there is also an absorption window in the photoabsorption (i.e. photodissociation) cross sections of Na_2^+. Such absorption window provides an answer to the puzzle. Excellent agreement between our theoretical results of Na (with Z=11) and the experimental results demonstrates that the electron correlations and the relativistic effects are treated adequately on equal footing in our calculations. Using the the bound and continuum state wavefunctions with sufficient accuracy, the relative bound-bound radiative transition rates, bound-free photoionization cross sections and electron impact cross sections, which are vitally important in relative fields, can be calculated with adequate precision. The stringently tested Breit-Pauli R-matrix code should be useful to provide the indispensable fine-structure-resolved atomic physical data of intermediate-Z elements such as C, N, O, Ne, Na, Si, S, etc., which play important roles in astrophysics.

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P25

Laser Induced Fluorescence Spectroscopy of Excited Neon Atoms in a Liquid-nitrogen-temperature Glow Discharge Plasma under a Strong Magnetic Field

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Domain : Low Temperature Laboratory Plasmas

The analysis of inter- and intra-multiplet transitions induced in atom-atom collisions within the framework of a molecular theory was discussed in many papers (e.g. [1]) and textbooks (e.g. [2]). In particular, angular momentum relaxations of polarized atoms due to atom-atom collisions, give a good indication about the accuracy of anisotropic molecular potentials.

We measured the decay rate of axially polarized neon atoms (alignment) in the $2p_2$ (in Paschen notations) state due to helium atom collisions in a temperature controlled glow discharge cell with laser induced fluorescence spectroscopy (LIFS). The experimental results were compared with those from the full quantum calculations of the alignment relaxation cross sections [3] based on the model potential of Hennecart and Masnou-Seeuws [4]. Above 77 K the theory and experiment were found to be in excellent agreement while the experimental values showed a more rapid decrease with the decrease in temperature from 40 to 15 K than the theoretical results. This finding suggests that the cross section rapidly decreases as decrease in the collision energy below a few meV.

Effects of a magnetic field on alignment relaxation collisions may be of interest because the Zeeman splitting make the collision inelastic. Recent development of cryogen free superconductive magnet systems has made us possible to perform optical measurements in a strong magnetic field with high flexibility. With such a magnet system, we may examine the magnetic-field dependence of the alignment relaxation at a cryogenic temperature. In this paper, we report the LIFS measurement of alignment relaxation of the $2p_2$ neon atoms at the liquid nitrogen temperature under a strong magnetic field.

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P26

Cross Sections and Rate Constants of Resonant Electron Collisions with Molecular Hydrogen and Hydrogen Halides

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Domain : Low Energy Electron Molecule Interactions

A collection of cross sections and rate constants of resonant collisions of electrons with some diatomic molecules calculated using the most recent nonlocal resonance models [1–5] is now available via anonymous FTP [6] and a new web interface is currently under the construction.

Processes of associative electron detachment, dissociative electron attachment and vibrational excitation of hydrogen halides (HF, DF, HCl, DCl, HBr, DBr, HI and DI) and molecular hydrogen (H_2 and D_2) are included. Data are calculated for many initial rovibrational molecular states at collision energies 0 eV – 4 eV for hydrogen halides and 0 eV – 5 eV for molecular hydrogen.

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[6] ftp://utf.mff.cuni.cz/QMGroup/CS_DBASE/

P27

Fine Structure Effective Collision Strengths for the Electron Impact Excitation of Ca VI

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Domain : Astrophysics

Ca VI emission lines arising from transitions among the $3s^2 3p^3$ levels of lowly ionized ions of the phosphorus isoelectronic sequence have been widely detected in the optical and near-infrared spectra of planetary nebulae (see, for example, Hyung & Aller [1-4]. In principle, these transitions provide excellent density and/or temperature diagnostics for the emitting plasma (Czyzak, Keyes & Aller [5]; Stranghellini & Kaler [6]). These observational data require accurate atomic data in the form of electron impact excitation rates (effective collision strengths) for analysis and interpretation. However, for this ion there are currently no such data available in the literature. To address this gap in the literature, we have therefore carried out a sophisticated *R*-matrix calculation.

An 18-state calculation has been performed. The target states are represented by configuration interaction wavefunctions and consist of the 18 lowest *LS* states, having configurations $3s^2 3p^3$, $3s3p^4$ and $3s^2 3p^2 3d$. These target states give rise to 39 fine structure levels and 741 possible transitions. The fine structure collision strengths were obtained by transforming to a jj-coupling scheme using the JAJOM program of Saraph and have been determined at a sufficiently fine energy mesh to delineate properly the resonance structure. The effective collision strengths are calculated by averaging the electron collision strengths over a Maxwellian distribution of velocities. The non-zero effective collision strengths for transitions between the fine structure levels are given for electron temperatures (T_e) in the range $\log_{10} T_e(\mathrm{K}) = 4.5 - 6.5$. Data for transitions among the 5 fine structure levels arising from the $3s^2 3p^3$ ground state configurations will be presented. These calculations are the first evaluations of collision strengths and effective collision strengths for this ion.

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P28

Evaluation of Xe Ions Transition Probabilities

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Domain : Astrophysics

Spontaneous emission is often the basis for optical emission diagnostics. Whenever a plasma is far from coronal equilibrium spontaneous emission is an important decay process, leading to significant plasma cooling as well as an optical diagnostic. Xe plasmas are becoming more common in the laboratory and in industry applications (plasma thrusters, plasma reactors, lightning) because of the low ionization energy of the Xe atom and of its ions. At the same time the high atomic number (Z=54) produces very rich spectra of plasmas containing Xe I to VI species with excitation of the outmost six noble gas 5p electrons possible.

Unlike the more common cases of He or Ar plasmas, which have been extensively studied some time ago, the Xe spectra, even for the neutral atom, are poorly known. The existing compilations of the corresponding transition probabilities and collision cross sections have many gaps. Relativistic effects are important for Xe, complicating the development of satisfactory Collisional Radiative (C-R) type models for low temperature plasmas. Because of the importance of Xe plasmas for contemporary industrial applications, especially for electric propulsion and in the divertor region of Tokamak plasmas, we are systematically addressing the C-R modeling [1], seeking the most extensive comparison of our theoretical results with values measured in various experimental devices in our l aboratory and/or observations available in the literature.

We have applied the same theoretical methods applied to the Ar case [2] to build the atomic database needed for our C-R model for Xe. A compilation of energy levels for the Coulomb approximation has been recently made available [3]. In the present work we restrict ourselves to the case where the local electron temperature (Te) of the plasma is sufficiently low for the Xeq+ ions with q¿4 to have a negligible effect on the line intensities calculated by the C-R model for the Xe I and Xe II spectra. Note that the appearance of the four times ionized species for Xe occurs at lower temperatures than for Ar due to the lower ionization limits of the Xe ions and the increased importance of the inner shells. A simple coronal model [4] calculation shows that including the ion stages Xe I to IV in the C-R model is expected to be sufficient for the study of the plasma properties up to about 10 eV.

For our theoretical Xe I to IV spectra, comparisons with experimental spectra mainly for the 6s 6p, 7p and 6p 5d, 6d multiplets show satisfactory agreement. In building the atomic database for our C-R model care was taken to include a complete set of data for all transitions between multiplets. Special care was devoted to transition probabilities belonging to the experimentally observed leading transitions. Samples of the data compilation will be shown in the Conference.

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P29

Establishment of new database engine for experimental-charge-exchange-collision cross-sections

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Domain : Fusion

A new database engine, which provides experimental-charge-exchange-collision cross-sections through SQL queries free of charge, has been established. It provides an electric version of cross-section data compilation for ion-atom and ion-molecule collisions, done under the collaboration of the Japan Atomic Energy Agency (JAEA) and our laboratory since 1983. [1,2]

Data stored in the database are total electron capture and loss cross-sections published since 1983 and partial cross-sections since 1992, compiled from journals of our selection. Experimental cross-sections for some related interactions since 1995, like inner-shell ionization of target, ion-ion collisions, cluster collisions and so on, are also compiled and stored. These compilations have been done without limiting the projectile ion or target species of the collision system, aiming at larger area of applications as well as fusion research.

The database is consisted of 8 tables, COL, DATA, DOC, REF, AUTH, AFF, MAT and PROC. The collected papers are indexed by document number key "docno" and the data are indexed by a combination of document and collision system number keys "docno, sysno", for cases that single paper includes multiple collision systems. The most important 3 tables COL, DATA and DOC store collision system information, numeric data and bibliographic indexes, respectively. In case that cross-section data for some collision system are required, "docno, sysno" keys for the desired system should be looked up in the table COL, and the numeric data are derived from the table DATA using those "docno, sysno" keys. If the bibliographic information is additionally required, it can be looked up in the DOC table with the "docno" key. Reference with specifying the known paper's information is also possible by looking the "docno" key up in the table DOC and look into COL and DATA tables.

In the present, the database query is available only through SQL queries and user-friendly interface is not provided, but we continue establishing http-based user-interfaces.

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P30

Effect of directional energetic electrons on the density diagnostic of hot plasmas

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Domain : Astrophysics, Fusion

The intensity ratio $R=z/(x+y)$ of the He-like forbidden line z ($1s2s\,^3S_1 \rightarrow 1s^2\,^1S_0$) and intercombination lines x and y ($1s2p\,^3P_{2,1} \rightarrow 1s^2\,^1S_0$) is often used as a diagnostic of the electron density in a variety of astrophysical and laboratory plasmas. Most of the reported studies on this diagnostic tool have dealt with an isotropic Maxwellian distribution for the plasma electrons. In this work, we investigate how the presence of a small proportion of directional energetic electrons in hot plasmas affects the R ratio and so can modify the density diagnostic as compared to a pure Maxwellian plasma.

We have calculated the R ratio of Ne^{8+} as a function of the total electron density in the 10^9-10^{13} cm^{-3} range, taking into account the polarization and anisotropy of the line emission. The calculations have been carried out considering various values of the temperature T_e ($2-5\times10^6$ K) of the Maxwellian component as well as the energy E ($1-5$ keV) and fraction f ($1-5\%$) of the directional electron component. The rate coefficients for excitation from the $1s^2\,^1S_0\,M_J=0$ ground and $1s2s\,^3S_1\,M_J=0,\pm1$ metastable magnetic sublevels, due to both thermal and beam electrons, were obtained from data reported in [1] and [2], respectively. We find that the electron density deduced from the R ratio under the assumption of a pure Maxwellian distribution can be very significantly overestimated or underestimated depending on the angle observation with respect to the direction of the electron beam present in the emitting plasma.

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P31

Anisotropic proton velocity distribution function in plasmas by means of polarization measurement on magnetic dipole transitions

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Domain : Fusion

Polarization of emission lines from atoms or ions in plasma contains information of anisotropy of the electron velocity distribution function [1]. The intensity and the longitudinal alignment of helium emission lines have been used to estimate the anisotropic electron velocity distribution function in a plasma heated by an electron cyclotron resonance microwave[2]. In the magnetic confined plasma various heating mechanism may produce the anisotropy on electron and proton velocity distribution function. Proton impact excitation contributes the upper level population production of the magnetic dipole transitions in ground state configuration. Visible spectral emission lines from magnetic dipole transitions in highly charged argons are observed from plasmas heated by neutral beam injections (160 keV) in the Large Helical Device. The orthogonal linearly polarized components of the emission lines are separated and the line profiles are recorded. The observed polarization degree of the transitions is analyzed with population-alignment collisional-radiative model. The alignment production cross section by the proton impact excitation is scaled with that of the electron impact excitation calculated by means of flexible atomic code[3].

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P32

Cross Sections for Collisions of Charged Particles with n-Butane

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Domain : Combustion

Hydrocarbon plasmas are found in ignition, combustion and industrial reactors, as well as in interstellar medium and planetary atmospheres. The modeling of these plasmas requires a basic data set on the collision processes of charged particles as well as neutral particles. Recently we have measured absolute cross sections of electron impact ionization of n-butane in an energy range of 10 to 200 eV. The energy dependencies of the total and partial cross sections will be presented for the dissociative ionization channels forming thirteen ions including the parent ion and major fragment ions of $C_2H_{3-5}^+$, $C_3H_{3,5-7}^+$ and $C_4H_9^+$. The cross sections for the collisions of selected fragment ions with their parent gas molecule also have been measured. The ion-molecule reactions studied proceed mainly via a H^- transfer mechanism. Based on the observation of the H^- transfer reactions and the calculated heats of reactions using the thermochemical data available in the literature, the structures of two of the major fragment ions from the electron impact ionization of n-butane, $C_3H_3^+$ and $C_3H_6^+$, are expected to be cyclic forms.

P33

NIFS databases for atomic and molecular collisions and plasma-wall interaction

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Domain : Fusion, Low Temperature Laboratory Plasmas, Plasma Processing

NIFS databases include cross sections and rate coefficients for electron and heavy particle collisions with atoms and molecules and sputtering yields and reflection coefficients of solids. The data can be retrieved via web browsers (database server: *https://dbshino.nifs.ac.jp*). Graphic output and bibliographic information about data sources are also available. The database server machine and system has been renewed in 2005 to meet increasing data needs and access to the database. Access is free for academic research purposes, once registered [1].

A working group of atomic and molecular physicists is organized under the auspices of NIFS to coordinate data research and compilation. Molecular data are required for fusion, process, atmosphere and radiotherapy. Since 2001, molecular databases (AMOL: electron collision and CMOL: heavy particle collision) have been developed. Cross section data for electron and ion collisions with the molecules of hydrogen, hydrogen isotopes, nitrogen, oxygen, hydrocarbons, water and carbon oxide were updated by the working group [2].

[1] A part of the database for electron-impact ionization and excitation of atoms (AMDIS-EXC/ION) is available without registration in a data retrieval system of IAEA, GENIE (*http://www-amdis.iaea.org/GENIE/*).

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The GAPHYOR Data Center

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Domain : Astrophysics

The GAPHYOR (GAz-PHYsique-ORsay) Data Center, located in Orsay at the Laboratoire de Physique des Gaz et des Plasmas (Laboratory of Physics of Gases and Plasmas, LPGP), was established by Prof. Delcroix in 1976. Its main activity was to develop and maintain an atomic and molecular data base of interest to physico-chemical research and applications (http://gaphyor.lpgp.u-psud.fr). This wide scope includes information on the properties of atoms, molecules, gases and plasmas and on their reactions. The data are indexed in consultation with a body of experts. Five separate sections compose this database, each addressing a distinct field of interest, namely properties of isolated atoms and molecules; collisions with photons; collisions with electrons; collisions and reactions between atoms and molecules; macroscopic properties of gases including plasma-surface interactions. The data base includes bibliographic entries citing journals, reports, books and proceedings of conferences covering the fields of atomic and molecular physics, of plasma physics and of chemical physics. Advanced query languages with on-line help are available for searching the five sections of the data base in English or French. In addition, the DANSE (Data Around the Net Search Engine [1]) code for on-line bibliographic searches, available through the International Atomic Energy Agency (IAEA) can be used to query the GAPHYOR data base on-line.

In addition to data base development, the GAPHYOR Data Center has the following activities:

- Implementation and management of a complementary numerical data base containing data of interest to selected applications, including thermonuclear fusion, plasma reactors, electric propulsion and optical diagnostics.
- Calculation, measurement and evaluation of atomic and molecular data, mainly for rare gases.
- Diagnostics and modeling of rare gases plasmas, supported by the code CLOEO (Calculation of high resolution Light Optical Emission at Orsay [2]) calculating the atomic level population in rare gas plasmas by Coronal and Collisional-Radiative models.

The latest data evaluations, on which we will report at the Meeting, in support of optical emission spectroscopy diagnostics. Towards this aim we are evaluating the following two data sets:

a) Transition probabilities Aij of rare gases atoms and ions, based on the Coulomb approximation in jK and LS coupling [3], in collaboration with the LUTH Laboratoire de Meudon, Observatory of Paris, where the SUPERSTRUCTURE code [4] is used giving Aij in intermediate coupling IC; The IAEA and the Los Alamos National Laboratory (LANL) also jointly calculating ab initio the structure and Aij of atoms and ions using the CATS [5] code,.

b) Electron collision ionization and excitation cross sections of lowly ionized Ar and Xe species. For evaluating these data we are using a calculational package of few body CTMC type codes [6] and the ACE [7] code of

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P35

Absorption spectra of gaseous indium monohalides: experiments and simulations

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Domain : Lamps and Lasers

We measured highly resolved absorption spectra of gaseous InCl, InBr and InI molecules in the wavelength region of the A $^3\Pi_0^+$ - X $^1\Sigma_0^+$ and B $^3\Pi_1$ - X $^1\Sigma_0^+$ band systems. The derived absorption cross-sections were analysed theoretically with the help of spectral simulation models at different levels of sophistication. As results we obtain radially dependent electronic transition moments D(R) for the A-X and B-X band systems of these three indium monohalides. The corresponding radiative lifetimes of the A and B states are in the range of 2 to 10 microseconds.

P36

Stark lineshape calculations with different atomic physics data

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Domain : Laboratory data needs and applications

One of the widely used techniques for diagnosing a gas or a plasma is that consisting on the comparison of experimental spectra of emitted lines with calculated line profiles. The accuracy of the results which can be obtained with this method depends not only on the used line shape model but also on the quality of both the measurements and the atomic data. For plasma conditions where Stark broadening is the dominant broadening mechanism, the lineshape code PPP [1,2] developed in our laboratory has proven to give excellent results especially for plasmas of moderate coupling. We propose in this paper to examine how line profiles calculated with the same code PPP are affected by the choice of atomic physics data and how this can affect the deduced plasma parameters. This will be illustrated through profiles of the He I 1s2p ^{3}P-1snd ^{3}D lines (n$\geq$8) [3] calculated with PPP using different atomic physics data (especially the reduced matrix elements of the dipolar transitions). In particular we use singly excited helium data obtained with a hydrogenic approximation and data of Theodosiou [4].

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P37

NIST's Bibliographic Databases on Atomic Spectra

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Domain : Other

In June 2006, the Atomic Spectroscopy Data Center of the National Institute of Standards and Technology (NIST) released three new Bibliographic Databases containing references to papers with data on atomic properties needed for controlled fusion research, modeling and diagnostics of astrophysical and terrestrial plasmas, and fundamental properties of electronic spectra of atoms and atomic ions.

The NIST Atomic Energy Levels and Spectra Bibliographic Database [1] is the first online version of the NIST bibliographic resources on atomic energy levels and spectra, earlier published on paper as NIST Special Publication 363, last published in 1985. This database includes references to articles on energy levels, transition wavelengths, ionization potentials, isotopic shifts, hyperfine structure, quantum field effects, and Zeeman and Stark splittings in atoms and atomic ions. The main emphasis is given to experimental papers. It also includes papers containing high-precision theoretical calculations of these atomic properties. The database is fairly complete for the period 1967 through 1994. The work is currently in progress to include papers for the period 1994 through 2006. Total number of references is more than 8400.

The NIST Atomic Transition Probability Database, version 8.1 [2], is an update of the previously published version 7.0 of this database published in October 2003. The database is now fairly complete for the period 1964 through 2005. About 500 new references have been added compared to the previous version, bringing the total number of stored references to more than 7000.

The NIST Spectral Line Broadening Bibliographic Database, version 2.0 [3], is a major upgrade of the previous online version 1.0. The total number of references is more than 3550, while version 1.0 contained only 800 references. The database is fairly complete for the period 1978 through 2005.

All three databases are now maintained in a unified database management system based on a MySQL server. This system allows us to quickly update the contents of the databases. Any new reference added to the database becomes available to the public on the next day. A robust Data Entry module makes it easy to enter the data and classify the papers by relevant categories. This work is supported in part by the National Aeronautics and Space Administration and by the Office of Fusion Energy Sciences of the U. S. Department of Energy.

[1] http://physics.nist.gov/Elevbib
[2] http://physics.nist.gov/Fvalbib
[3] http://physics.nist.gov/Linebrbib

P38

Reflection and chemical sputtering spectra at fusion edge plasma facing carbon

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Domain : Fusion

We study interactions of deuterium atoms and vibrationally excited deuterium molecules with deuterated amorphous and crystalline graphite surfaces at a range of low impact energies (5-30 eV/D). Molecular dynamics simulations of this complex system yields reflection spectra of D and D_2, chemically sputtered hydrocarbon and D_2 yields, as well as their energy and angular spectra [1]. Particular attention is paid to preparation of surfaces (by particle irradiation), to internal (rovibrational) state of impinging particles and to the choice of hydrocarbon potentials (REBO [2] and AIREBO [3]). Our data are in good agreement with available experimental results [4,5].

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P39

Benchmark measurements of differential cross-sections for electron-impact excitation using a time-of-flight approach

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Domain : Low Energy Electron Molecule Interactions

The threshold region continues to be an interesting target for investigations of low-energy electron scattering from atoms and molecules. However this energy region, which is also important in many technological applications of electron collisions, proves to be very challenging both to theory and experiment. Measurements of the angular-differential cross section are often performed in crossed-beam spectrometers using an electrostatic analyzer and optics, whose electron transmission efficiency must be known at all scattered energies. While it can be reliably established at high scattered energies, near a threshold the kinetic energies for the elastic and inelastic channels can differ by more than one order of magnitude. This makes determination of the transmission function difficult at best, and is the dominant source of experimental error in this energy range. We have therefore developed a crossed-beam time-of-flight spectrometer, which by the complete absence of electrostatic optics for the scattered electrons has an almost uniform electron transmission, regardless of energy. Contrary to other TOF spectrometers [1,2], we use a pulsed electron gun which can access scattering angles of $47-129^{\circ}$ and which incorporates a monochromator, thereby improving energy resolution from 500 meV to $120-150$ meV.

Using this spectrometer we have performed a benchmark measurement of the differential cross-sections for electron impact excitation of helium atoms at incident energies of 20.30, 22.05 and 23.48 eV, and have compared the results with a convergent close-coupling calculation [3], as well as with an R-matrix [4] and a B-Spline R-matrix [5] calculation. In general we have found good agreement between the theories themselves, as well as between experiment and theory. However, remaining differences indicate that the treatment of the ionization continuum, as well as the quality of the multiconfiguration expansions used to describe the target states are of most importance for the reproduction of the measured cross-sections. Currently, additional near-threshold measurements are being carried out on the vibronic excitation of nitrogen molecules, and for electronic excitation of argon atoms.

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P40

Data base for dissociative recombination processes

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Domain : Low Energy Electron-Atom Interactions

There has been a lack of a data base for dissociative recombination of molecular ions with electrons. Very recently a review of the topic was published in Physics Reports [1]. This review also contains tables with data from experiments. We have used these tables as starting point for a web based data base [2]. In case of discrepancy between the data base and the tables in ref. 1, we have given the data from the orginal journal article.

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[2] http://www.mol.physto.se/DRdatabase/

P41

Spectral measurements in the experiments with additional plasma heating on the tokamak FT-2

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Domain : Fusion

The effective Lower Hybrid Heating (LHH) with L-H transition and experiment concerned with the Fast Plasma Current Ramp Up (CRU) has been studied on the FT-2 tokamak [1,2]. Unique diagnostic equipment allows us to obtain the required detailed information of plasma parameters on the FT-2 tokamak [2].

Spectral measurements in the visible region spectra are made by two monochromators providing observation of fast transport changes at the periphery of the plasma core during additional heating in hydrogen plasma. One of these monochromators with high spectral and temporal resolution ($\sim 0.5\,ms$) has been used for measurements of an ion temperature and poloidal rotation of plasma by registration of Doppler broadening and the Doppler shift of the impurity spectral line emission. Such spectroscopic measurements are realized shot by shot using a series of typical discharges of the tokamak. Monitoring of the line-chord-integrated intensity during such spectral measurements is provided by the second monochromator.

The observed intensity ratio of hydrogen emission lines H_α and H_β was used for the determination of the ratio of molecular-to-atomic hydrogen densities in region of the plasma periphery. Changes of this ratio is analyzed for Lower Hybrid Heating and L-H transition, when recycling of the working gas fast decreases. Such measurements of profiles of the hydrogen line emission during one short are provided by applying a television video camera (VC) as a radiation detector. Registration of the monochromator outward slit image with the VC has been carried out with $2.5\,ms$ time intervals.

The role of impurity in the plasma energy balance is analyzed by taking into account Z_{eff} profile evolution. These data are obtained from bremsstrahlung continuum measurements of plasma emission in infrared spectrum band. The details of Z_{eff} measurements are presented. Further ASTRA code modeling using experimental Z_{eff} profile evolution provides more correct analysis of the plasma core transport changes.

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P42

Importance of atomic and molecular data in strong field laser matter interaction

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Domain : Other

The past decade has shown an enormous progress in ultrafast laser technology. Extremely short pulses down to 0.2×10^{-15}s have become reality[1]. These pulses are now applied to unveil innermolecular electronic motion. Sub-femtosecond time resolved studies of inner-atomic transients have become reality. The extension of such technologies towards more complex systems like small to medium sized molecules, clusters and solid surfaces is presently pushed forward within our institute. On the very basis of this fascinating application of attosecond technology stands the recollision of the laser field liberated electron with its parent ion. Prediction and interpretation of experimental results is therefore strongly dependent on the availability of electron-ion collision data and xuv photoionization cross sections. As a feedback into the community we can presumably extract time dependent differential cross sections from such rescattering processes. We have suggested that we will be able to steer angle, timing and energy of the recollision processes with high precision[2]. Such measurements become possible when cold target ion recoil coincidence spectroscopy (COLTRIMS) can be successfully combined with strong laser field ionization based on sub-5 fs carrier-envelope phase stabilized laser fields.

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P43

The role of chemi-ionization in fluorescent lamp discharge

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Domain : Low Temperature Laboratory Plasmas

Chemi-ionization processes resulting from the interaction of two excited Hg atoms have been widely used in numerical models of fluorescent lamp discharges. In particular, the Penning process Hg(6p $^3P_2$) + Hg(6p $^3P_2$) $\rightarrow$ Hg^+ + Hg(6p $^1S_0$) has been invoked as an important contribution to ionization and to the maintenance electric filed. There is no experimental measurement of the cross section for this process and experiments to measure cross sections of other chemi-ionization rections have been shown to be unreliable [1]. Numerical calculations of cross sections for these processes [2] indicate that they are much smaller than those previously assumed. We present a series of computations showing the influence of the calculated cross sections on the ionization balance over a range of discharge parameters. For discharge parameters appropriate to fluorescent lamps under standard operating conditions, it is necessary to invoke alternative ionization mechanisms, such as ladder like ionization via higher Rhydberg states, in order to reproduce the experimental results.

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P44

Systematic measurements in closed electron shell interaction particles

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Domain : Other

The absolute value of differential and integral cross section for charge exchange, ionization and stripping (electron loss) processes in collisions of single charge alkali metal ions with rare gas atoms and some atmospheric molecules (N_2, H_2) are measured. Despite the many studies devoted to this systems carried out by a variety of methods, the data available on the absolute cross section of mentioned above processes are contradictory and in some cases unreliable. In the present work a precise measurements are performed by improved transverse electric field and collision spectroscopy methods. Experimental techniques and measurement procedures have been discussed in details in our recent papers $[1-2]$. The energy range of these measurements is $0.7-10keV$ and angular range of the differential cross section measurements is $0-30^0$. The data obtained in this study have been used to elucidate possible mechanism of the corresponding processes. Where possible a comparison is made to the result of available theory. From these differential cross sections the threshold character for the most realizing inelastic processes are revealed. The contributions of partial inelastic channels to the total cross sections of ionization are clarified.

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[2] M.Gochitashvili, R.Lomsadze et al, Proceedengs of I.Javakhishvili Tbilisi State University, Physics 39, (2004) 162.

P45

Calculation of Collision Cross Sections with CTMC Codes

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Domain : Astrophysics

The Classical Trajectory Monte Carlo (CTMC) method has been used successfully in cross section calculations in various cases of collisions involving electrons, atoms, ions and molecules [1]. Besides being designed to calculate these cross sections, the CTMC method is of interest in the study of chaotic systems [2]. The various versions of the application codes differ mainly in the number of bodies taken into account (currently three-, four- and five-body problems), the potential allowed for the bodies (of which the Coulomb potential is the most evident choice) and the treatment of the distribution function(s), initially a purely micro-canonical one.
We report here recent work calculations of CTMC collision cross sections of interest to thermonuclear fusion. One aspect of the work involves ion ion collision cross sections at energies from approximately one keV/u up to several MeV/u. Collisions of metallic and of Ne ions with hydrogen atoms were previously studied using this CTMC code [3]. This work is now extended to the study of collisions of rare gas species in various ionization stages. Parametric potentials [4] are used throughout for the collision centers.
Another class of CTMC calculations in progress involves somewhat lower energy collisions of neutral sodium atoms constituting a neutral beam, colliding with low Z atoms and ions. As was the case with previous calculations involving He atoms [5], use of Coulomb potentials is expected to be sufficient in this case.
The CTMC method has the advantage of allowing the calculation of ionization and charge transfer cross sections simultaneously. The problem of excitation evaluation is more complicated, due to the large number of possible exit channels. However, the method has been used in cases where only a small number of excitation channels are important [6].
Calculated results for these two cases will be presented and discussed during the Conference.

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[6] K. Katsonis, T. Minea, A. Siskos, K. Dimitriou *Evaluation of Atomic and Molecular Data for C-R Modeling Applications*, in ESCAMPIG 16 and ICRP 5 Joint Conference, N. Sadeghi et H. Sugai Edts., Grenoble, July 14 18 (2002), p. II-37.

P46

Observation and interpretation of $4f^{12}$-$4f^{11}5d$ transitions in the Tm^{3+} free ion spectrum

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Domain : Low Temperature Laboratory Plasmas

The present work is the first interpretation of triply ionised thulium spectrum. About 300 lines have been identified as transitions from 95 levels of $4f^{11}5d$ to 10 levels of the $4f^{12}$ ground configuration in the free ion Tm^{3+}. The spectrum of thulium has been recorded in the 800-1800Åwavelength region on the 10.7 m VUV normal incidence spectrograph at the Paris-Meudon Observatory. This instrument is equipped with a 3600 lines/mm holographic grating and provides a unique plate factor of 0.25Å/mm in the first order. The ionised thulium spectrum in emission was obtained using a vacuum sliding spark source with an anode of pure thulium. To vary the discharge conditions, a self-inductance coil was placed in series with the spark source. For each wavelength region, three exposures were recorded with three values of the inductance $(63\mu F, 38\mu F, 11\mu F)$. The wavelengths calibration used known wavelengths of impurities present in spark, namely C, O, Si, Al. The estimated error of 0.003Åon the wavelengths of unperturbed lines was later confirmed by the wavenumber consistency of the classified TmIV array $4f^{12}$-$4f^{11}5d$.

The analysis was guided by predicted energy level values and transitions probabilities calculated by means of the methods and codes by Cowan [1]. Fitted parameters are consistent with those of neighbouring spectra.

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P47

OPserver: opacities and radiative accelerations on demand

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Domain : Astrophysics

We report on current developments carried out within the Opacity Project (OP) to upgrade atomic database services to comply with e-infrastructure requirements. We give a detailed description of an interactive, online server for astrophysical opacities, referred to as `OPserver`, to be used in sophisticated stellar modelling where Rosseland mean opacities and radiative accelerations are computed at every depth point. This is crucial, for instance, in chemically peculiar stars and in the exploitation of the new asteroseismological data.
`OPserver`, downloadable with the new OPCD_3.0 [1] release from the Centre de Données Astronomiques de Strasbourg, France, computes mean opacities and radiative data for arbitrary chemical mixtures from the OP monochromatic opacities. It is essentially a client–server network restructuring and optimization of the suite of codes included in the earlier OPCD_2.0 release [1, 2]. The server can be installed locally or, alternatively, accessed remotely from the Ohio Supercomputer Center, Columbus, Ohio, USA. The client is an interactive web page [3] or a subroutine library that can be linked to the user code. The suitability of this scheme in grid computing environments is emphasized, and its extension to other atomic database services for astrophysical purposes is discussed.

[1] `http://vizier.u-strasbg.fr/topbase`
[2] Seaton M. J., 2005, MNRAS, 362, L1
[3] `http://www.osc.edu/hpc/opacities/`

P48

Fine-structure resolved photoionization of metastable Be-like ions C III, N IV, and O V

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Domain : Atomic Data for Astrophysics

Be-like ions offer a number of scientifically interesting aspects. With the two loosely bound electrons in the L-shell and two tightly bound K-shell electrons, they are almost perfect objects for investigating two-electron effects. The metastable ^{3}P states can be easily populated and provide access to well isolated excited states which are known to be of high importance in the modeling of finite density plasmas. The present work aims at experimental distinction between the fine-structure levels of the ^{3}P term. High-resolution photoionization experiments were carried out with beams of C^{2+}, N^{3+}, and O^{4+} containing roughly equal amounts of ground-state and metastable ions. The energy scales of the experiments are calibrated with uncertainties of 1 to 10 meV depending on photon energy. By employing energy resolutions of the order of 20000, cross section features characteristic for individual states $^3P_0$, $^3P_1$, $^3P_2$ and, of course, the $^1S_0$ ground state are observed.

P49

Breit-Pauli Oscillator Strengths and Transition Probabilities for Transitions among the Fine-Structure Levels of Cl I

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Domain : Astrophysics

We are currently undertaking an extensive large-scale calculation to obtain the oscillator strengths and transition rates for all E1 transitions in Cl I between the fine-structure levels of the odd-parity configurations $3s^2 3p^5$, $3p^4(^1D)4p$, $3p^4(^3P)np(4 \leq n \leq 5)$ and the even-parity configurations $3s3p^6$, $3p^4(^3P, ^1D, ^1S)ns(4 \leq n \leq 5)$, $3p^4(^3P)6s$, $3p^4(^3P, ^1D)3d$, $3p^4(^3P)4d$, within the *Breit-Pauli* approximation, using the method of interaction of configurations (CI) enveloped in the general atomic structure code CIV3 of Hibbert [1,2]. The CI wavefunctions have been constructed from a common orthogonal set of twenty-two one-electron functions (OEFs), which have been carefully selected to ensure that the *LS*-dependency of the orbitals and all important correlation effects have been accurately represented. Specifically, the 1s→3p orbitals were taken to be the *Hartree-Fock* functions [3] of the Cl I ground state; the 3d, 4s, 4p, 5s were optimised as real *spectroscopic* orbitals, while the remaining functions served as '*correcting*' and '*correlation*' orbitals. In the *LS*-coupling regime, the configuration state functions (CSFs) included in the atomic wavefunction expansions were obtained by performing single and double electron replacements for each symmetry from the available orbitals *nl* in the set of dominant configurations $3s^2 3p^5$, $3s3p^6$, $3p^4 nl$. This ensures the inclusion of all *internal* and *semi-internal* correlation effects and the satisfactory convergence of *all-external* effects.

Results are compared with experimental and other available theoretical data. In the *LS*-coupling scheme our theoretical excitation energies are consistent with the experimental NIST [4] compiled values. We also observe excellent agreement in the dipole length and velocity forms of the calculated oscillator strengths (a measure of the uncertainty in the results), demonstrating a marked improvement over the corresponding results of Ojha [5]. We will present preliminary *ab initio* calculations of the oscillator strengths for transitions between the *LSJ*-coupled fine-structure levels within the Breit-Pauli approximation, which will be compared with the most recent work of Singh et al. (2006) [6].

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P50

NIST Atomic Databases and Units Markup Language

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Domain : Other

At the National Institute of Standards and Technology (NIST), the Office of Electronic Commerce in Scientific and Engineering Data (ECSED) coordinates and facilitates the electronic dissemination of Physics Laboratory (PL) information. ECSED is responsible for PL World Wide Web (WWW) pages at http://physics.nist.gov. ECSED is also engaged with PL 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
- Handbook of Basic Atomic Spectroscopic Data
- SAHA Plasma Population Kinetics Database
- Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibrations
- Ground Levels and Ionization Energies for the Neutral Atoms
- Bibliographic Databases are available for Atomic Energy Levels and Wavelengths, Atomic Transition Probabilities, Atomic Spectral Line Broadening, and Fundamental Constants.

ECSED has been developing an XML (eXtensible Markup Language) schema for encoding measurement units in XML. Adoption of this schema will allow for the unambiguous storage, exchange, and processing of numerical data. This project, http://unitsml.nist.gov, has three components:

- UnitsML - an XML schema
- UnitsDB - a database containing detailed information on scientific units of measure
- Tools - to facilitate the incorporation of UnitsML into other markup languages

An OASIS Technical Committee has been initiated to address any needed changes in the schema and to publish a final recommendation.

P51

Atomic structure calculations of chlorine like titanium

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Domain : Fusion

P52

Stark profile measurements using degenerate four-wave mixing (DFWM) laser spectroscopy and laser Thomson scattering

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Domain : Low Temperature Laboratory Plasmas

The critical review of the experimental data on Stark broadenings, recently published by Konjevic *et al.* [1], indicates that the experimental techniques have not advanced considerably over the last decade to result in the data of better accuracy. This situation limits progress in the field of astrophysics, laboratory plasma research and its applications, and also in line profiles calculations.

In fact, the experimental results are almost exclusively based on optical emission spectroscopy (OES). A simple experimental setup and non-intrusive measurement are its major advantage. On the other hand, only intensity integrated along a line of sight can be directly measured. So determination of local plasma parameters is often difficult or even impossible. Moreover, the spectral accuracy of the OES method is greatly reduced due to influence of the Doppler effect on the measured line profiles.

Therefore we have made an effort to apply nonlinear laser spectroscopy to the measurements of Stark profiles. Degenerate four-wave mixing (DFWM), the method referred to, is a method of high spatial resolution thus ideal for local studies of plasma. The DFWM in configuration with two counter propagating laser beams (backward phase-conjugate geometry) gives spectral profiles with significantly reduced Doppler broadening.

The separate problem in studies of Stark profiles is plasma diagnostic. Electron concentration and temperature are determined using Stark profiles (mainly H_α and H_β of hydrogen), the total intensity of spectral lines or the intensity of plasma radiation background. The precision of many diagnostics techniques also depends on accuracy of the electron transition probabilities for the investigated spectral lines when, for instance, the Boltzmann-Saha plot is constructed.

The method we use for measurements of plasma parameters is laser Thomson scattering (LTS) method. Its main advantages are good spatial resolution and relatively simple relation between the characteristic of the measured spectrum and electron density and temperature. Furthermore, the final result is independent on the plasma state.

The high experimental accuracy in our measurements of Stark profiles, is achieved by simultaneous measurements of DFWM profiles and LTS spectra using a spectrograph and a gated ICCD camera. However, due to the small cross sections for some of the laser scattering processes the experiments require high power pulsed laser which can result in strong plasma disturbance. It follows that the results need careful approach and often simple linear extrapolation of final results to the laser pulse energies can give misinterpretation of physical phenomena.

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P53

Water-vapor Continuum Absorption: Experiment and Modeling in the THz Region

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We present recent experimental results on the spectroscopic continuum study in the far-IR region from 10 to 90 cm^{-1} (0.3 - 2.7 THz). This effort addresses the needs of few terrestrial and satellite projects for an accurate model of the water-vapor continuum to insure reliable data on atmospheric transmittance in available THz windows for a wide range of temperatures and relative humidities. For typical absorption coefficient of $k_c(\nu,T) < 10^{-5}$ cm^{-1}, the measurement of such weak absorption is only possible with long optical pathlengths in situ or in well-controlled laboratory conditions. The presentation will include an analysis of experimental THz techniques such as broadband Fourier transform spectroscopy, high resolution tunable THz laser scans [1] and enhanced absorption in a temperature-controlled multipass cell. The contributions to absorbance resulting from both structureless H_2O - H_2O and H_2O - N_2 continua have been measured in the temperature range 293 to 333 K over a wide pressure range with resolution of 0.04 to 0.12 cm^{-1}. Continuum data are compared to several theoretical predictions. A few models that explore the HITRAN databases as well as available experimental data in the THz region [1], lineshape analysis, broadening and cut-off factors are evaluated for accurate account of resonance contribution from water vapor absorption lines.

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P54

Triple differential cross section data of (e, 2e) processes on Be, Mg and Ca atoms

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Domain : Low Energy Electron-Atom Interactions

The ionization of atoms, ions and molecules by electron impact are the basic processes of atomic and molecular physics, with fundamental applications in different areas as fusion physics, plasma physics, advanced fusion technologies, condensed matter physics, surface science etc. Electron coincidence experiments in which an incoming electron knocks out a bound electron in a collision with target and the two outgoing electrons are then detected in coincidence with defined kinematics are known as (e, 2e) experiments. Such types of investigations have been done to study the momentum distribution of valence electrons in atoms and molecules [1]. Extensive studies of (e, 2e) processes have been reported on various targets including hydrogen, helium, rare gases and alkali targets [2-3]. Recently, Purohit et al [4-5] have calculated triple differential cross sections (TDCS) and spin asymmetry in (e, 2e) processes for lithium like ions and helium like ions using distorted wave Born approximation (DWBA) formalisms. We present in this communication the results of our calculation of TDCS in (e, 2e) processes for alkaline earth targets Be, Mg and Ca atoms in coplanar symmetric geometry. We have performed the calculation in DWBA [1] formalism using spin averaged static exchange potential. We compare the results of our calculation of TDCS for Ca atom with the available experimental data [6].We also present the results of our calculation of TDCS for the inner- shell (e, 2e) processes on Be, Mg and Ca atoms. The inner-shell ionization provides an understanding of the effect of nuclear charge on angular profile of TDCS, particularly on the recoil peak. We will discuss silent features of the inner-shell ionization which are different from outer-shell ionization. The effects of incident electron energy, distortion, polarization on the inner-shell and outer shell ionization will also be discussed for the alkaline earth atoms investigated by us

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P55

NIST Numerical Databases for Atomic and Plasma Physics

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Domain : Other

The Physical Reference Data program [1] at the National Institute of Standards and Technology (NIST) supports about 20 numerical and bibliographic databases of importance for atomic and molecular physics. Here we report on a number of newly developed or recently updated numerical databases for atomic and plasma physics. In July 2006 the most comprehensive of our atomic databases, the NIST Atomic Spectra Database (ASD), was upgraded to version 3.1 [2]. The total number of energy levels and spectral lines is about 76,600 and 141,000, respectively. Transition probabilities are available for about 74,000 spectral lines. The recently added data include extensivedata for Be II, Ne II, Ne III, Ne VIII, and all ionization stages of Kr. A large number of spectral lines and transition probabilities was added for Al VI-XII and Si I-XIV. A number of corrections for configurations of complex ions were made as well, including level compositions in Ho and Yb ions and term grouping in rare earth elements. Among other modifications in ASD 3.1 is addition of the bibliographic reference for the primary source of data.

In May 2006 we released a new SAHA Plasma Population Kinetics Modeling Database [3] which contains the benchmark results for simulation of plasma population kinetics and emission spectra. The data calculated by 14 different codes were contributed by the participants of the 3rd Non-LTE Code Comparison Workshop [4]. The list of the available physical parameters includes, for example, mean ion charges, central momenta, ionization distributions, and rates of physical processes. A newly developed user interface allows one to easily perform selection and retrieval of data. The results can be visualized by using a graphical interface which also allows data presentaion in different formats.

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P56

Spectrum and Energy Levels of Mo VI

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Domain : Fusion

Molybdenum continues to be of interest for controlled fusion reactors as it is used as a first wall material in a number of tokamaks and may play a role in the construction of ITER. In the plasma edge and divertor regions, the spectra of moderately ionized atoms will be especially important. In response to this application we investigated the spectrum and energy levels of Mo VI. This ion belongs to the Rb isoelectronic sequence and as such has a simple one-electron spectrum ($4s^24p^6nl-4s^24p^6n'l'$) as well as a more complicated spectrum arising from inner-shell excitations ($4s^24p^54d^2$ and $4s^24p^54d5s$).

An extensive description of the one-electron spectrum was given by Edlén et al. [1] in 1985 based on observations with a sliding-spark. By using long-wavelength yrast-type transitions observed by Romanov and Striganov [2] with a Penning discharge, Edlén et al. [1] determined an accurate value for the ionization energy. However, Kancerevicius et al. [3] re-observed the spectrum with a low-inductance spark. They extensively revised the identification of transitions arising from inner-shell excitations [4] as well as some odd-parity levels of the one-electron spectrum [1]. As a result, several levels used by Edlén et al. [1] for the ionization energy were called into question and thus also the value for the limit itself. This was derived from the 6h, 7i, and 8k levels.

A few years ago we re-observed the spectrum of Mo VI with a sliding-spark discharge and the 10.7-m normal- and grazing-incidence spectrographs at NIST. The observations covered the range 200-5300 Å. Although we revised a number of the even levels of the one-electron spectrum, we did confirm the identification of the 5g-6h multiplet of Edlén et al. [1] This had been used by them to connect the 6h, 7i, and 8k levels, established by Romanov and Striganov, [2] to the main set of one-electron levels. We also observed most of the lines given by Romanov and Striganov [2] and confirmed those used to determine the 7i and 8k levels. The ionization limit of Edlén et al. [1] was thus confirmed. However, a number of Romanov and Striganov's line identifications had to be revised.

More recently, in an effort to complete our work on this spectrum, we re-visited the line identifications for transitions to the $4s^24p^64d$ ground configuration from the $4s^24p^54d^2$ and $4s^24p^54d5s$ configurations [3] and the energy levels of these configurations. Although almost all of these levels were confirmed, a few revisions were called for. Improved values were obtained for all of the energy levels and a new least-squares fit for the odd configurations was carried out.

This work was supported by the Office of Fusion Energy Sciences of DOE.

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P57

High Resolution Vacuum Ultraviolet Emission Spectrum of D_2 from 78 to 103 nm

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Domain : Other

The emission spectrum of the D_2 molecule has been recorded using the high resolution $10m$ VUV spectrograph in the wavelength range $(785-1700\mathring{A})$. This instrument is equipped with 3600 lines/mm holographic grating and provide a plate factor of $0.25\mathring{A}/mm$. The spectrum is produced by a Penning electric discharge source and contains about 24 000 lines.

The previous similar experimental study was limited to $1000\mathring{A}$ upwards by Bredohl and Herzberg[1] on Lyman and Werner bands.

The analysis of the new spectrum is being carried out with the support of theoretical calculations of term values and line intensities for the $B^1\Sigma_u^+ - X^1\Sigma_g^+$, $C^1\Pi_u - X^1\Sigma_g^+$, $B'^1\Sigma_u^+ - X^1\Sigma_g^+$, $D^1\Pi_u - X^1\Sigma_g^+$ bands taking into account nonadiabatic coupling terms and for the $B''\overline{B}^1\Sigma_u^+ - X^1\Sigma_g^+$, $D'^1\Pi_u - X^1\Sigma_g^+$ and $D''^1\Pi_u - X^1\Sigma_g^+$ bands in the adiabatic representation.

Since the large rotational intervals of the small D_2 molecule result in a complex line spectrum similar to a complex atom spectrum, the program suite **IDEN** [2], based on pattern recognition and developed for analysis of complex atomic spectra has been experienced for identifying spectral lines, finding energy levels and optimizing their energy values. The current analyses led to determination of 302 energy levels among which 175 are new.

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P58

Databases for radiative emission probabilities of molecular hydrogen and simulation of experiments.

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Domain : Astrophysics, molecular processes, molecular data

We present tables of emission probabilities from Rydberg states of H_2 , D_2 and HD published in publicly available databases. The tables can be used to simulate various VUV spectra observed in astrophysical environments or obtained in laboratory experiments. (A recent example is displayed by VUV emission from H_2 excited by monoenergetic electron beams [1].) As pure ab-initio calculations may give rise to significant discrepancies with very high resolution experiments, we have combined a semi-empirical treatment and ab-initio informations to compute line emission transition probabilities and the corresponding wavenumbers. Lyman B-X, Werner C-X, B'-X, D-X VUV emission probabilities of H_2 and D_2 are available in the MOLAT database [2]. Tables of the radiative lifetime and spontaneous radiative dissociation probabilities of excited electronic levels of H_2 are obtained from the CDS base [3]. We have performed ab-initio calculations of VUV emission probabilities of HD and published the data in the CDS database [4].
We present here a comparison between experiments performed at JPL at a resolution of 3 AA [5] and recent calculations of infrared and visible emission probabilities of H_2 arising from excited gerade Rydberg electronic states. Such an emission may only take place from electron excitations followed by radiative cascades. The radiative transitions occur between the upper g-states (EF, GK, HH, P, O, I, R, J, S) and the intermediate u-states (B, B', C, D) in the infrared or visible window, and subsequently in the VUV via the transition to the X ground electronic state.

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P59

Generation of Atomic Data for Complex Many-Electron Atoms and Ions

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Domain : Fusion

The universal method of generation of fairly accurate atomic data (wave functions, energy spectra, wavelengths of electric and magnetic multipole electronic transitions, oscillator strengths, transition probabilities and life-times of excited levels) for complex atoms and ions of various ionisation degrees is presented. It is based on the angular momentum theory, graphical methods, second quantisation in coupled tensorial form, irreducible tensors in three spaces (orbital, spin and quasispin) and completely reduced matrix elements of irreducible tensorial operators [1]. The efficiency of the methods of accounting for correlation and relativistic effects is analysed. This approach is implemented in the form of fairly universal special mathematical software for atomic calculations, allowing to generate the fairly accurate atomic data in principle for any atom of Periodical Table, ions with open f-shells included. The accuracy of the data generated for various complex atoms and ions of various ionisation degrees is evaluated and its high efficiency is demonstrated.

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P60

The $4d^9 5p^2$ Configuration in the In III, Sn IV, Sb V and Te VI Spectra

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Domain : Other

The Ag - like ions In^{+2} - Te^{+5} have a ground state $4d^{10}5s\ ^2S_{1/2}$. Low energy levels of one electron excited states $4d^{10}nl$ are known for a long time [1]. Later the $4d^{10}5s$ - $4d^9 5s5p$ transitions were analyzed and the energies of the $4d^9 5s5p$ configuration with the electron excitation from the $4d^{10}$ core were found [2-4]. Recently (see [5] and references therein) mostly in absorption transitions from the autoionizing configurations $4d^9 5snl$ (n up to 11, l = p and f) and $4d^9 5pnl$ ($n > 5$, l = p and f) were studied. The $4d^9 5p^2$ configuration up till now was not known in the Ag I isoelectronic sequence.

High resolution spectra of the elements from In through Te excited in a vacuum spark (C = 12 - 7500 μF, L = 0.75 - 25 μH, U = 0.22 - 4 kV) have been recorded in the 200 - 600 $\AA$ wavelength region. A 3 m grazing incidence spectrograph with a 3600 l/mm grating was used for the 200 - 350 $\AA$ region (plate factor respectively 0.36 - 0.45 Å/mm). In the longer region the spectrum was recorded on the 6.65 m normal incidence spectrograph with a plate factor 1.25 Å/mm. The $4d^{10}5p$ - $4d^9 5p^2$ transitions were identified and the energies of the $4d^9 5p^2$ configuration were found. The $4d^9 5p^2$ configuration changes its position with respect to the ionization limit $4d^{10}$ along the isoelectronic sequence. In Te VI it is located below the ionization limit whereas in In III all levels of this configurations are situated in autoionization region. The autoionization widths of the lines were observed and measured and compared with the Cowan Code calculations.

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P61

Atomic properties of Li, Na, K, Rb, Ga, Cs, Tl, Fr, Mg^+, Ca^+, Sr^+, Cd^+, Ba^+, Hg^+, and Ra^+

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Domain : Other

We conducted a systematic high-precision calculation of the atomic properties of systems with one valence electron above closed core using a relativistic all-order method. This method is a linearized coupled-cluster method, where single and double excitations of Dirac-Fock wave functions are included to all orders of perturbation theory. Partial triple excitations are also included in some of the calculations. The energy levels, fine-structure intervals, electric-dipole and electric-quadrupole matrix elements, lifetimes, hyperfine constants, static and dynamic polarizabilities, isotope shifts, as well as other properties are calculated for various systems. Systematic comparison with available experiment is carried out and excellent agreement is found in most cases. This work provides benchmark values for a large number of yet unmeasured properties.

As a result of these calculations, we have created an extensive theoretical database of more than 500 reduced electric-dipole matrix elements of the alkali-metal atoms and other systems with one valence electron above the closed core. The database includes all allowed electric-dipole transitions between four lowest *ns* states and four lowest $np_{1/2,3/2}$ states, four lowest $np_{1/2}$ states and three lowest $nd_{3/2}$ states, and four lowest $np_{1/2,3/2}$ states and three lowest $nd_{3/2,5/2}$ states for the alkali-metal atoms. A number of transitions for other systems are included as well. The database includes three values for each transition: lowest-order DHF values and two state-of-the-art calculations: all-order calculation with single and double excitations and all-order calculation with single, double, and partial triple excitations. Listing all three values in the database allows to evaluate the accuracy of the results as it allows to calculate the approximate relative size of the correlation correction and estimate the importance of certain classes of the higher-order terms.

P62

Transition properties of plasma embedded ion: a multi-configuration Dirac-Fock study

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Domain : Other

P63

Polarization resolved plasma spectroscopy on LHD: Emission locations, temperature and flow of neutral hydrogen

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Domain : Fusion

We have observed polarization-resolved spectra of atomic hydrogen, Balmer$_\alpha$ λ656.3 nm, with an absolutely-calibrated high-resolution spectrometer on the Large Helical Device at National Institute for Fusion Science [1]. The spectral profile have been analyzed by fitting the observed spectra, with a consideration of magnetic fields in the LHD plasma assuming two atom temperatures and we determined 2-dimensional emission locations, atom temperatures and hydrogen influxs for several lines of sight on a poloidal cross section. Discharges in configurations with and without the use of local island diverter head gave different results. The analyses on those results suggested to modify the present assumption used in the calculation. From the comparison of the observed spectra with the generated ones by a neutral-particle transfer code simulation including molecular hydrogen, the processes between the hydrogen atoms, molecules and ions are also discussed in details.

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P64

M-shell dielectronic recombination and ionization of Fe ions

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Domain : Fusion, Astrophysics

M-shell dielectronic recombination and ionization of Fe ions are issues of study concerning EUV spectroscopy of solar corona by the Solar-B satellite [1] and impurity concentration of the Large Helical Device. Energy levels, radiative transition probabilities and autoionization rates for Mg-like and Na-like Fe ions were calculated by the Hartree-Fock-relativistic method (Cowan code) and the relativistic many-body perturbation theory method (RMBPT code) [2].

Experimental measurements of charge-state distribution of Fe ions in an Electron-Beam-Ion-Source/Trap (EBIS/T) is also being prepared. In the experiment, extracted ion intensities from the EBIS/T are measured by a magnet analyzer and a position-sensitive detector. Assuming the coronal equilibrium in the EBIS/T, the charge-state distribution is simulated by theoretical recombination and ionization cross sections. Comparison between the experiment and the simulation serves as validation of the theoretical cross sections. Resonant-Excitation-Double-Autoionization cross sections of Li-like I ions were measured by the similar method with the faith of theoretical cross sections for Radiative-Recombination, Direct-Ionization and Excitation-Autoionization [3].

Authors acknowledge with gratitude financial support from the Matsuo foundation.

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P65

Spectroscopy of Interstellar Carbon Molecules: From Laboratory to Space. Recent Advances in Laboratory Studies and the Search for Carbon Molecules in Interstellar Spectra

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Domain : Astrophysics

Large carbon molecules are an important and ubiquitous component of carbon-bearing materials in space. A long-standing and major challenge for laboratory astrophysics has been to measure the spectra of large carbon molecules in laboratory environments that mimic (in a realistic way) the physical conditions that are associated with the interstellar emission and absorption regions [1]. This objective has been identified as one of the critical Laboratory Astrophysics objectives to optimize the data return from space missions [2]. An extensive laboratory program has been developed to assess the properties of PAHs in such environments and to describe how they influence the radiation and energy balance in space. We present and discuss the gas-phase electronic absorption spectra of neutral and ionized PAHs measured in the UV-Visible-NIR range in astrophysically relevant environments and discuss the implications for astrophysics [1]. The harsh physical conditions of the interstellar medium - characterized by a low temperature, an absence of collisions and strong VUV radiation fields - have been simulated in the laboratory by associating a pulsed cavity ringdown spectrometer (CRDS) with a supersonic slit jet seeded with PAHs and an ionizing, penning-type, electronic discharge. We have measured for the first time the spectra of a series of neutral [3, 4] and ionized [5, 6, 7] interstellar PAHs analogs in the laboratory. An effort has also been attempted to quantify the mechanisms of ion and carbon nanoparticles production in the free jet expansion and to model our simulation of the diffuse interstellar medium in the laboratory [8, 9]. These experiments provide unique information on the spectra of free, large carbon-containing molecules and ions in the gas phase. We are now, for the first time, in the position to directly compare laboratory spectral data on free, cold, PAH ions and carbon nano-sized carbon particles with astronomical observations in the UV-MIR range (interstellar UV extinction, DIBs in the NUV-NIR range, UIR bands in the IR). This new phase offers tremendous opportunities for the data analysis of current and upcoming space missions geared toward the detection of large aromatic systems i.e., the "new frontier space missions" (Spitzer, HST, COS, JWST, SOFIA,...).

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P66

Charge Transfer in Homonuclear Collisions of Heavy Ions

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Domain : Fusion

Charge-changing collisions due to intra-beam scattering can have a high impact on modern high intensity accelerators and storage rings [1-3]. Using the crossed-beams technique we have measured absolute cross sections for charge transfer in homonuclear collisions of Ar, Kr, Xe, Pb and Bi ions with charge states q = 2+, 3+ and 4+ and centre-of-mass energies between 2 keV and 94 keV. Typical cross section values are in the order of 2×10^{-17} – 3×10^{-16} cm^2 depending on the collision velocity and Q-value of the reaction. Many systems show a direct correlation of the cross section with the Q-value such that lower Q-values lead to higher cross sections. For the heavier ions and higher charge states however a significant influence of metastable ions is found. Transfer from excited metastable states into the ground state or possible excited target states usually leads to a significantly smaller Q-value then from the ground state. This explains the missing dependence of the measured data on the collision velocity observed for the heavier ions and higher charge states.

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P67

Reactive collisions of electrons with molecular cations: computation and comparison with storage ring and plasma experiments

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Domain : Low Energy Electron-Molecule Interactions

Electron-impact dissociative recombination, ro-vibrational (de-)excitation and dissociative excitation of molecular cations play a major role in the kinetics and energy balance of various ionized media, occuring in interstellar molecular clouds, supernovae, planetary atmospheres, (plasma assisted) combustion, divertor region of the fusion devices and atmospheric re-entry of spacecrafts [1,2]. We will show - and compare with plasma-type and storage ring experiments - our recently computed [3,4] cross sections and rate coefficients on H_2^+, HD^+, DT^+ and NO^+, for several energy regions and ro-vibrational target states of interest, obtained by using a method [5,6] based on the Multichannel Quantum Defect Theory (MQDT). The rapid progress in energy, state-to-state and angular distribution resolution occuring in the storage-ring technique [1,7] allows presently to address these collisions in increasingly detailed aspects, of huge relevance for practical applications. We will illustrate our progress in the developpment of the existing MQDT tool, as well as on the wave-packet method [8], and compare the theoretical results with the recent TSR storage-ring measurements.

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Electron Impact Excitation of Fe-peak Ions of Astrophysical Interest

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Domain : Astrophysics

Electron-impact collision strengths and corresponding effective collision strengths are of crucial importance in the interpretation of spectra of low-ionisation stages of the iron peak elements Fe, Co and Ni, which occur in numerous laboratory and astrophysical plasmas. However, accurate calculation of these quantities is complicated by the open d-shell structure of these ions, which give rise to many low-lying target states that are strongly coupled. This, in turn, leads to a large number of coupled channels which must be retained in the model, posing a formidable computational challenge. Recently a new parallel R-matrix package, PRMAT [1], has been developed to address this problem, and we are in a position to study successfully much larger collision problems than previously possible. In particular, we have a unique opportunity to gain a deeper insight into the role of configuration interaction effects in both the $(N+1)$-electron collision wavefunction, as well as the N-electron target state wavefunction.

Previous studies on Fe II [2] and Fe III [3] have illustrated the importance of the inclusion, in the CI expansion, of electronic configurations allowing for 'two-electron' excitation from the $3p$ to the $3d$ shell. In addition, recent work on Ni V [4] has demonstrated the rôle of broad 'two-particle-one-hole' resonance features, arising from the intermediate states of Ni IV. These features can act to significantly affect the collision strength results. Latest findings for ions of Fe, Ni and Co will be presented at the conference.

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P69

Absolute emission cross section of dissociative products in $He^+ - N_2, O_2$ collisions

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Domain : Other

Absolute emission cross section of excited products was determined in vacuum ultraviolet $50-130nm$ end visible $400-800nm$ spectral region. The measurements were carried out by optical spectroscopy method in the $1-12keV$ energy range of He^+ions. An estimation of uncertainties of the absolute value of all cross sections given here did not exceed $20-25\%$ and the accuracy of relative measurements was $4-5\%$.
Emission cross-section and linear polarization of the excitation of helium atomic $HeI(388.9nm)$ and nitrogen ionic $NII(500.1-500.5nm)$ lines have been measured. High degree of the polarization $P=-20\%$ was observed in the case of helium line. Such a great negative value of the degree of polarization indicates that $m_l=\pm 1$ sublevels of the excited state $3p(^3P)$of helium atom are preferably populated. Analysis of the experimental results indicates that the electron density formed in He^* during the collision is oriented perpendicularly with respect to the incident beam direction. Strong correlation is revealed between inelastic channels of the formation of excited helium and nitrogen particles. To discuss the results of the formation of inner shell vacancy the quasidiatomic approach has been used. In terms of this approximation the excitation of inelastic channels is induced by transitions of electrons at crossings between an initially occupied and promoted molecular orbital (MO) with empty MO's.In our case initial vacancy in $He(1s)$ orbital becomes an inner vacancy of the quasimolecule, hence core-excited, one-hole molecular states can be formed.In particular, in the case of He^+-O_2 the decay of one-hole$2\sigma_g^{-1}$ high excited molecular states$^2\Sigma_g^-$or $^4\Sigma_g^-$ of oxygen cause the excitation of intense oxygen ionic line $OII(83.4nm)$,while in the case of He^+-N_2 intense line $NI(120.0)$ are excited as result of decay of one-hole $2s\sigma_g^{-1}$ intermediate molecular state of N_2^+. The energy dependence of the excitation cross section of the most intense atomic $NI(120,0nm))(3s^4P$- $2p^3\ ^4P))$ and ionic $NII(108.4nm,\ 2p^3\ ^3D$- $2p^{23}P)$ lines exhibit a similar shape with maxima below $1keV$. Moreover, the absolute values of the excitation cross sections for these lines are close to each other. Probable it means, that the excitation mechanisms of the molecular states which dissociate into $N^*(3s\ ^4P)$ and $N^{+*}(2p^3\ ^3D)$ products are the same.

P70

Rotational excitation of CS and SiO molecules by collisions with Helium

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Domain : Astrophysics

Observations of molecular emission at millimeter and infrared wavelengths, supplemented by careful and detailed modeling, are powerful tools to investigate the physical and chemical conditions of astrophysical objects. The modeling of the line intensities requires comparison with model excitation calculations using radiative as well as collisional rates. In the relatively cold environments, collisional excitation is dominated by collisions with the most abundant neutral species, He and H_2.

We present here new 2D potential energy surfaces for the SiO-He and CS-He systems, calculated at r-distance frozen at their experimental minimum energy distance. Both are obtained at the CCSD(T) level using aug-cc-VQZ basis sets for the three atoms and supplemented by bond functions. Close coupling calculations of the collisional excitation cross sections of the rotational levels of SiO and CS by He are calculated from kinetic energies ranging from 0.1 to 1500 cm^{-1}. The propensity rules between rotational levels are studied. For SiO, ΔJ even cross sections are much larger than ΔJ odd cross sections. At the opposite, for CS, ΔJ odd cross sections are much larger than ΔJ even cross sections. Excitation rates among the 31 first rotational levels of SiO and CS are calculated for temperatures ranging from 5-300K.

P71

Electron Collision Excitation of O II, O IV, and Fe XIV

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Domain : Astrophysics

Electron collision excitation cross sections for infrared, optical, and ultraviolet lines arising from transitions between the 47 levels of O II, 54 levels of O IV, and 135 levels of Fe XIV have been calculated using the Breit-Pauli R-matrix approach [1]. Configuration-interaction wave functions have been used for an accurate representation of target levels. There is a strong term dependence of valence orbitals in O II. The non-orthogonal orbitals in the multiconfiguration Hartree-Fock approach have been used to account for term-dependence of O II wave functions and to describe important correlation corrections and relaxation effects. These wave functions yield excitation energies which are in close agreement with experiment. Oscillator strengths and transition probabilities for various transitions also compare very well with previous calculations and measurements. The B-spline R-matrix approach [2,3] has been used to calculate electron excitation collision strengths and rates in O II. The calculated excitation cross sections show very good agreement with the available measured absolute excitation cross sections for all three ions. Several line intensity ratios involving O II, O IV, and Fe XIV lines are density and/or temperature sensitive and can be used for diagnosing the physical conditions of planetary nebulae, seyfert galaxies, symbiotic stars, and solar transition region and corona. This research work is supported by NASA Grant NAG06GD39G from the Astronomy and Physics Research Analysis program.

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Cross sections for low energy electron impact excitation of the electronic states of water

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Domain : Low Energy Electron Molecule Interactions

We report differential and integral cross sections for excitation of the lowest lying $^3B_1$, $^1B_1$, $^3A_1$, and $^1A_1$ electronic states of water. The energy range of these measurements is 15-50eV and the angular range of the DCS measurements is 10°-90°. From these DCS the corresponding ICS is calculated using a molecular phase shift analysis technique to extrapolate the data to 0° and 180°. Where possible, comparison is made to the results of available theory. One of the main objectives of this study is to perform statistical equilibrium calculations to determine if the origin of the OH Meinel bands in our atmosphere are due, at least in part, to electron driven processes.

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High resolution XUV laser spectroscopy of HD and D_2

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Domain : Astrophysics

Using a narrowband (~ 0.01 cm^{-1}) and tunable extreme ultraviolet (XUV) laser source, spectral lines in the Lyman and Werner bands of the HD and D_2 hydrogen isotopomers were re-investigated in high resolution. The XUV transitions were monitored via a 1 XUV + 1 UV multiphoton ionization and detection of ions after time-of-flight mass separation. The narrwoband XUV radiation was obtained through third harmonic generation of the frequency-doubled output of a pulsed dye amplifier, seeded by a CW ring dye laser. The goals of these measurements are twofold. Firstly, a comparison is made to test the *ab-initio* calculations on the $B^1\Sigma_u^+$ - $X^1\Sigma_g^+$ and $C^1\Pi_u$ - $X^1\Sigma_g^+$ systems of HD and D_2. Secondly, the present high-resolution results serve to calibrate the emission spectra of the Lyman and Werner bands with the 10 m classical spectrometer present in the Observatoire de Paris, Meudon.

P74

Towards Better Assessment of Atomic Transition Probabilities

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Domain : Atomic Data

Large amounts of atomic transition probabilities have been obtained from atomic structure calculations, but normally without uncertainty estimates. To obtain some guidance for the expected uncertainties, many authors have undertaken comparisons with available experimental data, usually on a very limited basis, and have, by extrapolation, made risky assumptions for other transitions. This applies especially to extrapolations from strong, prominent lines to weaker transitions.

It is still a great challenge to produce realistic, well-justified uncertainty estimates for theoretical transition probability data. Recently, many calculated results, especially for light elements, have been presented both in the dipole length and dipole velocity forms (which should ideally produce identical results), and it has been suggested that the difference between the two results should be a measure of the uncertainty. We have tested this suggestion for various transitions in light and medium-heavy elements, for which such results as well as experimental comparison data were available. We have found that this measure of uncertainty works fairly well, and could also be further refined.

P75

Observation and interpretation of emission spectra of free ions Nd^{3+} and Nd^{4+}

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Domain : Low Temperature Laboratory Plasmas

Spectra produced by a sliding spark with a pure Nd anode were observed in the spectral range from 60 to 120 nm on the normal incidence 10.7m vacuum ultraviolet spectrograph at the Paris-Meudon Observatory. Earlier spectral plates produced at NBS, Gaithersburg on a similar instrument have completed our data at longer wavelengths. The source operating conditions were varied in order to select lines of Nd III to Nd V. Polynomial interpolation from impurity lines of ionized elements C, N, O, Al and Si led to Nd wavelengths with estimated errors of $\pm 0.003\AA$ near $1300\AA$. In spite of many studies of Nd^{3+} in compounds, the atomic energy levels of this famous Nd-laser ion had never been derived from spark spectra. In a first step, 37 (out of 41 possible) levels of $4f^3$ were determined from $4f^3$-$4f^2 5d$ transitions and were described in various theoretical approximations [1]. The running extension of this work includes more than a half of the $4f^2 6s$ and $4f^2 6p$ levels but a complete theoretical description of Nd IV is hampered by the overlap of the latter configuration with $5p^5 4f^4$.

More recently, all levels of $4f5d, 4f6s$ and $4f6p$ have been determined in Nd V and only the highest level of the ground configuration $4f^2$ is missing.

Trivalent lanthanide ions have many applications, for which the knowledge of the free ion spectra, atomic energy levels, radial parameters and transition probabilities are crucially important. After Nd IV and Tm IV [2], the spectra of Eu IV and Er IV will be investigated shortly.

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P76

Modeling for Non-equilibrium plasma diagnostics for LHD and Solar-B

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Domain : Spectroscopic diagnostics, Fusion, Solar physics

This year, Solar-B satellite in order to observe the Sun will be launched in Japan. Solar-B has three kinds of detectors for optics, EUV, and X-ray observations. Very high-resolved spectra are measured with the EUV imaging spectrometer (EIS). EIS measures two bands of 170A-210A and 250A-290A where many lines of M and L shell Fe ions are detected. Analysis of these lines without assuming ionization equilibrium is required to understand coronal heating mechanism in transition-coronal region. However construction of non-ionization equilibrium plasma model is difficult if we take into account the transport of plasma particle.
In this paper, comparisons with calculated spectra by CHIANTI and our model assuming ionization equilibrium, and useful intensity ratios for plasma diagnostics are presented. Our model includes energy levels from H-like to Ca-like Fe ions and atomic processes with cross sections calculated by the HULLAC code. For excitation processes of Si-like Fe ions we use recommended data. Time-resolved EUV spectra in ionization non-equilibrium plasma are measure from large helical device (LHD) at NIFS. Spectral lines are identified and time dependence of line intensities is studied.

P77

CRAAMD Atomic and Molecular Database

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Domain : Fusion

China Research Association of Atomic and Molecular Data (CRAAMD) aims at organizing physicists and groups on atomic and molecular (AM) physics in China to measure, calculate, collect, compile and assess AM data. Since the ICAMDATA 04 held in Toki, Japan, more than ten groups in different Chinese universities and institutes joined the CRAAMD and contributed a lot to the CRAAMD AM database, an extensive AM data were produced, compiled and assessed, such as atomic energy levels and radiative transition properties, molecular spectra, precise ionization potential and viberational energy levels of molecular ions, data of collision between electron and atom/molecular, heavy particles collision data, opacity data , and so on. These activities will be introduced in detail in present paper.

P78

Recent Progresses of Plasma Property (Atomic and Molecular) Database for Industrial Plasma

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Domain : Low Temperature Laboratory Plasmas

Since the characteristics of plasmas depend strongly on the interactions between plasma particles such as electron, ions, and neutrals, a well-established atomic and molecular database is needed to understand and produce various types of plasma. Although atomic and molecular cross section data have been generated for a long time, they have not yet been integrated well into a user-friendly database which is increasingly needed especially for nuclear fusion and industrial plasma applications as well as pure plasma science. Thus here we introduce the NFRC and KISTI activity, how tried to collect, analyze and integrate the atomic and molecular cross section data into a database that is easily accessible for users through the internet.

P79

Systematic calculations of oscillator strengths in noble gases.

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Domain : Astrophysics

The B-spline box-based close-coupling method [1,2] was applied for extensive calculations of the transition probabilities in the noble gases Ne, Ar, Kr, and Xe for energy levels up to $n = 12$. Individually optimized, term-dependent sets of non-orthogonal one-electron radial functions were used to account for the strong term dependence in the valence orbitals. The core-valence correlation was introduced through multi-channel expansions, which include the ns^2np^5, $nsnp^6$, and $ns^2np^4(n+1)\ell$ target states. The inner-core correlation was accounted for by employing multi-configuration target states. Energy levels and oscillator strengths for transitions from the np^6 ground-state configuration as well as transitions between excited states were computed in the Breit-Pauli approximation. The present calculations provide the most systematic *ab initio* radiative data for noble gases: they include the lifetimes and oscillator strengths for 299 states and 11300 transitions in Ne, 359 states and 19000 transitions in Ar, 212 states and 6450 transitions in Kr, and 125 states and 2550 transitions in Xe. We obtained excellent agreement with existing experimental data in the case of Ne and overall very good agreement for Ar and Kr, except for a few transitions to closely spaced $(n+1)s$ and nd states. In Xe, very close agreement with experiment was obtained for excitation of the lowest $6s$ and $6s'$ states. However, noticeable discrepancies for excitation of the nd states indicate the limitation of the Breit-Pauli approximation in this case. Good agreement with other calculations was obtained for transitions from the ground states, whereas significant discrepancies were found for transitions between excited states. Our results show that the B-spline method with non-orthogonal orbitals can be used for accurate calculations of oscillator strengths for states with intermediate n-values, i.e., exactly in the cases for which it is difficult to apply standard MCHF methods.

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Multi-Configuration Distorted-Wave Approximation in Electron-Impact Ionization of Ar_6^+

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Domain : Low Energy Electron Atom Interactions

A quasi-relativistic distorted-wave approximation is developed to investigate the direct electron-impact ionization processes, in which the configuration interactions are considered in the initial and final states of target. As an example, the direct detailed-level electron-impact ionization cross sections for the ground and low excited states of $Ar^{6+}(3s^2, 3p^2, 3s3d)$ are calculated in the energy range from 1.02 to 15Ith (Ith the ionization threshold). Comparison with the available data demonstrates that our results are reasonable. The effects of configuration interactions are discussed, and the validity of transformation principles by statistical weights between configuration-averaged and detailed-level electron-impact ionization cross sections is analysed.

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Excitation of CO by Electron Impact

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Domain : Low Energy Electron Molecule Interactions

The BEf scaling [1]—which converts plane-wave Born (PWB) cross sections for electron-impact excitations of atoms to accurate results at low incident electron energy T—also provides reliable vibrational excitation cross sections for the A $^1\Pi$ v′ = 0–7 ← X $^1\Sigma^+$ v″=0 transitions
of CO in excellent agreement with experimental cross sections at T = 50–200 eV obtained by integrating energy-loss angular distributions measured at the Sophia Univ. and the Flinders Univ. The generalized oscillator strength calculated by Chantranupong et al. [2] was used to generate PWB cross sections. The scaled Born cross sections are also in excellent agreement at T = 300–1500 eV with the experimental results available in the literature [3,4]. Preliminary data on the application of the BEf scaling to H_2 and H_2O indicate that the scaling method is applicable to a wide range of molecules. The theoretical method is valid only for integrated cross sections of electric-dipole and spin allowed excitations.

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