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Review lectures

Atomic data collection with the new 4th generation x-ray light sources

R. W. Lee[1,*],
P. Audebert, M. Bergh, C. Caleman, R. Cauble, P. Celliers, M.H. Chen, H.-K. Chung, M. Fajardo, R. Falcone, R. Fedosejevs, E. Foerster, J. Gauthier, S. Glenzer, G. Gregori, J. Hajdu, P. Heimann, L. Juha, J. Krzywinski, H.-J. Lee, S. Moon, B. Nagler, Y. Ralchenko, R. Redmer, D. Riley, S. J. Rose, F. Rosmej, W. Rozmus, R. Schuch, H. A. Scott, D. Schneider, J. R. Seely, R. Sobierajski, K. Sokolowski-Tinten, T. Stoelker, S. Toleikis, T. Tschentscher, S. Vinko, H. Wabnitz, J. S. Wark

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The construction of short-pulse tunable XUV and x-ray free electron lasers based on the self-amplified spontaneous emission process provides a major advance in capability for generating atomic data from atoms / ions both isolated and in dense plasmas. These sources will provide up to 10^{12} photons in a pulse that is 10 to 100 fs in duration, are tunable, have full transverse coherence and have repetition rates of $\geq$ 10 Hz. There are several areas where these x-ray sources provide unique opportunities. First, one can focus the x-rays to intensities unavailable previously, thus opening the way for multiple ionization that can form hollow ions, and when tightly focused one can generate two-photon processes previously inaccessible in the x-ray region. Second, with the high photon flux one can photo-ionize the inner-shell of atoms in a gas and attempt to invert the hollow atom population to create lasing. This is a prototype of any lasing scheme that requires inversion produced by, e.g., collisions in a plasma, as here the FEL can test the kinetics simulations. Third, the FEL can be used to irradiate atomic clusters. In the unfocused mode each atom becomes ionized and the Coulomb explosion, which has been produced with short pulse optical lasers, will be more efficient in that the entire cluster will be ionized producing fast electrons, fast ions an x-rays. In a highly-focused beam the cluster continues to ionize until it is fully stripped. Interest in the tightly focused cluster irradiation arises from the need to understand detail processes, as these are central to proposals intent on imaging bio-molecules. Finally, the study of dense plasma population kinetics has suffered from the fact that, until the x-ray FELs recently became available, there was no way to selectively pump a transition in situ. With the advent of the these FELs one will be able to perform plasma spectroscopic experiments on ion species with the same control that one can use an optical laser to probe the states of neutral atoms. Here we discuss experiments to probe and manipulate ions in plasma.

The Virtual Atomic and Molecular Data Centre: A new way to disseminate A.&M. data

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Atomic and molecular (A&M) data are of critical importance across a wide range of applications such as astrophysics, atmospheric physics, fusion, environmental sciences, combustion chemistry, and in industrial applications from plasmas to lighting. Currently these vital and fundamental A&M data resources are highly fragmented and only available through a variety of highly specialized interfaces, thus limiting the full exploitation of their scientific worth. This in turn hinders research across a wide range of topics including space exploration (the characterization of extrasolar planets, understanding the chemistry of our local solar system and of the wider universe, see e.g. Fig 1); the study of the terrestrial atmosphere and quantification of climate change; the development of the international fusion programme for energy, and our understanding of radiation damage within biological systems, to give just a few examples.

The Virtual Atomic and Molecular Data Centre (VAMDC) [1, 2] is a major new European initiative now building a unified, secure, documented, flexible and interoperable e-science environment-based interface to existing A&M data. VAMDC combines the expertise of existing A&M databases, data producers and service providers with the specific aim of creating an infrastructure that is easily tuned to the requirements of a wide variety of users in academic, governmental, industrial or public communities. The project encompasses the construction of the core consortium, the development and deployment of the infrastructure and the development of interfaces to existing A&M databases. VAMDC partners are responsible for many of the world's major A+M data resources. The paper describes the current 'Level 1' service deployment of the VAMDC data infrastructure across a wide range of VAMDC partner provided resources and outlines our objectives.

Acknowledgement. VAMDC is funded under the "Combination of Collaborative Projects and Coordination and Support Actions" Funding Scheme of The Seventh Framework Program. Call topic: INFRA-2008-1.2.2 Scientific Data Infrastructure. Grant Agreement number: 239108.

References

[1] Dubernet, M.L., et al, 2010, JQSRT, in Press (http://dx.doi.org/10.1016/j.jqsrt.2010.05.004)

[2] http://www.vamdc.eu

Computation of atomic data for astrophysics and fusion

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From a theoretical atomic perspective, electron collision processes in both astrophysical and magnetic fusion plasmas have much in common, both require data for excitation, ionization and recombination for a multitude of elemental ions, although there are differences in the relative importance of light elements, e.g. magnesium vs beryllium. There are longstanding fundamental differences, the most significant (from an electron-ion perspective) being that of electron density. For the most part, the coronal approximation suffices for astrophysics while for magnetic fusion collisional-radiative modelling is crucial and this places additional requirements upon the data and its producers, for example, total ionization and recombination rate coefficients are not directly usable. With the advent of ITER, a new difference and challenge arises viz. complex heavy species. Tungsten, xenon etc will be commonplace and so will their diagnostic modelling. Such ions place new demands on modelling suites, such as ADAS [1], which in turn place new requirements on atomic data and its producers. For example, relativistic effects cannot be treated as lightly, while the complexity of the ions mean that the most sophisticated collision methodology and codes (e.g. R-matrix) will be unable to deliver the level of coverage of data that is possible for astrophysics.

We will review methodologies and associated computer codes for atomic data generation for astrophysical and magnetic fusion plasmas, including new developments, viz. Dirac R-matrix with pseudo-states [2], massively parallel R-matrix codes, including radiation damping [3], AUTOSTRUCTURE 'distorted-wave'; and how they can be used to benchmark and constrain simpler approximations which can easily be applied to the full complexity of the diagnostic modelling of heavy species.

Finally, we report-on a program of systematic calculations for R-matrix electron-impact excitation of isoelectronic sequences [4–6], AUTOSTRUCTURE dielectronic recombination of M-shell ions [7–8] and its benchmarking by experiment [9].

References

[1] H.P. Summers, *The ADAS User manual version 2.6* (2004) http://www.adas.ac.uk/

[2] N.R. Badnell, J.Phys.B **41**, 175202 (2008)

[3] C.P. Ballance and D.C. Griffin, J.Phys.B **39**, 3617 (2006)

[4] G.Y. Liang, A.D. Whiteford and N.R. Badnell, Astron. Astrophys. **500**, 1263 (2009)

[5] G.Y. Liang, A.D. Whiteford and N.R. Badnell, J. Phys. B **42**, 225002 (2009)

[6] G.Y. Liang and N.R. Badnell, Astron. Astrophys. At Press (2010)

[7] D. Nikolić, T.W. Gorczyca, K.T. Korista and N.R. Badnell, Astron. Astrophys. At Press (2010)

[8] N.R. Badnell, Astrophys. J. Lett. **651**, L73 (2006)

[9] M. Lestinsky et al, Astrophys. J. **698**, 648 (2009)

Benchmark calculations of electron-impact differential cross sections

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The fundamental motivation behind the study of collisions in atomic and molecular physics is the requirement for accurate interaction data in a variety of applications. These include fundamental and applied sciences, as well as industry. Astrophysics, fusion, lasers, lighting, and other plasma physics applications can all benefit from the quantitative knowledge of the underlying interactions.

In order to be useful the collision data required in plasma modelling needs to be accurate. The level of precision required may vary from one application to another, but reducing the uncertainties to just a few percent enables the modellers to concentrate solely on the physics of their models, and not be distracted by concerns about the accuracy of the inputs.

Typically, the required collision data takes the form of integrated cross sections, which are obtained by integrating differential cross sections. Unfortunately, obtaining accurate cross section data in the field of atomic and molecular physics is not a simple task. For many targets of interest even the structure is too complicated, let alone collisions with such targets. Even for the simpler targets, whose structure is readily obtained, the long-standing formal problems associated with the long-ranged nature of the Coulomb potential also abound. Targets in the field having an infinite discrete spectrum and a continuum adds another layer of complexity. Yet we require accurate results irrespective of the kinematics or the transition of interest.

The ever increasing computational resources have allowed collision physicists to tackle the above-mentioned problems head-on. There are now several computational techniques whose foundation is such that they have the capacity to generate accurate results. The most widely used approaches are based on the R-matrix method [1], and yield excellent results particularly when supplemented with pseudostates to take into account the target continuum [2, 3]. This approach has also been extended to the relativistic domain [4]. The time-dependent close-coupling approach has also enjoyed considerable success in more recent times, see the review of Pindzola et al. [5]. The convergent close-coupling (CCC) method [6] utilises a complete Laguerre basis for the generation of the target states and solves the close-coupling equations in momentum space. Its strength is that convergence can be systematically studied by simply increasing the size of the basis. This approach has also been extended to the relativistic domain [7].

In the talk we will review recent progress in the field, and show some comparison between benchmark calculations and experiment. We will also indicate that there are still very many targets for which a joint experimental and a theoretical investigation is necessary.

References

[1] P. G. Burke and W. D. Robb, Adv. Atom. Mol. Phys. **11**, 143 (1975).

[2] K. Bartschat, E. T. Hudson, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 115 (1996).

[3] N. R. Badnell and T. W. Gorczyca, J. Phys. B **30**, 2011 (1997).

[4] N. R. Badnell, J. Phys. B **41**, 175202 (2008).

[5] M. S. Pindzola, F. Robicheaux, S. D. Loch, J. C. Berengut, T. Topcu, J. Colgan, M. Foster, D. C. Griffin, C. P. Ballance, D. R. Schultz, et al., J. Phys. B **40**, R39 (2007).

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

[7] D. V. Fursa, C. J. Bostock, and I. Bray, Phys. Rev. A **80**, 022717 (2009).

Atomic and molecular data needs for radiation damage modeling underlying radiotherapy

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A multiscale approach to radiation damage due to irradiation of living cells with photons or energetic ions is needed to understand the whole range of physical, chemical, and biological phenomena that take place during and following radiotherapy. Understanding of different mechanisms leading cell death on phenomenological level makes it possible to sort out advantages of choosing particular type of radiotherapy, e.g., photons vs. carbon ions or vice versa. The main difficulty of this problem is that the events are happening in a large range of time, distance, and energy scales. Therefore, the multiscale approach is designed to consider these effects within one framework.

In our first series of works devoted to the development of the multiscale approach to radiation damage and its application to the treatment of atomic and molecular mechanisms underlying the ion beam cancer therapy [1-5], we defined our goals, considered the effects of ion stopping in the medium, secondary electron production, and the transfer of the latter to DNA segments. We addressed different aspects of the Bragg peak and energy spectra of secondary electrons. An improved approach to these issues is published recently in [4]. DNA damage by secondary particles (electrons, holes, and radicals) is deemed to have a supreme importance for killing cells. Therefore, our next goal was to consider different pathways of DNA damage. Since in high-linear-energy-transfer (high-LET) irradiation events, associated with ion-beam therapy, the direct damage by electrons is one of the most important, we started with the analysis of the transport of secondary electrons to DNA [2, 3]. We were able to estimate the number of double strand breaks (DSBs) per μm of the ion's trajectory which reasonably comparable to the experiments. This analysis only included low-energy electrons and an improved approach is under development. In the next round, we are interested in calculating of the radial dose distribution to compare it with the radial distribution of probability of complex damage. The complexity of DNA damage is a special feature of high-LET irradiation. It is related to a much higher number density of secondary particles and presents a qualitative leap, advantageous for ion-beam therapy. The quantification of the complexity of damage is a part of the multiscale approach and it is one of the subjects of our most recent work.

The multiscale approach opens many opportunities for analysing different conditions due to various particle beams, and tissues. In the future we hope to be able to calculate the relative biological effectiveness locally and thus make this approach practical for treatment planning. This analysis relies on a significant amount of atomic and molecular data, which are currently available only partially.

References

[1] E. Surdutovich, O. Obolensky, E. Scifoni, I. Pshenichnov, I. Mishustin, A.V. Solov'yov, and W. Greiner. Eur. Phys. J. D **51**, 63–71 (2009)

[2] A. V. Solov'yov, E. Surdutovich, E. Scifoni, I. Mishustin, and W. Greiner. Phys. Rev. E **79**, 011909 (2009)

[3] E. Surdutovich and A. Solov'yov. Europhys. News 40/2, 21 (2009)

[4] E. Scifoni, E. Surdutovich, and A.V. Solov'yov, Phys. Rev. E **81**, 021903 (2010)

[5] M. Toulemonde, E. Surdutovich, and A.V. Solov'yov, Phys. Rev. E **80**, 031913 (2009)

Progress reports

Database and related activities in Japan

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The National Institute for Fusion Science (NIFS) has constructed an atomic and molecular numerical database for collision processes and makes it available via the internet at URL=http://www.nifs.ac.jp/. Data compilation was started in the 1970s at the Institute of Plasma Physics, Nagoya University and has a long history. We have organized a working group of atomic and molecular physicists to search and evaluate atomic data to be included in our database. The database was started to compile atomic data relevant for fusion plasma research, but recently we extend our interests to wider research areas such as astrophysics, applied-science plasma with low temperature, and so on. Since 2001 we have constructed databases for electron collision and heavy particle collision processes involving molecules. Recently we also collect atomic data of heavy elements, such as Ar, Fe, Ni, Kr, and Xe [1], and have started to search for atomic collision data for hydrogen isotopes which are important for fusion research.

We have been interested in plasma diagnostics using Fe ion intensity ratios for research on solar and laboratory plasmas [2–4]. Atomic data of Fe ions have been compiled for kinetic modeling. Electron-impact excitation rate coefficients for Fe ions were assembled and recommended data is available as electronic files for for kinetic modeling [5, 6].

Proton-impact excitation processes are important for exciation within fine-structure levels of ground state or metastable states and these processes affect population kinetics and spectral line intensities. Plasma diagnostics of electron density using Fe ion spectral line ratios are affected by proton-impact excitation for solar and laboratory plasmas. Proton-impact excitation rate coefficients for M-shell and L-shell Fe ions were evaluated and recommended data was fitted with an analytic formula [7]. We also calculated the rate coefficients of proton-impact excitation for Fe^{19+} ion using a close-coupling method [8].

We compiled recommended data of photo-absorption cross sections for 9 atoms and 23 molecules [9] and the database is now available from the web page [10].

Recently we organized the Forum of Atomic and Molecular Data and Their Applications in Japan to communicate and exchange information on atomic and molecular data between atomic and molecular physicists, data users such as plasma application researchers, company researchers, or plasma software developers and/or suppliers, and our database groups. We use emails and the web page for communication and have a workshop every year. We hope the Forum will help to distribute atomic and molecular data and will activate the research using atomic and molecular data in Japan.

References

[1] M. Kitajima et al., in preperation for NIFS-DATA (2010)
[2] N. Yamamoto et al., Astrophys. J. **689**, 646 (2008)
[3] T. Watanabe et al., Astrophys. J. **692**, 1294 (2009)
[4] I. Murakami et al., Plasma Fusion Research, in press (2010)
[5] I. Skobelev, I. Murakami, T. Kato, NIFS-DATA-99 (2007)
[6] I. Murakami et al., in preperation for NIFS-DATA (2010)
[7] I. Skobelev, I. Murakami, T. Kato, Astron. Astrophys. **511**, A60 (2010)
[8] A. Ulantsev and I. Murakami, in preperation for NIFS-DATA (2010)
[9] N. Sakamoto et al., NIFS-DATA-109 (2010)
[10] http://dpc.nifs.ac.jp/photoab/

Atomic data for solar corona studies

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In recent years due to the increased sophistication of space instrumentation ever more detailed spectra from a large variety of coronal structures are available. While interpreting such spectra some unexpected properties of coronal plasmas were discovered. Although in general close inspections of recorded spectra show good agreements between observations and code predictions, there are cases were discrepancies between observations and calculations do exist. During my talk I will discuss some of the unexpected observational results that were recently discovered, some of the discrepancies between observations and measurements and allude to unsolved issues in the properties of coronal structures that could be helped by ideas from the atomic physics community.

Measurement of EUV spectra of high Z elements from Large Helical Device

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Optically thin high-temperature plasmas produced in the Large Helical Device (LHD) at the National Institute for Fusion Science can be utilized as a characteristic research light source including substantial extreme ultra-violet (EUV) emissions from intentionally injected high Z elements. A number of reliable diagnostics installed in LHD are advantageous to a source of the experimental database of the EUV spectra. In this study we will focus on the EUV spectra from highly charged tin, xenon and tungsten ions measured by a 2 m Schwob-Fraenkel type grazing incidence spectrometer [1] in LHD. Tin and xenon have been studied as candidate materials in the development of EUV light source for the next generation semiconductor lithography, and tungsten as a plasma facing component in the forthcoming ITER (International Thermonuclear Experimental Reactor) project.

The EUV spectra have been observed mainly in the wavelength ranges around 13 nm, 11 nm and 5 nm for tin, xenon and tungsten, respectively, where emissions from open N shell ions are expected. The measured spectral feature largely depends on whether the discharge is stably sustained or is approaching a radiation collapse [2, 3]. Figure 1 shows an example for the case of tin. When the plasma edge is cooled as a precursor of a radiation collapse, a broad spectral feature around 13.5 nm arising from unresolved transition array (UTA) from open $4d$ subshell ions is superposed on sharp discrete lines from higher charge states with open $4s$ or $4p$ subshell ions [3]. As for tungsten, contribution of open $4f$ subshell ions should also be considered to interpret the whole spectra.

Since various charge states are observed at the same time in LHD, comparisons with charge selected spectral data (experimental/theoretical) are indispensable for the analyses of the measured spectra. Assignments of the complicated broad features and the strong discrete lines from tin, xenon and tungsten ions have been performed with the help of comparisons with the experimental spectra in charge exchange collisions [4] and electron beam ion trap (EBIT), and the theoretical calculations by Cowan code.

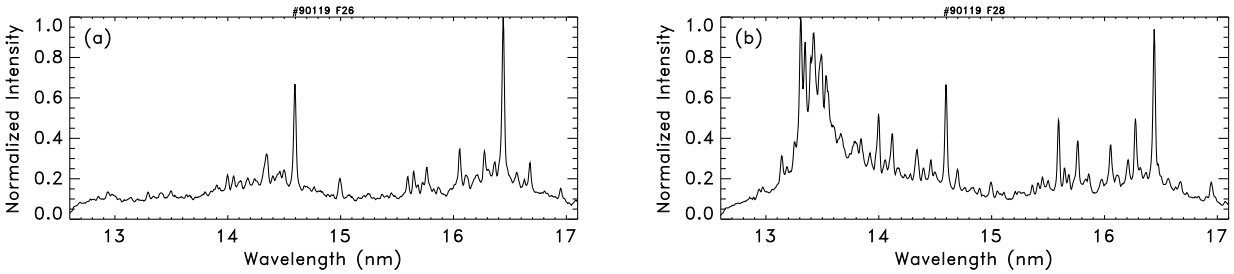

Figure 1: EUV spectra from highly charged tin ions measured in LHD plasma (a) in a stable phase and (b) approaching a radiation collapse.

References

[1] J. L. Schwob, A. W. Wouters, S. Suckewer, Rev. Sci. Instrum. **58**, 1601 (1987)
[2] T. Kato *et al.*, J. Phys. B: At. Mol. Opt. Phys. **41**, 035703 (2008)
[3] C. Suzuki *et al.*, J. Phys. B: At. Mol. Opt. Phys. **43**, 074027 (2010)
[4] H. Ohashi *et al.*, J. Phys. B: At. Mol. Opt. Phys. **43**, 065204 (2010)

Recent developments in the NIST Atomic Databases

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New versions of the NIST Atomic Spectra Database (ASD, v. 4.0) and three bibliographic databases (Atomic Energy Levels and Spectra, v. 2.0, Atomic Transition Probabilities, v. 9.0, and Atomic Line Broadening and Shapes, v. 3.0) have recently been released. In this contribution I will describe the main changes in the way users get the data through the Web. The contents of ASD have been significantly extended. In particular, the data on highly ionized tungsten have been added from a recently published NIST compilation. The tables for Fe I and Fe II have been replaced with newer, much more extensive lists (10000 lines for Fe I). The other updated or new spectra include H, D, T, He I-II, Li I-III, Be I-IV, B I-V, C I-II, N I-II, O I-II, Na I-X, K I-XIX, and Hg I. The new version of ASD now incorporates data on isotopes of several elements. I will describe some of the issues the NIST ASD Team is facing while updating the data.

Atomic and molecular data for astrophysics: VALD3 and VAMDC projects

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I will describe some typical applications of atomic and molecular data in modern astrophysics and highlight the different requirements to the completness and accuracy of the data. The examples will include high-resolution synthesis of stellar spectra for mapping stellar surface chemical composition and magnetic fields, search for exoplanets with radial velocity techniques and reliable estimates of radiative cooling and heating rates in large-scale hydrodynamic simulations of stars and circumstellar medium. All of these examples will be illustrated by the calculations based on the latest version of the Vienna Atomic and molecular Database VALD3 and direct comparision with the observations.

I will also show that the range of physical parameters and processes encountered in such applications is often beyond any single collection of atomic and molecular data and, therefore, an infrastructure such as the Virtual Atomic and Molecular Data Center (VAMDC) has a crucial role in uderstanding e.g. planet formation or final evolutionary stages of solar-type stars where the radiation carries energy across phase transition boundaries of matter.

Spectroscopy of ionized atoms for nanotechnology

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Extreme ultraviolet (EUV) lithography has been accepted as the successor to optical lithography for large-scale chip manufacturing. A light source is one of the major functional blocks of the lithography tools. High power EUV radiation can be emitted mostly by a high temperature plasma. A task of atomic spectroscopy is to find an appropriate "fuel" material and to obtain fundamental atomic data needed for optimization of the source at particular wavelength region.

The EUV lithography at 13.5 nm is presently under intense development with tin as the most probable fuel for the light source. The emission spectrum of tin excited in a plasma with electron temperature ∼50 eV has a very intense peak in the 130–140 Å range consisting from the transitions in Sn^{+8}–Sn^{+14} ions with the ground configuration $4p^6 4d^k$ (k = 6–0). Results of the study (wavelength identification, energy level location, transition probability calculation) of high resolution spark Sn IX – Sn XV spectra in the region 120–160 Å as well as corresponding isoelectronic spectra of Rh, Pd, Ag and Cd are reported. The physical effects related to the studied spectra such as configuration crossing and interaction, emissive zone formation and relativistic effects are discussed.

Some results of the study of other chemical element spectra as possible fuel for lithography sources at shorter wavelengths will be presented.

Challenges of theoretical spectroscopy of heavy and superheavy atoms and ions

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The development of modern technologies, particularly - nanotechnologies, poses new tasks for contemporary theoretical atomic physics. Progress in experimental physics allows to synthesize super-heavy atoms, for example, ununnilium (Uun Z=110), unununium (Uun Z=111) and ununbium (Uun Z=112). Because of the very short lifetimes it is impossible to detect by experiment even the basic states, ionization potential and other characteristics of these atoms. The theoretical (ab initio) methods require very accurate wave functions of heavy elements. That is why it is essential to further develop ab initio methods allowing to generate very accurate characteristics of atoms and ions, whose accuracy could compete or even exceed that of the experimental results.

In this presentation, the different methods, leading to the calculation scheme which allows us to perform the large scale theoretical studies of complex atoms and ions, are discussed. The approach is based on the multiconfiguration Dirack-Fock and relativistic configuration interaction methods [1] in which for calculations of spin-angular parts of matrix elements the second quantization method in coupled tensorial form and quasispin technique were adopted [2]. In case of complex electronic configurations, having several open shells, particularly open d- and f-shells, the main difficulties lie in calculations of the spin-angular parts of the relevant matrix elements of the operators considered. This phenomenon is even more pronounced if to extensively use the superposition of configurations methods, single and double excitations included. The use of the abovementioned second quantization and quasispin techniques, leading to triple tensors (in orbital, spin and quasispin spaces), enables to efficiently overcome these difficulties and to achieve the breakthrough in the field, to essentially increase the efficacy and the speed of the calculations, opening the possibilities to consider extremely complex electronic configurations leading to the matrices of very large orders. Their diagonalization requires the extremely large computing resources.

Non-relativistic and relativistic approaches are considered as well as the accounting for quantum electrodynamics effects. Various methods accounting for correlation effects are discussed, too. The universal computer codes to calculate the matrix elements for electric and magnetic multipole transition operators, having not-specified value of the gauge condition of the electromagnetic field potential, are written. They allow to study the general case of electronic transitions of any multipolarity.

A number of numerical results, obtained while using the above mentioned methods for heavy and superhavy atoms as well as for ions, are presented and discussed as the examples [3, 4]. They demonstrate the practical possibilities of theoretical studies of complex atoms and ions, the highly charged ions included as well as the prospects to efficiently generate various spectroscopic parameters of fairly high accuracy.

References

[1] Z. Rudzikas, *Theoretical Atomic Spectroscopy* (Cambridge university Press, 1997, 2nd ed. 2007) p. 427

[2] G. Gaigalas, Z. Rudzikas, C. Froese Fischer, J. Phys. B **30**, 3747 (1997)

[3] G. Gaigalas, E. Gaidamauskas, Z. Rudzikas, N. Magnani, R. Caciuffo, Phys. Rev. A **79**, 022511 (2009)

[4] G. Gaigalas, E. Gaidamauskas, Z. Rudzikas, N. Magnani, R. Caciuffo, Phys. Rev. A **81**, 022508 (2010)

Atomic data and modelling for fusion: The ADAS Project

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The paper is an update on the Atomic Data and Analysis Structure, ADAS [1], since ICAMDATA2006 and a forward look to its evolution in the next five years. ADAS is an international project supporting principally magnetic confinement fusion research. It has participant laboratories throughout the world, including ITER and all its partner countries. In parallel with ADAS, the ADAS-EU [2] Project provides enhanced support for fusion research at Associated Laboratories and Universities in Europe and ITER. OPEN-ADAS [3], sponsored jointly by the ADAS Project and IAEA, is the mechanism for open access to principal ADAS atomic data classes and facilitating software for their use. EXTENDED-ADAS comprises a variety of special, integrated application software, beyond the purely atomic bounds of ADAS, tuned closely to specific diagnostic analyses and plasma models.

The current scientific content and scope of these various ADAS and ADAS related activities are briefly reviewed. They span a number of themes including heavy element spectroscopy and models, charge exchange spectroscopy, beam emission spectroscopy and special features which provide a broad baseline of atomic modelling and support. Emphasis will be placed on 'lifting the fundamental data baseline' – a principal ADAS task for the next few years. This will include discussion of ADAS and ADAS-EU coordinated and shared activities and some of the methods being exploited.

References

[1] http://www.adas.ac.uk
[2] http://www.adas-fusion.eu
[3] http:/open.adas.ac.uk

Atomic data and their application in calculation of radiative properties of plasmas

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The Atomic and Molecular Data Research Center in the Institute of Applied Physics and Computational Mathematics have developed systemic code suites to calculate the atomic data including energy levels, cross sections and/or rate coeffcients for radiative transitions and electron collision with ions. Based on these data, codes were developed to calculate the radiative properties of both LTE and non-LTE plasmas in the framework of detail-configuration-accounting model and detail-level-accounting model. I will introduce the recent work of above aspects, as well as the recent activities of Chinese Research Association of Atomic and Molecular Data.

Recent database activities on basic plasma research

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Since the characteristics of plasmas depend strongly on the interactions between plasma particles such as electron, ion, and neutrals, a well-established atomic and molecular database is needed to understand and produce various types of plasma. Thus, here the work conducted at the Data Center for Plasma Properties over last 5 years on the systematic synthesis and assessment of fundamental knowledge on low-energy electron interactions with plasma processing gases is briefly summarized and discussed. This work mostly emphasis on the electron interaction processes.

Heavy particle collision data for fusion and astrophysics

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A wide range of applications, for example, diagnostics and modeling of fusion plasmas, interpretation of astronomical observations and modeling of astrophysical environments, and simulation of material processing plasmas, require large, accurate, and complete collections of electron, photon, heavy particle, and surface interactions. Consequently, over several decades, experimental and theoretical efforts have been developed in order to produce the required data, to drive the development and refinement of the techniques used to measure or calculate the data, and to explore the fundamental physical mechanisms that underlie interactions at the atomic scale.

In the present talk, I will illustrate some of the recent progress in the development of techniques and their use in describing heavy particle collisions, in particular those involving ions interacting with atoms and simple molecules, with specific applications of the resulting data in fusion energy and astrophysics. For example, interest in understanding recently observed X-ray emission from comets and from planetary atmospheres originating from ion-molecule charge transfer has motivated calculation of both large databases of required state-selective capture cross sections needed for modeling these environments (e.g., [1]), as well as more focussed comparison of theoretical data with measurements to serve as benchmarks for the calculations (e.g., [2, 3]).

Similarly, modeling light emission from radiative decay following charge transfer to excited states of ions in fusion devices has led to a valuable set of plasma diagnostics, motivating development of new theoretical treatments for several fundamental systems such as He^{2+} (from injected helium beams or born in the dt fusion) and Be^{4+} (originating from sputtered plasma-facing material) colliding with atomic hydrogen [4, 5]. Heavy particle collisions data is also needed, for example, for modeling transport in the cool, dense regions of plasma devices, spurring the need for large scale calculations of elastic and related transport cross sections (e.g., [6] and references therein), and providing another illustration of the production of large data sets needed in plasma science applications.

References

[1] Y. Hui, D.R. Schultz, V.A. Kharchenko, A. Bhardwaj, G. Branduardi-Raymont, P.C. Stancil, T.E. Cravens, C.M. Lisse, and A. Dalgarno, Journal of Geophysical Research **115**, A07102 (2010).

[2] R. Ali, P.A. Neill, P. Beiersdorfer, C.L. Harris, D.R. Schultz, and P.C. Stancil, The Astrophysical Journal **716**, L95 (2010).

[3] J. Simcic, D.R. Schultz, R.J. Mawhorter, I. Čadež, J.B. Greenwood, A. Chutjian, C.M. Lisse, and S.J. Smith, Phys. Rev. A **8**1, 062715 (2010).

[4] T. Minami, T-G. Lee, M.S. Pindzola, and D.R. Schultz, J. Phys. B **41**, 135201 (2008).

[5] T. Minami, M.S. Pindzola, T-G. Lee, and D.R. Schultz, J. Phys. B **39**, 2877 (2006).

[6] P.S. Krstić and D.R. Schultz, Physics of Plasmas **16**, 053503 (2009).

Quantum electrodynamics effects in heavy ions and atoms

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Quantum electrodynamics theory of heavy ions and atoms is considered. The current status of calculations of the binding energies, the hyperfine splittings, and the g-factor values in heavy few-electron ions is reviewed. The theoretical predictions are compared with available experimental data. A special attention is focused on tests of quantum electrodynamics in strong electromagnetic fields and on determination of the fundamental constants. Recent progress in calculations of the parity nonconservation effects with heavy atoms and ions is also reported.

Accurate cross-section calculations for low-energy electron–atom collisions

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The low-energy electron scattering from atoms and ions, which is often dominated by resonance structure, proves to be very challenging to both theory and experiment. Over the past decade, we have developed a highly flexible B-spline R-matrix (BSR) method [1] that has some advantages compared to the standard R-matrix (close-coupling) approach. The two essential refinements are (i) the removal of orthogonality restrictions, which allows for the use of nonorthogonal orbital sets to represent both the bound and continuum one-electron orbitals, and (ii) the use of B-splines as a universal and effectively complete basis to generate the R-matrix functions. These features often allow us to achieve a high accuracy in the description of the target states, as well as a truly consistent description of the scattering system. The BSR code, in both its non-relativistic and semi-relativistic (Breit-Pauli) forms, was successfully applied to many problems of electron collisions from atoms and ions, including photoionization and photodetachment, and often considerable improvements were obtained in comparison to previous calculations.

Relativistic effects are well known to be crucially important in the treatment of electron scattering from heavy targets. In the present talk we report an extension of the BSR complex to the fully relativistic Dirac scheme. It was described in detail in recent applications to e-Cs [2] and e-Hg [3] collisions. The new DBSR code retains all the advantages of the previous semi-relativistic version, including its generality as an all-electron code and the flexibility associated with the use of nonorthogonal orbital sets. The application of the fully relativistic scheme allowed us to obtain, for the first time, close agreement with experiment for electron scattering from such complex targets as Kr and Xe. Illustrative examples are also presented for recent applications of the DBSR code to valence and core excitation of Au and Cu, as well as elastic scattering from Pb and I.

These example results exhibit the flexibility of the B-spline R-matrix method to describe both the N-electron target and the $(N+1)$-electron collision problems, which is of critical importance for obtaining highly accurate cross sections, particularly in the low-energy regime. The relativistic *ab initio* calculations of electron collisions with complex targets are computationally very extensive and were performed with parallelized versions of the DBSR code.

References

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

[2] O. Zatsarinny and K. Bartschat, Phys. Rev. A **77**, 062701 (2008)

[3] O. Zatsarinny and K. Bartschat, Phys. Rev. A **79**, 042713 (2009)

Cold light from hot atoms

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From the time man made his first steps on earth, he has been fascinated by light. Early man relied on light from the sun for his daily activities, and the moon and stars provided the only relief from darkness at night. From the time he first learned to tame fire to provide the first artificial light, mankind has constantly striven to improve the quality of light to assist his ever increasing needs as civilization developed. At the same time, his fascination with the stars led him to develop more sophisticated equipment to observe and understand them. Today's sophisticated technology allows us to manufacture miniature lamps in ceramic vessels, and to reach ever further into space to investigate our stellar neighbors. One of the important aspects of the development of both technologies has been an understanding of one section of the periodic table, the rare earth elements. The need for reliable atomic an spectral data has led to a fruitful collaboration between the astrophysical and lighting research communities over the last decade. There is an ever growing need for fundamental data, and this talk will discuss some applications of such data on the Mega and miniature scale.

Rare earth atoms such as Dy, Ho and Ce provide excellent radiation sources for lighting applications, [1] with strong radiation bands in the visible spectrum, such that a suitable combination of these elements can provide high quality white light. The relatively low ionization threshold of these atoms ($\sim$5 eV) means that a high electron density discharge can be readily produced, provided sufficient rare earth atoms are present in the gas phase. This is achieved by heating metal halide salts to a high temperature (>1300 K) at the wall the lamp, to provide sufficient vapor above the molten salts to allow the molecules to dissociate into atoms at the axis of the discharge ($\sim$5000 K) . The process is enhanced if the wall temperature can be increased, without melting or damaging the wall, and this can be achieved using a ceramic material, such as polycrystalline alumina (PCA). Optimization of lamp performance relies on an improved understanding of the discharge properties, including thermo-chemical, transport and spectral data.

Rare earth elements also have important advantages for astrophysical observations [2]. The open f-shells of these elements yield a rich energy level structure with many low lying even- and odd-parity levels. This level structure results in a very rich visible spectrum which is accessible to ground based telescopes. Elemental abundance values can be determined from many spectral lines, at least some of which are very clean (unblended) and of near ideal strength. The ideal strength length >spectral line is strong enough to have a good S/N ratio, but not so strong as to be saturated. The papers by Sneden *et al.* and Lawler *et al.* summarize more than a decade of work on rare earth ions which has yielded a robust r(apid)-process n(eutron)-capture abundance pattern. The pattern is the same in the Sun (from subtracting the modeled s-process pattern from total abundance values) and five r-process rich metal-poor Galatic halo stars. This pattern provides a powerful constraint for future efforts at modeling the r-process.

References

[1] G. G. Lister, J. E. Lawler, W. Lapatovich and V. Godyak, Rev. Mod. Phys. **76**, 541 (2004)
[2] J. E. Lawler, C. Sneden, J. J. Cowan, I. I. Ivans and E. A. den Hartog, Astron. J. Suppl. Ser. **182**, 51 (2009)

Atomic and molecular collisional radiative modelling for spectroscopy of both low temperature and magnetic fusion plasmas

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The robust and easy-to-use diagnostic tool of emission spectroscopy is a widely used in many plasma applications. For the determination of plasma parameters such as electron density, electron temperature and particle fluxes the quantitative analysis of measured atomic or molecular photon fluxes requires an appropriate population model. Low temperature, low pressure plasmas used in industrial applications and the cold plasma edge of magnetically confined fusion plasma are described by collisional radiative (CR) models which balance excitation and de-excitation mechanisms of the excited states of the particle. Re-absorption of emission lines, i.e. opacity, can be taken into account by introducing escape factors. The densities of the ground state and the ion(s) are determined by mainly by diffusion; thus these densities typically are assumed to be constant and are used as input parameters for such a CR model. The accuracy of CR models depends strongly on the availability and accuracy of the input date, i.e. the cross sections and rate coefficients for the individual processes. In order to solve the corresponding rate equations the flexible solver Yacora has been developed which is also capable to couple different heavy particles to the excitation and treat heavy particle collisions [1]. The usage of cross sections allows studying the influence of the electron energy distribution on the results.

Yacora has been used to construct CR models for several atoms such as H, He, Ar, and for diatomic molecules such as H_2, N_2, CH, BeH, BH most of them for interest to both the low pressure plasmas and the fusion plasma edge. For the latter isotope effects in CR models for molecules are studied as well.

Of particular relevance to many applications is the CR model for hydrogen in which the model for molecular hydrogen is linked to the model of atomic hydrogen. Both models have been benchmarked individually by experimental data from dedicated laboratory experiments. The coupling allows the quantification of dissociative excitation on Balmer line emission which is of importance in plasmas with low dissociation degree [2]. The transition from ionising to recombining plasmas is studied on the example of divertor plasmas of fusion experiments and linear divertor plasma devices for plasma wall interaction studies as well as ion sources which rely on the tandem concept. The influence of the dissociative recombination on data interpretation will be highlighted. By coupling the CR model to negative hydrogen ions via the mutual neutralisation process, a diagnostic tool for negative hydrogen ions in ion sources is developed [3].

References

[1] D. Wünderlich, S. Dietrich, U. Fantz, J. Quant. Radiat. Spec. Trans. **110**, 62 (2009)

[2] K. Behringer, U. Fantz, New J. Phys. **2**, 23 (2000)

[3] U. Fantz, D. Wünderlich, New J. Phys. **8**, 301 (2006)

Recent investigations of heavy elements. Results and needs

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The investigation of the atomic structure of the lanthanide ions is often prevented by the complexity of the configurations involved implying an open 4f-shell. Their knowledge however is vital and strongly needed in astrophysics in relation with problems of abundance determination, cosmochronology and nucleosynthesis, these elements appearing frequently overabundant in CP stars.

In order to clarify the relative importance of the r and s processes for the production of heavy elements in the Galaxy, the astrophysicists need also accurate atomic data (transition probabilities, oscillator strengths, radiative lifetimes, ...) particularly for the heavy elements belonging to the sixth row of the periodic table. An element like tungsten, which is important for thermonuclear fusion research because it is used as a delimiter in Tokamak devices, belongs also to this group.

The heavy refractory elements of the fifth row, frequently difficult to produce in the laboratory, require also further investigations, many gaps subsisting concerning the available atomic data.

For these reasons, we have decided to start a systematic investigation of the radiative properties (oscillator strengths, A-values, lifetimes, branching fractions, Lande factors,...) of these three groups of elements (more precisely, the first three ionization stages have been considered) combining the experimental determination of lifetimes with theoretical calculations of branching fractions. About 650 lifetimes have been measured by TR-LIF spectroscopy at the Lund Laser Centre, in Sweden, for the elements Rb to Xe, Cs to Rn and for the lanthanides and, in many cases, the corresponding branching fractions have been calculated using a Relativistic Hartree-Fock approach modified for inclusion of core-polarization effects [1, 2].

This combination of lifetime measurements with theoretical (and, when possible, experimental) branching fraction determination has led to transition probabilities for about 65 000 (lanthanides) and 13 000 transitions (fifth and sixth rows of the periodic table), respectively. These new results are stored in two databases, DREAM [3] and DESIRE [4], which are regularly updated on web sites of Mons University in Belgium.

We will present, during the meeting, a summary of the results obtained so far and we will illustrate the difficulties encountered and the success met by considering a few specific cases.

References

[1] É. Biémont and P. Quinet, Phys. Scr. **T105**, 38 (2003)

[2] É. Biémont, Phys. Scr. **T119**, 55 (2005)

[3] É. Biémont, P. Palmeri and P. Quinet, Astrophys. Space Sci. **269-270**, 635 (1999); http://www.umh.ac.be/∼astro/dream.shtml

[4] V. Fivet, P. Quinet, P. Palmeri, É. Biémont and H.L. Xu, J. Electron. Spectrosc. Relat. Phenom. **156-158**, 250 (2007); http://www.umh.ac.be/∼astro/desire.shtml

Importance of atomic data for precision physics of simple atoms, determination of fundamental constants and search for their variations

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Determination of values of fundamental constants and precision tests of fundamental theories, such as bound-state quantum electrodynamics, need various atomic, nuclear and molecular data. In my talk I will discuss which data are necessary for that and what is specific requirement for them.

Meantime, another area related to the fundamental constants, where precision atomic and molecular data are needed is search for variation of fundamental constants. Specific needs of this area will be also presented in my talk.

Radiative transition probabilities in neutral cerium and the problem of complete data sets for complex spectra

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The complex spectra of rare-earth elements and the use of rare-earth spectroscopic data in the lighting industry present a somewhat different set of requirements for data producers than those to which they may be accustomed. Of course, the most accurate data values are desirable. However, the lighting industry's goal of simulating low-resolution spectral distributions of radiant power emitted by proposed discharge lamp designs also demands that the data set be sufficiently complete[1]. In this case, missing values can be just as deleterious as major errors in values that are present. The usefulness of a data set depends on both the accuracy of individual lines *and* the completeness of the set.

For complex spectra, like those of the rare-earths, achieving completeness can be a daunting task. Neutral cerium, of considerable recent interest in the lighting industry, is only partially described by a classified line list containing some 20,000 lines [1]. Lawler and co-workers [2] at the University of Wisconsin have just published a list of high-quality transition probabilities in neutral cerium for nearly 3000 lines. This is a prodigious output, but clearly far smaller than the enormous extent of this spectrum.

For some applications, the complexity of a spectrum naturally compensates for random/uncorrelated errors in individual data values. For complex spectra in which there may be 10, 20, or 30 significant lines within a 1 nm span (more than sufficient spectral resolution for many applications), the error in the total radiant power in that span may be as much as 3, 4, or 5 times smaller than the random uncertainty in the individual lines.

As a possible path to obtaining a considerably larger data set of radiative transition probabilities for neutral cerium, we are measuring relative line intensities in high-resolution Fourier transform spectra acquired in the mid-1980s by Conway and co-workers [3]. Plotting $\ln \frac{I_\lambda \lambda}{g_u A_{ul}}$ *vs* E_u for the lines measured by Lawler [2], we obtain an intensity scale and discharge temperature from a linear least-squares fit to the data under the assumption that the line intensities can be described by a Boltzmann model

$$I_\lambda \propto \frac{g_u A_{ul}}{\lambda} \exp \frac{-E_u}{kT} \tag{1}$$

where I_λ is the intensity of a line of wavelength λ, A_{ul} is the radiative transition probability between upper level u and lower level l, g_u and E_u are the degeneracy and energy of the upper level, k is Boltzmann's constant, and T is the excitation temperature that best describes the data.

The small uncertainty that we obtain for the temperature (less than $\pm$ 1 %) indicates that the Boltzmann model is a suitable description for at least some of these spectra. Using the temperature and intensity scale we obtained from the fitting process, we are obtaining additional radiative transition probabilities from intensities of lines not measured by Lawler [2]. We will report on our progress in terms of the completeness of the data set and the estimated uncertainties.

References

[1] W. C. Martin, unpublished

[2] J. E. Lawler et al., J. Phys. B: At. Mol. Opt. Phys. **43**, 085701 (2010)

[3] Available at http://nsokp.nso.edu/

[1] It is recognized that this term may only defined by the application.

Coordinated research projects of the IAEA Atomic and Molecular Data Unit

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The Atomic and Molecular Data Unit, part of the Nuclear Data Section at the IAEA, is dedicted to the provision of databases for atomic, molecular and plasma-material interaction data that are relevant for nuclear fusion research [1]. As part of this work the Unit encourages new research, and the principal mechanism for that purpose is the Coordinated Research Project (CRP). These projects normally run for about 4 years and involve 10-15 research groups that are carrying out research towards a shared goal, which is usually the development of data for a well-defined class of A+M/PMI processes. Participants meet 3 times at about 1.5-year intervals over the course of the CRP for a Research Coordination Meeting (RCM). Meeting reports and, in many cases, presentation materials may be found through the CRP web pages [2]. Ongoing and planned CRPs include the following:

- *Data for surface composition dynamics relevant to erosion processes.* This CRP (2007-2011) is concerned with the behavior of mixed materials, such as C-Be-W, in a fusion vacuum vessel. The 3rd and final RCM is planned for 13-15 September 2010.
- *Characterization of size, composition and origins of dust in fusion devices.* (2008-2012.) Dust from plasma-material interaction and tritium retention in dust are concerns for ITER and for a reactor.
- *Light element atom, molecule and radical behavior in the divertor and edge plasma regions.* (2009-2013.) Concerned with data for collisional processes of molecules and molecular ions, especially hydrides, of first row elements.
- *Spectroscopic and collisional data for tungsten from 1 eV to 20 keV.* (2010-2014.) Dedicated to data for collisional and radiative properties, including electron impact and heavy particle collisions. The 1st RCM is scheduled for Dec 2010.
- *Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma.* The proposal for this CRP (2011-2015) is being prepared. The focus will be on processes of rovibrationally excited states of the molecules and molecular ions.

Beyond these we anticipate a CRPs on erosion and tritium retention of beryllium surfaces, one on PMI for tungsten alloys and irradiated tungsten, and one on kinetic modelling of hydrocarbons in plasma. Highlights of the ongoing CRPs and plans for future CRPs will be descibed in the talk.

References

[1] http://www-amdis.iaea.org/
[2] http://www-amdis.iaea.org/CRP/

Detailed atomic structure of neutral or near-neutral atomic systems

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An accurate treatment of electron correlation is crucial in the calculation of atomic properties. When wave functions are expressed in terms of expansions of configuration state functions, the convergence of the results can be very slow, particularly for systems close to the neutral end of an isoelectronic sequence. Away from the neutral end, a limited CI expansion is often sufficient, if the configurations are chosen wisely. Again, even for near-neutral elements, properties such as oscillator strengths can be determined with some degree of convergence, for transitions between energetically low-lying levels. But many transitions of interest involve more highly excited levels in moderately heavy ions (see, for example [1]). In the process of obtaining wave functions for these levels, it is necessary also to obtain wave functions for all lower-lying levels, so the calculation can become enormous. There is an inevitable compromise between size and accuracy. Some amelioration of the situation can be achieved by the use of extrapolation techniques, in order to attempt to improve the accuracy of the final results without increasing the size of the calculation.

In the talk, we will discuss some of those methods in the context of specific calculations of neutral and singly ionised systems. One example will be a series of calculations we have undertaken [2] for neutral chlorine. There had been persistent, but unresolved, interest in the identification and relative strengths of the lines of astrophysical interest at $\lambda\,1088, 1097$. Previous theoretical [3–6] work had been hampered by the strong CI mixing of the upper levels of the transitions, while experimental [7] or observationally derived [8, 9] oscillator strengths were not in sufficient agreement with each other or with the calculations to provide a clear guide. Our calculations show that a further line at $\lambda\,1095$ needs to be taken into account and results in a different assignment of state labels to the upper levels of the transitions, as well as affecting the calculated oscillator strengths. Further experimental analysis has recently been carried out at NIST [10] and we shall discuss the implications.

We will also point to two posters being presented at the conference, on Fe II (important for its astrophysical implications) and on Sn II (of relevance to impurity diagnostics in plasmas), where strong CI mixing is a critical factor in obtaining accurate results.

References

[1] G. Corrégé, A. Hibbert, ApJ **636**, 1166 (2006)
[2] P. Oliver, A. Hibbert, J. Phys. B **40**, 2847 (2007)
[3] C.F. Fischer, G. Tachiev, A. Irimia, Atom. Data Nucl. Data Tables **92**, 607 (2006)
[4] P.C. Ojha, A. Hibbert, Phys. Scr. **42**, 424 (1990)
[5] E. Bièmont, R. Gebarowski, C.J. Zeippen, Astron. Astrophys. **287**, 290 (1994)
[6] N. Singh, A.K.S. Jha, M. Mohan, Astron. Astrophys. **328**, 285 (2006)
[7] R.M. Schectman, S.R. Federman, D.J. Beideck, D.G. Ellis, Astrophys. J. **406**, 735 (2006)
[8] S.R. Federman, Astrophys. J. **309**, 306 (1986)
[9] P. Sonnentrucker, S.D. Friedman, D.G. York, Astrophys. J. **650**, L115 (2006)
[10] J.M. Bridges, W.L. Wiese, Phys. Rev. A **78**, 062508 (2008)

Posters, session A

NIST atomic and molecular databases and the UnitsML markup language

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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 [1].

In collaboration with the Atomic Physics Division the databases available online include:

- Fundamental Physical Constants Database
- Electron-Impact Ionization Cross Section Database
- Handbook of Basic Atomic Spectroscopic Data
- NLTE Databases and Codes

Databases recently updated include:

- The Atomic Spectra Database
- Bibliographic Database on Atomic Transition Probabilities
- Bibliographic Database on Atomic Spectral Line Broadening and Shifts
- Bibliographic Database on Atomic Energy Levels and Spectra

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

ECSED has started a collaboration with Lawrence Berkeley National Laboratory to develop an XML (eXtensible Markup Language) schema for encoding measurement units in XML [2]. Adoption of this schema will allow for the unambiguous exchange of numerical data over the World Wide Web.

References

[1] http://physics.nist.gov/data

[2] http://unitsml.nist.gov

Progress on atomic transition probabilities for weak spectral lines

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Critical data compilations of the National Institute of Standards and Technology (NIST) [1, 2] have shown that uncertainties for the atomic transition probabilities of weak lines are usually much larger than for strong lines. This is clearly seen in a number of graphical comparisons in these tabulations for data from various sources. Recently, new sophisticated atomic structure codes, with very extensive multi-configuration treatments, have been developed and applied to strong and weak transitions [3, 4]. For many weak transitions, the numerical differences between the dipole length and dipole velocity forms of the transition integral have been greatly reduced. To test a few of the results, we have carried out emission measurements of spectral line intensities for several weak N I, Cl I, and Ne II lines [5–7]. For the strong, persistent lines in these spectra, we found excellent agreement with other recent measurements and the new calculations, so that these values are accurately established and may serve to establish reference scales. We then focused our measurements on lines that are weaker by factors in the range from 10 to 100, and for which substantial disagreements among earlier experimental and theoretical data were observed. In our work, critical factors have been the accurate determination of the often large continuum background under the weak lines and the de-convolution of the weak lines with the extended wings of strong neighboring lines. This sometimes required the use of order-separation filters, a detail that was not always included in earlier work. The agreement between our new measurements and the recent advanced structure calculations is indeed greatly improved, as will be shown in several comparison graphs and tables.

References

[1] W. L. Wiese, J. R. Fuhr and T. M. Deters, J. Phys. Chem. Ref. Data, Monograph 7 (1996)

[2] W. L. Wiese and J. R. Fuhr, J. Phys. Chem. Ref. Data **36**, 1287 (2007)

[3] C. F. Froese Fischer and G. Tachiev, At. Data Nucl. Data Tables **87**, 1 (2004)

[4] P. Oliver and A. Hibbert, J.Phys. B: At. Mol. Opt. Phys. **40**, 2847 (2007)

[5] J. M. Bridges and W. L. Wiese, Phys. Rev. A **76**, 022513 (2007)

[6] J. M. Bridges and W. L. Wiese, Phys. Rev. A **78**, 062508 (2008)

[7] J. M. Bridges and W. L. Wiese, to be published

State of the development of the STARK-B database in the framework of the European Project VAMDC (Virtual Atomic and Molecular Data Center)

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Stark broadening theories and calculations have been extensively developed for about 50 years. The theory can now be considered as mature for many applications, especially for accurate spectroscopic diagnostics and modelisation. This requires the knowledge of numerous collisional line profiles, especially for very weakly abundant atoms and ions which are used as useful probes for modern spectroscopic diagnostics. Nowadays, the accces to such data via an on line database becomes indispensable.

STARK-B [1] has been a collaborative project between the Astronomical Observatory of Belgrade and the Laboratoire d'Etude du Rayonnement et de la matière en Astrophysique (LERMA) for a few years. It is a database of calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions (i.e. impacts are separated in time). This database is devoted to modelisation and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is relevant to laboratory plasmas, laser equipments and technological plasmas. Hence, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion.

STARK-B is a part of VAMDC [2]. VAMDC (Virtual Atomic and Molecular Data Centre) is an European Union funded collaboration between groups involved in the generation and use of atomic and molecular data. VAMDC aims to build a secure, documented, flexible and interoperable e-science environment-based interface to existing atomic and molecular data.

STARK-B has been fully opened since September 2008 though not yet complete. We will present the advancement of its development at the Conference.

References

[1] http://stark-b.obspm.fr

[2] http://www.vamdc.eu

The MCHF/MCDHF Database, Version 2

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The MCHF/MCDHF Database [1] is a collection of transition energies ΔE, line stregths S, oscillator strengths f_{ik}, and transition probabilities A_{ki} from "spectrum" calulations in which the same computational procedure is used to obtain for all levels up to a given excited level. The database facilitates the evaluation of different procedures for accuracy. Two indicators of accuracy are the agreement with observed ΔE or wavelengths and the discrepancy in the length and velocity form of the line strength. The two forms are only available for the electric multipole transitions but they are the sole indicator when observed ΔE are not available.

Version 2 [2] has implemented some important improvements and options. Theoretical calculations of A_{ki} and f_{ik} are often based on computed values. The line strength S is the preferred property for comparison but experimental data usually provides A_{ki} or f_{ik} values or possibly branching fractions. Since the A_{ki}i rate for an E2 transition, for example, depends on ΔE^5, errors in ΔE can result in large fluctuations in reported A_{ki} rates. In the present version, the user may request data be recomputed with the observed ΔE and displayed according to sorting options. Some new data for ionizated atoms has also been included.

Theoretical data is often classified according to the method or code used for the calculation. More important is the correlation that has been included. Figure 1. shows how the length and velocity forms of S for the $3p^2\ {}^3P_2$–$^1D_2$ E2 transition in Fe^{+12} change as the set of orbitals that represent corrections to the wave function is increased from $n = 3$ to $n = 7$ [3]. Many early calculations were some form of $n = 3$ calculations, others using similar codes were n=5 calculations. Clearly evident is the improvement in the agreement between the length and velocity form of the line strength. Because a limited computational strategy may not converge to the observed ΔE, Figure 1. also shows the velocity form when adjusted for the observed transition energy.

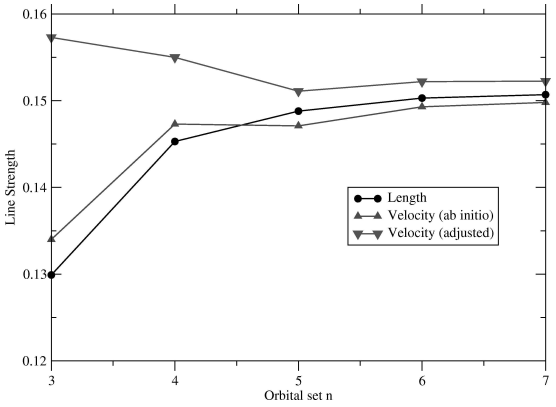

Figure 1: Trends in length and velocity forms of S for the $3p^2\ {}^3P_2$–$^1D_2$ E2 transition in Fe^{+12} as a function of the orbital set.

References

[1] http://atoms.vuse.vanderbilt.edu/, MCHF/MCDHF Database, Version 1

[2] http://nlte.nist.gov/MCHF/, MCHF/MCDHF Database, Version 2

[3] C. Froese Fischer, J. Phys. B: At. Mol. Opt. Phys. **43**, 074020 (2010)

Production of atomic data using relativistic multiconfiguration methods

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GRASP2K is a package for large scale relativistic atomic structure calculations based on the multiconfiguration Dirac-Hartree-Fock theory [1]. By an extensive use of default options, together with a naming convention for the files, the package is user friendly with a minimum of input data. However, a large number of non-default options can still be invoked when the need arises. The package implements a biorthogonal transformation method that permits initial and final states in a transition array to be optimized separately, which, in many cases, leads to more accurate values of the resulting rates [2]. In addition to energy structures and transition rates a number of other properties such as hyperfine structure, isotope shift, and splittings in external magnetic fields can be computed [3].

To illustrate the potential and restriction of the package for large scale production of atomic data we present results for a number of systems and properties. Among the properties are energies, g_J factors, hyperfine structure, isotope shifts, and transition rates in oxygen, carbon, and boron-like ions [4,5,6].

References

[1] P. Jönsson, X. He, C. Froese Fischer and I.P. Grant, Comput. Phys. Commun. **177**, 597 (2007)

[2] J. Olsen , M. Godefroid, P. Jönsson, P.Å. Malmqvist and C. Froese Fischer, Phys. Rev. E **52**, 4499 (1995)

[3] M. Andersson and P. Jönsson, Comput. Phys. Commun. **178**, 156 (2008)

[4] P. Jönsson, J. Li, G. Gaigalas, and C. Dong, At. Data Nucl. Data Tables **96**, 271 (2010)

[5] P. Jönsson and J. Bieroń, J. Phys. B: At. Mol. Opt. Phys. **43**, 074023 (2010)

[6] P. Jönsson, P. Rynkun, and G. Gaigalas, At. Data Nucl. Data Tables, in press (2010)

The iron wolf of Vilnius howls about iron II

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According to legend, Vilnius was founded after the Grand Duke of Lithuania dreamt of an iron wolf howling on a hilltop at the site of the city. In this poster we explain why the iron wolf is still howling about his native material.

The Vienna Atomic Line Database (VALD), an on-line resource which offers easy access to atomic data such as oscillator strengths for literally millions of spectral lines, is of immense value and importance to stellar spectroscopy. Of the many data sets included in this database, those for neutral and once ionised iron are certainly among the most important because of the large number of iron lines in the optical and UV spectra of most stars. VALD includes data from a number of major experiments and computations for Fe II. These data have in general a fairly good level of overall agreement, but do not agree within their stated uncertainties. It is not clear which data to prefer. Further, for astrophysical spectroscopy it is very important to have sets of oscillator strengths that have overall consistency, so selecting data one spectral line at a time from various not fully consistent experiments leads to poor fits to observed spectra, to further uncertainties in the derived abundance of this very important element, and to uncertainties in other stellar parameters derived or tested using Fe II.

To try to improve the situation, we have constructed two new globally averaged datasets of oscillator strengths of Fe II. One is calibrated to the most recent large set of experimental data [1] and the other to the very large computational dataset of Raassen and Uylings ([2] - RU). Our procedure has been to make a linear fit and correction of other recent data to the fundamental calibration set as a function of $\log gf$, and then create from all renormalised recent data a single weighted average calibration dataset. It is found that the various data sets generally agree well for large $\log gf$ values (around 0) but diverge at the 0.1 or 0.2 dex level for small values (around -2 or -3). This renormalisation has also allowed us to estimate the uncertainties of relative $\log gf$ values in datasets without stated uncertainties, and to test the uncertainties claimed by datasets with errors.

Finally we created two weighted average sets of about 150 $\log gf$ values of Fe II ranging in wavelength from 2250 to 7700 Å, and in oscillator strength from +0.5 dex to -4.1 dex. These two alternative datasets are found to differ at roughly the 0.1 dex level over much of the range in $\log gf$, and, in paticular, in the optical region, for lines that are used in stellar abundance analysis. Both datasets have been tested for internal consistency by being used in Fe I/II analysis in the atmospheres of few stars: the Sun (5777 K), β Vir (6060 K), HD 49933 (6500 K), Procyon (6510 K), 21 Peg (10400 K), and π Cet (12800 K), with accurately known atmospheric parameters. Lines of Fe I with experimentally measured oscillator strengths were employed. Although both sets of Fe II $\log gf$ values provide standard deviations in abundance results which are compatible with the uncertainties of individual $\log gf$ values (mostly of order 0.05 dex) we find that all stars but Procyon are closer to Fe I/Fe II ionization equilibrium with the RU-calibrated set of Fe II oscillator strengths, while with the Schnabel-calibrated set of data the difference between Fe I and Fe II reaches 0.1 dex. Our results clearly show an urgent need for new accurate laboratory analysis of the optical Fe II lines.

References

[1] R. Schnabel, M. Schultz-Johanning, M. Kock, A&A **414**, 1169 (2004)

[2] A.J.J. Raassen, P.H.M. Uylings, A&A **340**, 300 (1998)

VAMDC: atomic data production, curation, management and preservation in data-intensive e-science

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As we are well aware, information and communication technologies have had a profound effect on scientific research in the past 30 years. In fact we are beginning to talk now of a new way of doing science, "e-science", characterized by globally distributed data-intensive collaborations on a second-generation Internet [1]. In this context, an international project has been recently launched to develop the Virtual Atomic and Molecular Data Center (VAMDC) [2, 3, 4], aiming to integrate and upgrade several distributed atomic and molecular (A&M) databases so as to cope with the increasing data demands from a new breed of clients: virtual organizations (e.g. the International Virtual Observatory Alliance [5]) and scientific social networks (e.g. MyExperiment [6]).

Inspired by the pioneering Opacity Project [7] and Iron Project [8] long-term atomic data production consortia, and under the VAMDC umbrella, we are currently exploring approaches in grid environments to produce and curate massive radiative and collisional data sets for complete isonuclear sequences, in particular of the iron group. In this respect, application deployment (for instance, for the atomic structure code AUTOSTRUCTURE [9], the *R*-matrix suite for electron–ion scattering [10] and atomic database-centric spectral modeling codes such as XSTAR [11]) is bound to evolve from the Unix shell to cloud-computing web services (e.g. SOAPLAB2 [12]) and workflows (e.g Taverna [13]). A&M data exchange is destined to become XML-based (see the newly proposed XSAMS A&M schema [14]), carrying comprehensive metadata to ensure data provenance, usability and preservation in diverse user communities. Moreover, we believe that the workflow will soon accompany the scientific publication as the blueprint of a verifiable and adaptable scientific method, and it will also become an essential tool in data-mining networks, the cornerstone of the new scientific paradigm.

References

[1] T. Hey, S. Tansley, K. Tolle (eds.), *The Fourth Paradigm: data-intensive scientific discovery* (Microsoft Research, Redmond, WA, USA 2009)
[2] C. Mendoza, L.A. Núñez, in *Proceedings of the First EELA-2 Conference* (Editorial CIEMAT, Madrid, Spain 2009) p. 219
[3] M.L. Dubernet, et al., J. Quant. Spectrosc. Radiat. Transfer, in press
[4] http://www.vamdc.org/
[5] http://www.ivoa.net/
[6] http://www.myexperiment.org/
[7] http://cdsweb.u-strasbg.fr/topbase/op.html
[8] http://www.usm.uni-muenchen.de/people/ip/iron-project.html
[9] N.R. Badnell, J. Phys. B **19**, 3827 (1986); **30**, 1 (1997)
[10] K.A. Berrington et al., Comput. Phys. Commun. **14**, 367 (1978)
[11] M.A. Bautista, T.R. Kallman, Astrophys. J. Suppl. Ser. **134**, 139 (2001)
[12] http://soaplab.sourceforge.net/soaplab2/
[13] http://www.taverna.org.uk/
[14] http://www-amdis.iaea.org/xsams/about.html

BASECOL and VAMDC: A new way to access and manipulate molecular collisional data for interstellar applications

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Understanding the language of Interstellar Molecules requires to combine observations and modelling of interstellar media. Many software applications have been or are being developed in order to analyse spectra (CASSIS project [1], CATS project [2], STARFORMAT[3]). These applications rely heavily on the knowledge of molecular spectroscopy data such as those found in the CDMS [4] and JPL [5] databases, and collisional excitation rate coefficients such as those found in BASECOL [6, 7].

The usual difficulty met by astrophysical users is to combine data from these different databases. Combination of data implies the possibility to match molecular states that are very often described differently in JPL, CDMS and BASECOL. In order to overcome this problem BASECOL has imported spectroscopic data from JPL/CDMS, for each molecule scientific work was done locally in order to transform CDMS/JPL molecular description into BASECOL internal description, and then a complete and coherent set of data including spectroscopic and collisional data were prepared for the users. This required lengthy manipulation of data for each individual molecule, that should not be necessary any more within the VAMDC [8,9] infrastructure.

VAMDC infrastructure implies an output of databases into an unified format for description of data, the possibility of finding resources through registries using unified query language and finally integrating different sets of data from different databases. The VAMDC's activities are based on the use of an XML schema XSAMS (XML Schema for Atomic & Molecular Spectroscopy) [10] which has been developed under the auspices of the IAEA and aims to describe atomic, molecular and particle-surface interaction data in distributed databases around the world. Molecular part of XSAMS is currently being improved within the VAMDC consortium. The specific case of BASECOL and CDMS/JPL within the context of astrophysical applications will be presented in this paper.

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References

[1] http://cassis.cesr.fr/

[2] http://www.astro.uni-koeln.de/projects/schilke/PublicCATS

[3] http://astro.ens.fr/index.cgi?exe=139434&xar=

[4] http://www.astro.uni-koeln.de/cdms

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

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

[7] M.L. Dubernet et al., Ro-vibrational Collisional Excitation Database BASECOL Proceedings Joint Meeting ITC14 and ICAMDATA 2004, Toki, Japan. Journal of Plasma and Fusion Research SERIES 2006;7:356-57

[8] M.L. Dubernet, et al., 2010, JQSRT, in Press; http://dx.doi.org/10.1016/j.jqsrt.2010.05.004

[9] http://www.vamdc.eu

[10] M.L. Dubernet, D. Humbert, R.E.H. Clark, Yu. Ralchenko, E. Roueff, D.R. Schultz, *XSAMS: XML schema for Atomic, Molecular and Solid Data*, eds. Dubernet M.L., Humbert D., Ralchenko Yu., Version 0.1, September 2009; http://www-amdis.iaea.org/xml/

Cross sections for charge changing collision of W ions as well as heavy particle impact cross section database

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We have measured electron capture cross sections for W^+ and W^{2+} ions colliding with He, Ne, Ar, Kr, H_2, N_2, CH_4, C_2H_6, C_3H_8 atoms or molecules at 5–15 keV. Measured cross sections show power-law dependence on the target first ionization potential, as have been demonstrated for collisions of light or medium ions of Be, B, C, Fe, Ni and so on [1], implying a possibility that electron capture of heavy and clothed ions could be understood as a distant crossing of "potentialed" particle with neutral targets. We have been also devoted to compilation of experimentally-derived charge changing cross sections for ion-atom collisions published in journals of our selection. A part of compiled data can be accessed online [2] through SQL queries.

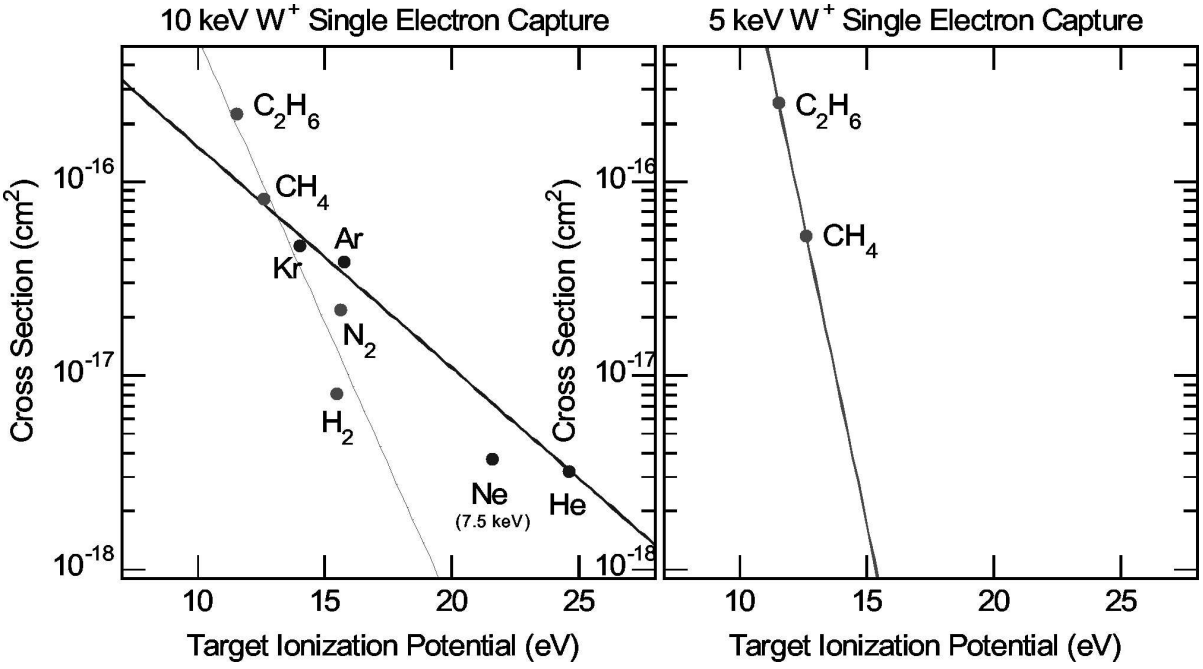

Figure 1: Single electron capture cross sections for W^+ ion colliding with gaseous targets, plotted against the first ionization potential of targets.

References

[1] M. Imai, T. Shirai, M. Saito, Y. Haruyama, A. Itoh, N. Imanishi, F. Fukuzawa and H. Kubo, J. Plasma Fusion Res. Ser. **7**, 323 (2006)

[2] http://toshi3.nucleng.kyoto-u.ac.jp:5560/isqlplus/ (username/password required)

The LXCat project

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Our long-term objective is the establishment of a set of web based tools and open access databases relevant to modeling low temperature plasmas and plasma chemistry. To this end, we have focused over the past year on developing web-based tools for access, display, and processing of data concerning the electrons in typical low temperature plasma conditions - this is the LXCat (or ELECtron SCATtering) project. From the web site in its present version [1], users can access compilations of complete sets of electron-neutral scattering data for various gases developed by different contributors (presently 34 different gases and 6 contributors). New contributors are welcome. Anyone wishing to up-load their cross section sets and/or swarm parameters to this site should contact lxcat.info@gmail.com to obtain an account and to receive instructions for how to use the on-line tools to upload data and plot/compare data. The available cross section compilations on the site at this time are "complete" in the sense that the major momentum and energy loss processes are included for each gas.

In many low-temperature plasma conditions, the electron energy distribution function (edf) is non-Maxwellian and a good parameter is the reduced electric field, E/N, the ratio of the electric field strength to the neutral density. The electron transport and rate coefficients are functions of E/N are obtained appropriate averages over the edf, which is itself determined by solving the electron-Boltzmann equation. Input to the Boltzmann equation solver consists of the complete set of cross sections for each gas and can be taken from the LXCat databases. We have developed an on-line version of BOLSIG+, a solver for the electron-Boltzmann equation in the two-term approximation [2] which is also available on the LXCat site. Thus electron transport and rate coefficients in pure gases and gas mixtures can be calculated on-line. Results are displayed in graphical form or in a text file that can be downloaded from the LXCat site.

References

[1] http://www.lxcat.laplace.univ-tlse.fr

[2] G.J.M. Hagelaar and L.C. Pitchford, Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models, Plasma Sources Sci. Technol. **14**, 722 (2005)

Atomic, molecular, plasma-surface interaction database development for fusion energy research

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Research on fusion energy devices requires a large amount of data for atomic, molecular and plasma-surface interactions. As current machines are updated and future machines are designed, data for a variety of different materials for a wide range of plasma parameters arise. The Atomic and Molecular (A+M) Data Unit of the International Atomic Energy Agency works to coordinate efforts to establish databases for this fusion research effort.

Current activities for database development include a number of Coordinated Research Projects (CRP), Technical Meetings, Consultant Meetings and a number of collaborations. These activities generate significant new data in support of fusion research. These data are published in journals as well as IAEA publications and are included in numerical databases ALADDIN accessible by all fusion researchers [1].

Historically a number of institutions have contributed to development of such databases and continue to participate in a Data Centre Network, supported by the A+M Unit. Members of this network maintain individual databases, many of which can be searched using the GENIE search engine. The A+M Unit host the OPEN-ADAS system that allows access to most of the numerical data stored within the ADAS system. An effort on development of an XML schema for data exchange among the databases is underway.

Many numerical data for specific processes in fusion relevant materials are not available. In many cases computer codes exist with the capability of generating such data as needed. An informal network of institutions with such capabilities is in the process of formation to provide a means quickly generating such data. The A+M Unit maintains on-line code capabilities to generate atomic and molecular data and serves as an access point to LANL atomic physics codes and FLYCHK [2] Non-LTE kinetics codes at NIST.

Currently, a wiki-style knowledge base is under the development. It will host a wealth of information on atomic, molecular, plasma-surface data for fusion research performed through the CRP and other activities. The knowledge base will complement the numerical and bibliographical databases.

References

[1] Details can be found on the Unit home page http://www-amdis.iaea.org/CRP

[2] H.-K. Chung, M.H. Chen, W.L. Morgan, Y. Ralchenko and R.W. Lee, High Energy Density Physics **1**(1), 3–12 (December 2005)

Theoretical approach for data generation for rare gas emission spectra in an alternating electric field

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In this work, the influence of an external electric field on shifts and splitting of spectral lines and transition probabilities between energy levels was investigated. The dependences of these characteristics on frequency and strength of the electric field were revealed and studied. Rare gas atoms under the effect of the circular polarized electric field (electric fields of such polarization are generated in a high-frequency inductive discharge and under laser excitation) were chosen as subjects for study. Rare gases are widely used in plasma physics, therefore, this problem is topical both from a theoretical point of view and for practical applications of the calculation results.

The attempts were made to derive formulas allowing calculation of shifts and splitting of energy levels in the electric field of any strength and frequency. However, these attempts were successful only in some particular cases: for the systems in the one-and two-level approximations, in the isolated atom approximation, only for the Rydberg states of atoms and so on (see [1] and references there). A theoretical approach suitable for calculating atomic and ionic spectra in an alternating circular polarized electric field of an arbitrary strength and frequency was suggested in [2]. This method, based on the energy matrix diagonalization, free from limitations inherent in perturbation theory and allowing to perform calculations in the many-level approximation, is applied to calculating emission spectra of rare gas atoms He, Ne, Ar and Kr in the electric field.

The algorithm of using this method is realized in a special software package written in FORTRAN. Input data of this package are the unperturbed energy level positions of the system under consideration, and the frequency and strength of the electric field. Output data obtained at sequential passing of the code blocks are following: the wave functions of the system, spectral line shifts and splitting, transition probabilities and Stark-level lifetimes in the electric field.

Based on the simulation results, the regularities inherent in the behavior of spectral line shifts and splitting of atoms and transition probabilities under a change in the frequency and strength of the electric field were revealed and investigated. It is found, the interaction of energy levels in the electric field plays a key role in the Stark effect and behavior of transition probabilities. This interaction leads to anomalies in the emission spectra and unequiprobable filling of atomic levels. Additionally, it was found that the transition probabilities have a polynomial dependence on the electric field strength.

The obtained theoretical results are useful for plasma diagnostics and for a solution of problems of plasma spectroscopy. These results allow us to explain the processes taking place in plasma. In particular, based on the calculated data one can determine the electric field strength inside a discharge, clarify a mechanism of filling of the excited levels and causes of the changes in spectral line intensities. The transition probabilities can be used as input data for calculations of lifetimes, spectral line intensities, and for solution of the population density balance equations.

References

[1] N.B. Delone, and V.P. Krainov, Uspekhi Fizicheskikh Nauk **169**, 753 (1999) [in Russian]

[2] E.V. Koryukina, J. Phys. D: Appl. Phys. **38**, 3296 (2005)

Experimental study of self-absorption phenomenon in LIBS

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Departure of the plasma conditions from thermal equilibrium, spatial and temporal inhomogeneities is closer to reality in LIBS experiment. As a result, the self-absorption phenomenon becomes more serious, under these conditions some basic assumptions (LTE, optical thinness, etc.) in treating laser-induced plasma are not work anymore. Therefore, the self-absorption effect must be taken into account in LIBS, especially for quantitative analysis [1–2].

The self-absorption phenomenon of different main group elements has been investigated in this work. It has been found that some emission lines of Mg, Ca and Sr have a stronger self-absorption effect even the laser power density enough low, as Fig. 1 shows.

This phenomenon has been successfully explained by using a semi-empirical model which is used to predict the spatial and temporal distributions of atom, ion, and electron number densities, evolution of an atomic line profile and optical thickness, and the resulting absolute intensity of plasma emission in the vicinity of a strong non-resonance atomic transition, but the reasons why the second main group elements appear stronger self-absorption effect than others are not very clear till now.

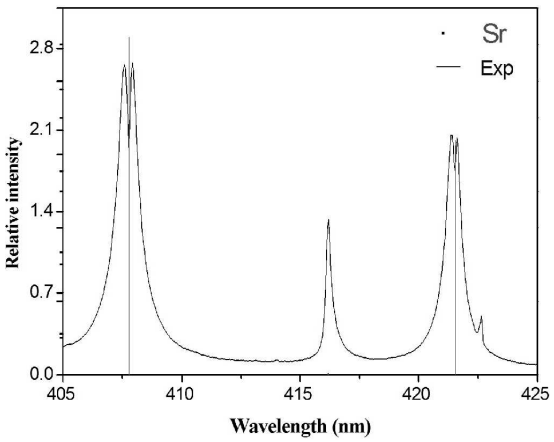

Figure 1: Partial LIBS spectra with self-absorption phenomenon

References

[1] I. B. Gornushkin, C. L. Stevenson, et al, Spectrochim. Acta Part B **56**, 1769-1785 (2001)

[2] F. Bredice, F. O. Borges, et al Spectrochim. Acta Part B **61**, 1294-1303 (2006)

Fractional abundance and cooling rate of W calculated with FAC code

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Tungsten is one of the leading candidates of plasma facing components for future fusion devices such as ITER. However, tungsten is a high-Z element, and is not fully ionized in the temperature range of fusion plasmas (5–20 keV), leading to high line-radiation. Hence, in ITER, in order to keep high-confinement mode plasmas against significant radiative power loss from tungsten ions, it is predicted that allowable tungsten density against electron density is 10^{-5}. Since this prediction heavily relies on the radiative power rate of tungsten ions, or the cooling rate, the accuracy should be assessed, for example, with code-code comparison [1]. The total cooling rate under ionization equilibrium, L_{W}, is expressed as follows,

$$L_{\mathrm{W}} = \sum_{q} F_a(q) \cdot L_{\mathrm{W}^{q+}} \ (\mathrm{Wm}^3)\,, \tag{1}$$

where $F_a(q)$ and $L_{\mathrm{W}^{q+}}$ are, respectively, a fractional abundance of W^{q+} under ionization equilibrium and a cooling rate of W^{q+}. Here, $F_a(q)$ is calculated with ionization, radiative recombination and di-electronic recombination rates (only for W^{44+}, W^{45+} and W^{46+}) calculated with the FAC code [2] and dielectronic recombination rates for the other charge states taken from Ref. [3] and $L_{\mathrm{W}^{q+}}$ is calculated with a collisional-radiative model based on the FAC code. The calculated $F_a(q)$, L_{W} and $L_{\mathrm{W}^{q+}}$ are shown in Fig. 1. With increasing electron temperature, the L_{W} decreases because the mean charge of the W ions under ionization equilibrium increases, and with increasing charge state, the cooling rate of W^{q+} decreases as shown in the figure. The cooling rate of Ref. [4] seems to be, in addition to difference by a factor of ~ 3, shifted toward the low temperature compared with that of the present work. This is due to a shift of $F_a(q)$ toward the low temperature, which was calculated with scaled ionization and recombination rates in Ref. [4]. Therefore, ionization and recombination rates are required to be evaluated, for example, with experimental data in EBIT and/or in tokamaks [3, 5].

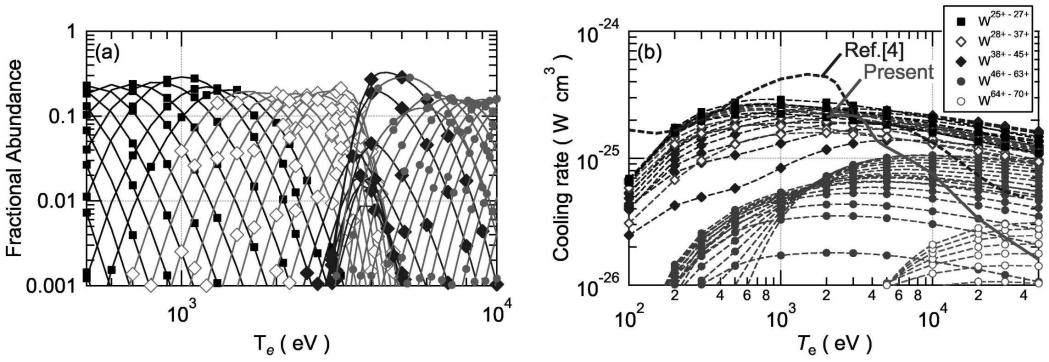

Figure 1: (a) Fractional abundance under ionization equilibrium and (b) total W cooling rates under ionization equilibrium calculated by FAC code and taken from Ref. [4] as a function of electron temperature.

References

[1] Y. Ralchenko et al., AIP Proceedings **1161**, 242 (2009)

[2] M. F. Gu et al., Astrophys. J. **582**, 1241 (2003)

[3] T. Pütterich et al., , Plasma Phys. Control. Fusion **50**, 085016 (2008)

[4] T. Pütterich et al., Nucl. Fusion **50**, 025012 (2010)

[5] T. Nakano et al., J. Nucl. Mater. (2010) [submitted]

Possibility of asymmetric charge transfer between doubly ionized ions and inert gases in low temperature plasma

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Large difference in impurity element effects on excitation of ions and atoms in argon inductively coupled plasma was observed. Even the elements with very close first and second ionization potentials can influence intensities of the spectral lines of other plasma components at very different extent. Presence of the excited levels of the doubly ionized impurity ion at energies above argon ionization potential relative to the ground state of the singly ionized ion was found of importance and Penning ionization by argon ions as a possible influence mechanism was proposed [1]. Due to almost total ionization and appreciable concentrations of the excited doubly ionized ions of the low first and second ionization potential atoms in the plasma possibility of the charge transfer between doubly ionized impurity ions and argon atoms, as the prevailing particle component, ought to be regarded also. In the report, overview of the infinite separation energy defects and semi-classical [2, 3] rate coefficients for asymmetric charge transfer between doubly ionized ions and inert gas atoms for lanthanides, Sc, V, Ti, Mn and some other ions, and analysis of the possible effect of the phenomenon on the plasma state will be presented.

References

[1] G.C.-Y. Chan, G.M. Hieftje, Spectrochimica Acta Part B **61**, 642 (2006)

[2] A. Bogaerts, K.A. Temelkov, N.K. Vuchkov, R. Gijbels, Spectrochimica Acta Part B **62**, 325 (2007)

[3] A.R. Turner-Smith, J.M. Green, C.E. Webb, J. Phys. B: At. Mol. Phys. **6**, 114 (1973)

Elastic cross sections for electron collisions with molecules relevant to plasma processing

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Gaseous electronics the term which is loosely applied to describe low temperature discharge physics is a broad and diverse area of research and development which encompasses both established and emerging technologies. These include semiconductor production, lighting, propulsion, environmental remediation and materials processing to name just a few. One of the major areas of application of gaseous electronics is in the plasma modification and processing of semi-conductor and other electronic materials. This industry worldwide had a turnover in excess of US 210 billion dollars in 2009 [1]. Absolute electron-impact cross sections for molecular targets including their radicals are important in developing plasma reactors and testing various plasma processing gases. However, low-energy electron collision data for these gases are sparse and only the limited cross section data are available.

In this report, elastic cross sections for electron-polyatomic molecule collisions are compiled and reviewed for 17 molecules relevant to plasma processing: CF_2, CF_4, C_2F_4, C_2F_6, C_3F_6, C_3F_8, cyclo-C_4F_8, C_6F_6, CHF_3, CH_2F_2, CH_3F, CF_3I, NF_3, SF_6, SiH_4, Si_2H_6, GeH_4. Elastic cross sections are essential for the absolute scale conversion of inelastic cross sections, as well as for testing computational methods. Data are collected and reviewed for elastic differential, integral, and momentum transfer cross sections and, for each molecule, the recommended values of the cross section are presented. The energy range of interest is up to and including 100 eV, with several exceptions. The literature has been surveyed through early 2010.

Reference

[1] http://www.sia-online.org

Fragile molecules in hostile environments: the physics of molecular filaments in cool-core clusters of galaxies

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Cool-core clusters of galaxies often show a network of fine filaments that surround the central brightest-cluster galaxy. HST observations reveal the filaments to be composed of very long and narrow clouds, suggesting magnetic confinement. These filaments show a remarkable optical emission-line spectrum that is quite unlike any observed in galactic nebulae. Infrared observations reveal exceptionally strong H_2 emission which indicates that a broad range of kinetic temperatures exists within the emitting gas. Radio observations show that nearly 10^{11} solar masses of molecular gas is present. I will discuss the challenges presented by the chemistry and plasma physics, especially the problem of protecting, but exciting, fragile molecules in the hostile cluster environment. The general problem is summarized in [1], while the atomic and chemical physics developments are being made to the plasma simulation code Cloudy [2], which is described in [3].

References

[1] G.J. Ferland, A.C. Fabian, N. Hatch, R. Johnstone, R. Porter, P. van Hoof, & R.J.R. Wiliams, MNRAS **392**, 1475 (2009)

[2] http://www.nublado.org

[3] G.J. Ferland, K. Korista, D. Verner, J. Ferguson, J. Kingdon, & E. Verner, PASP **110**, 761 (1998)

High resolution laboratory spectroscopy for astrophysical and atmospheric physics

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New and future spectrographs, some operating in underexplored wavelength regions, on ground and space-based telescopes have led to urgent needs for laboratory atomic and molecular data of at least matching accuracy and completeness for the interpretation of new astrophysical spectra.

Atomic spectroscopy: Our laboratory atomic astrophysics programme at Imperial College (IC) uses the IC VUV FTS [1] and also IR FTS at Lund University, Sweden, and NIST, USA, to study high resolution spectra of species of astrophysical importance. We report here on measurement of: (i) log gfs (to at least 10% accuracy) for low-mass stars (LMS), brown dwarfs and extra-solar planet analyses. We also target the near IR atomic data needs for future Gaia, E-ELT, and SDSS-III/APOGEE. (ii) new atomic data for visible and UV/VUV spectra of specific neutral, singly and doubly ionised atoms urgently needed for modern elemental abundance studies of the Sun and stars for investigations of Galactic chemical evolution.

High-precision laboratory wavelength measurements of the Ti II emission spectrum have been performed to provide a highly accurate standard for the study of absorption spectra from high-redshift quasars, with the aim of probing possible time variations in the fine-structure constant (α) [2].

Molecular spectroscopy: The molecular laboratory programme, using the IC UV FTS, has been concentrating on the UV absorption spectrum of SO_2. SO_2 plays an important role within the complex chemistry of both the upper atmosphere of Venus and the volcanically active Jovian moon Io. The lack of high resolution laboratory studies has prevented the full, accurate determination of absorption cross sections which are the basis for reliable photochemical models. Recently completed measurements have for the first time recorded the UV spectrum of SO_2 at high resolution ($\lambda/\Delta\lambda \approx 450{,}000$) at 295 K, 198 K, and 160 K [3–6].

We are currently undertaking the first high resolution measurements of the isotopologues of SO_2 to enable the photoabsorption cross sections of all the isotopologues to be included into photochemical models of the early Earth's atmosphere. These models will be used to more reliably interpret the sulphur isotope ratios found within ancient rock samples from the Archean period (2450 million years ago) [7], and examine the role of the isotopologues of SO_2 in mass independent fractionation seen in rock samples used in studies of the Earth's early atmosphere. Sulphur mass independent fractionation is currently being used to estimate levels of oxygen and other UV absorbers in the ancient Earth atmosphere.

References

[1] J.C. Pickering, Vib. Spectrosc. **29**, 27 (2002)
[2] J. K. Webb et al., Phys. Rev. Lett. **82**, 884 (1999)
[3] G. Stark et al., J. Geophys. Res. **104**, 16585 (1999)
[4] J. Rufus et al., J. Geophys. Res. **108**, 51 (2003)
[5] J. Rufus et al., J. Geophys. Res. **114**, E06003 (2009)
[6] D. Blackie et al., J. Geophys. Res. (2010) (submittied)
[7] J. R. Lyons, Geophys. Res. Lett. **34** L22811 (2007)

Chemical composition of kinematically identified Galactic stellar groups

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Chemical evolution of galaxies is a key topic of modern astrophysics which extensively uses achievements of theoretical physics in plasma modelling, atomic and molecular data computing and many other fields. The Vienna Atomic Line Data Base (VALD) is extensively used in preparing input data for synthetic stellar spectrum calculations [1]. Using the method of synthetic spectra we are analyzing a large sample of 86 Milky Way stars in order to find out their origin. They belong to three newly identified kinematic stellar groups, supposed to belong to remnants of dwarf galaxies which have merged with the Milky Way Galaxy during its formation or later.

The newly found coherent groups of stars were identified in a homogeneous data set of kinematical, age and metallicity parameters of about 14,500 solar-type stars [2] by investigation of their orbital parameters [3]. In order to understand the origin of those stars we make a detailed chemical analysis of each star and then compare to Galactic disk stars. From accurate elemental abundance patterns we expect to see fossil signatures of past mergers in our Galaxy.

High resolution spectra of the programme stars were obtained with the FIES spectrograph at the Nordic Optical Telescope at La Palma, Spain. The spectra were analyzed using a differential model atmosphere technique. A set of plane parallel, line-blanketed, constant-flux LTE model atmospheres ware computed with an updated version of the MARCS code [4].

Here we report on detailed chemical composition of the 16 stars so far investigated. It is clear that they are chemically homogeneous and abundances of oxygen, magnesium, silicon, calcium and titanium are overabundant in comparison to the Galactic stars and models of Galactic chemical evolution trends [5]. Our results provide further evidence that these stars are of extragalactic origin.

References

[1] N.E. Piskunov, F. Kupka, T. A. Ryabchikova, W. W. Weiss, C.S. Jeffery, A&AS **112**, 525 (1995)

[2] B. Nordström, M. Mayor, J. Andersen et al., A&A **418**, 989 (2004)

[3] A. Helmi, J. Navarro, B. Nordström, MNRAS **365**, 1309 (2006)

[4] B. Gustafsson, B. Edvardsson, K. Eriksson, et al., A&A **486**, 951 (2008)

[5] B.E.J. Pagel, G. Tautvaišienė, MNRAS **276**, 505 (1995)

Synthetic stellar energy flux modeling under gridified software SYNTSPEC

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We present a gridified stellar energy flux modeling tool SYNTSPEC for stellar spectra analysis. It is an example of data- and compute-intensive application running on the testbed of the Enabling Grids for E-sciencE (EGEE) GRID compatible infrastructure, which brings the new quality to the research in astrophysics [1]. The multi-job application is running within the Gridcom system – the user friendly interface that allows a common (virtual) work of a physically spread scientific group. Atomic and molecular structure of stellar photosphere redistributes the initial energy flux through the entire spectrum employing absorption, reemission, scattering processes and paints a unique shape of flux image of the specific star.

SYNTSPEC software calculates the energy flux and normalized to the continuum stellar spectra that are applied for stellar classifications and determinations of e.g. chemical compositions, effective temperatures and surface gravities of stars [2]. The specific energy flux modeling is an important tool for analysis of data, which will be produced by the European Space Agencys GAIA space observatory and other modern observatories.

A special added value is the compatibility to Virtual Observatory tools and operation of the application within the Gridcom interface which improved the job submission procedures and possibilities of user interaction [3, 4].

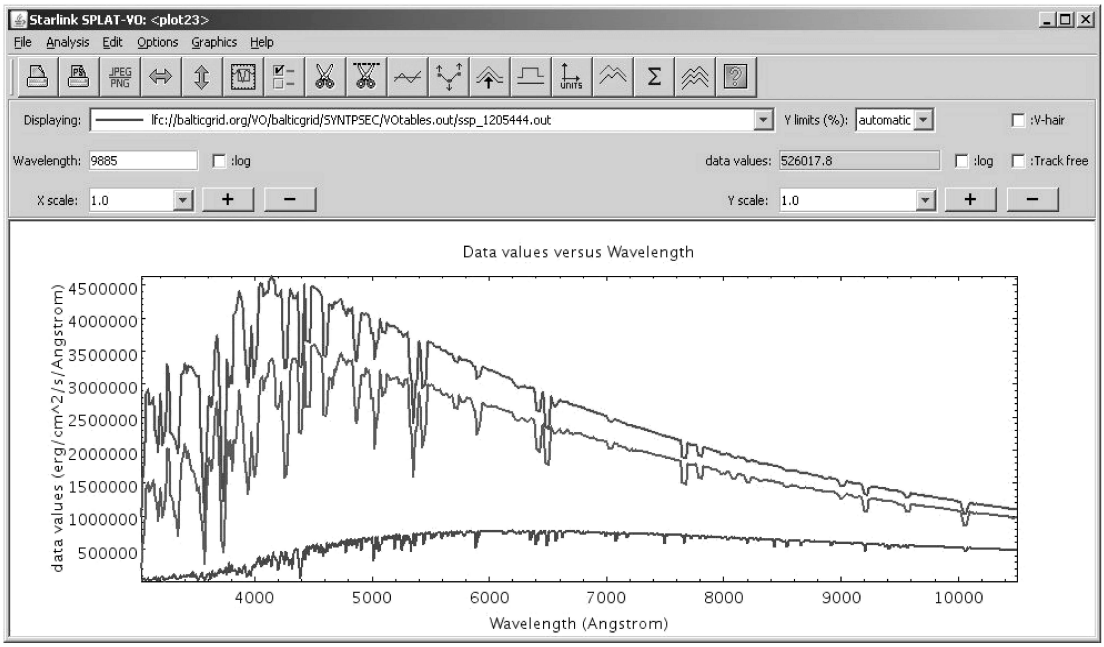

Figure 1: The interface example with synthetic spectra at 330–1050 nm for stars with ($T_{\rm eff}$, log g, [Fe/H]) equal to: (6400 K, 2.2, 0.0), (5700 K, 4.4, 0.0) and (4200 K, 2.0, 0.0), from the top downwards. The SPLAT-VO software was used for the visualization.

References

[1] G. Tautvaišienė, Š. Mikolaitis, E. Puzeras, Memorie della Societa Astronomica Italiana **80**, 534 (2009)
[2] G. Tautvaišienė et al., Astronomical Journal **134**, 2318 (2007)
[3] A. Juozapavičius, D. Mažeika, Baltic IT&T Review 3, 5 (2007)
[4] D. Šešok, R. Belevičius, A. Kačeniauskas, J. Mockus, Mechanika **82**, 63 (2010)

Analysis of Pr III and Nd II spectra with application to the study of chemically peculiar stars

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Theoretical calculations of Pr III and Nd II have been performed by means of the Cowan codes. In the parametric study of the experimental level energies, the most important configuration interactions were taken into account explicitly while influence of far lying configurations was accounted for by introducing extended set of effective parameters. The calculations confirm that a parametric fitting is not an impossible task in such very complex spectra of lanthanides.

In Nd II, 597 levels of the odd configurations and 233 levels of the even configurations were interpreted with a standard deviation of respectively 87 and 57 cm^{-1}. Calculated transition probabilities from odd upper levels are in fairy good agreement with available experimental data. A spectrum of the famous Przybylski' Ap star (HD 101065) was used to search for the presence of Nd II lines with even upper levels for which transition probabilities were previously unknown. Our results show that a large number of unidentified features in the star spectrum can be attributed to such Nd II transitions.

Using all available experimental data, comprising a list of about 7300 lines in the spectral range 821 to 10717 Å, and the present calculations, new analysis of the Pr III spectrum was performed. As a result, about 4900 lines are now classified in this spectrum in comparison with about 3300 previously known lines. The set of odd levels is extended to 403 (previously 234) and the one of even levels, to 235 (167). New classifications refer mostly to transitions from high lying levels where new configurations $4f^27p$, $4f^27d$, $4f^26f$, $4f^25g$, $4f^26h$ and 4f5d6p are located. Parametric calculations resulted in standard deviation of respectively 59 and 56 cm^{-1} for all odd and even levels. The ratio of the experimental to calculated lifetimes was found to be 0.99(7) for 8 odd levels after scaling the Hartree Fock dipole transition integrals by factors of 0.95 and 0.60 respectively for transitions from the $4f^26p$ and the $4f5d^2$ configurations. For levels of the even $4f^25d$ and $4f^26s$ configurations, neither experimental lifetimes nor transition probabilities are available. Therefore the oscillator strengths from these levels that are important in astrophysics have been calculated with unscaled values of the dipole transition integrals. An analysis of Pr II (experimental transition probabilities) and Pr III (present calculations) lines in high resolution high S/N ratio spectrum of Am star 32 Aqr indicates an ionization equilibrium Pr II/Pr III in its atmosphere that validates our calculations.

Calculation and application of R-matrix electron-impact excitation data for ions of interest to astrophysical diagnostic modelling

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A large number of high-resolution and high-quality spectra have been (will be) obtained in recent years (near future) from both the EUV (e.g. Hinode) and X-ray (e.g. Chandra, XMM-Newton, IXO) regions. Many emission lines observed in these spectra are potential diagnostics of the electron temperature and density of coronal-like hot plasmas. There are also many emission lines unknown and large discrepancies in line intensity ratios with unknown contaminations. Such diagnostics and associated line identifications require accurate atomic data, especially the electron-impact excitations.

The advantages of the intermediate-coupling frame transformation R-matrix method [1] make it feasible to provide excitation data along iso-electronic sequences covering a substantial range of astrophysically important ions at the high level of accuracy afforded by the R-matrix method. This is one of the key goals of the UK Atomic Processes for Astrophysical Plasmas (APAP) network[1]. Here we will address the effective collision strength along the Ne-like and Li-like iso-electronic sequences [2] and specified ion—Fe^{13+} [3], and assess the accuracy of the product.

Using the latest electron-impact excitation under the framework of R-matrix, we analyze the EUV and soft X-ray spectra of hot plasmas, e.g. stellar corona and electron beam ion traps. Several previous discrepant line intensity ratios in Fe^{13+} have been explained satisfactorily and some lines are identified in astrophysical sources for the first time with the aid of laboratory measurement performed at Heidelberg EBIT [3].

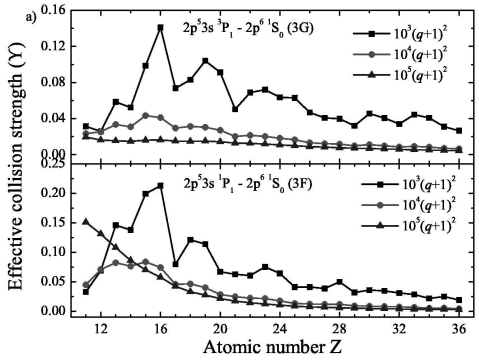

Figure 1: The effective collision strengths of 3s—2p line along the Ne-like sequence

References

[1] D.C. Griffin, N.R. Badnell, & M.S. Pindzola, *J. Phys. B: At. Mol. Opt. Phys.*3713 (1998)

[2] G.Y. Liang, & N.R. Badnell, A&A (2010) [in press]

[3] G.Y. Liang, N.R. Badnell, J.R. Crespo López-Urrutia, T.M. Baumann, G. Del Zanna, P. Storey, H. Tawara, & J. Ullrich, ApJ (2010)

[1] `http://www.apap-network.org`

Atomic data for spectral line calculation in HID lamps

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The knowledge of atomic and molecular data is essential to describe all gaseous applications such as discharges, arcs, gas lasers, gaseous dielectrics and the earths atmosphere. Obtaining such data has been the goal of many different laboratories and authors. In this work, we will show the importance of this data in radiation transport calculations of HID (High Intensity Discharge) lamps. These lamps generate light by applying an electrical current across an ionized gas. Different methods are used to calculate the radiative properties of these lamps [1]. A model for radiation transport calculation based on the ray tracing method has been adopted [2] in order to calculate the output flux, the net emission coefficient and the photometric characteristic of these lamps. The model is based on the resolution of the radiative transfer equation that describes the change of spectral intensity I_λ ($\mathrm{W\,m^{-3}sr^{-1}}$) along a path. The medium where radiation takes place is considered to emit and absorb radiation without scattering. Hence, knowing $\varepsilon_\lambda(\lambda, r)$ (the local spectral emission coefficient) at different position in the discharge and also κ (the local absorption coefficient) we are able to resolve the radiative transfer equation. In this model, the atomic data is the only resource to calculate both coefficients. For the first step, a pure mercury HID lamp is considered. For each spectral line, the local absorption and emission coefficients are strongly dependant on the broadening constants that are calculated from the atomic data of each spectral line. Calculations reported in the literature use different values for these constants, leading to marked differences in output of the models.

References

[1] S. C. Mishra and M. Prasad, Radiative heat transfer in participating media, Sadhana **23**(2), 213-232 (1998)

[2] M. Galvez, Ray-tracing model for radiation transport in three-dimensional LTE systems, J. Phys. D: Appl. Phys. **38**, 3011 (2005)

Investigation of highly excited and auto-ionizing atomic states for the resonance ionization laser ion source at ISOLDE

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The Resonance Ionization Laser Ion Source (RILIS) is the preferred method for ionizing the nuclear reaction products at the Radioactive Beam Facility ISOLDE. ISOLDE produces 'exotic' - unstable - isotopes used for fundamental research in nuclear physics, nuclear astrophysics, atomic physics, condensed matter physics, radiobiology and elementary particle physics. ISOLDE uses the Isotope Separator On-Line (ISOL) process whereby a proton beam impinges on a thick, heated target. A mixture of vaporized nuclear reaction products diffuses out of the target and must be ionized so that they can be accelerated, mass separated and sent to one of the various experimental stations.

The Resonance Ionization Laser Ion Source uses the highly selective method of stepwise resonant ionization of the element of interest, using up to three different laser wavelengths [1, 2]. The atomic selectivity of RILIS complements the mass selection process of the ISOLDE separator magnets and reduces the isobaric contamination which can be a limiting factor for the study of shorter-lived or lower yield isotopes.

Isotopes of 26 different elements have been laser ionized at ISOLDE. New ionization schemes are developed as they are requested by users of ISOLDE. An ideal ionization scheme makes use of strong atomic transitions and high ionization cross-section. In many atoms the ionization cross-section is much improved if the final wavelength is in resonance with an auto-ionizing state (AIS). Where no favorable transition to AIS is known, a high-power laser beam is used to pump the non-resonant ionization step. Previously the scope for development has often been limited to testing resonant transitions between well documented atomic levels and a non-resonant ionization step.

A generous grant has recently allowed a major upgrade of the RILIS laser system and the construction of a laser photoionization spectrometer in a separate development lab [3] where thorough ionization scheme studies can be performed. The spectrometer includes two broadly tunable optical parametric oscillators, a dye laser and two time-of-flight mass-spectrometers. This setup allows resonance ionization spectroscopy of atoms to be carried out in a wavelength range of 220–1680 nm.

We present here a three step resonance ionization study of Mn I. Spectra of transitions to AIS from different highly excited states have been measured. A large number of strong resonances has been observed in the energy region 66100–73400 cm^{-1}. The better ionization scheme is achieved using an excited state which open access to AISs that are not observed in the VUV absorption spectrum, which is the main source of accessible information of AIS.

References

[1] V.I. Mishin *et al*, Nucl. Instrum. Methods Phys. Res. B **73**, 550 (1993)

[2] V.N. Fedoseyev *et al*, Hyperfine Interact **127**, 409 (2000)

[3] B.A. Marsh *et al*, Hyperfine Interact. **196**, 129 (2010)

Magnetically controlled artificial minimal living cells

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The programmable artificial minimal living cells that are designed and synthesized in our former consortium are only a few (4-10) nanometers in size. In their simplest form, these cells consist of a micelle which acts as the container, a light driven metabolism, and a genetic system, whose functions are all very tightly coupled. The container consists of amphiphilic fatty acid (FA) molecules that self-assemble into a micelle or small vesicle. The hydrophobic interior of the micelle provides an alternative thermodynamic environment from the aqueous or methanol exterior and acts as a sticking point for the photosensitizer (neutral radicals), organic precursors of FA (pFA - food), and the genetic material molecules. Peptide nucleic acid (PNA) is chosen as the genetic material as it is far less polar than RNA or DNA and therefore should stick to the micelle, especially if hydrophobic chains are added to the PNA backbone. The electronic and structure, electron spin densities and isotropic Fermi contact coupling (EPR) of neutral radical molecules implemented in the artificial cells was obtained by the quantum mechanical methods installed in GAMESS-US or Turbomole packages of our Theoretical Molecular Electronics and Spintronics research group. The molecular spintronics devices are based on electron spin density shift in various excited states (see Figures below).

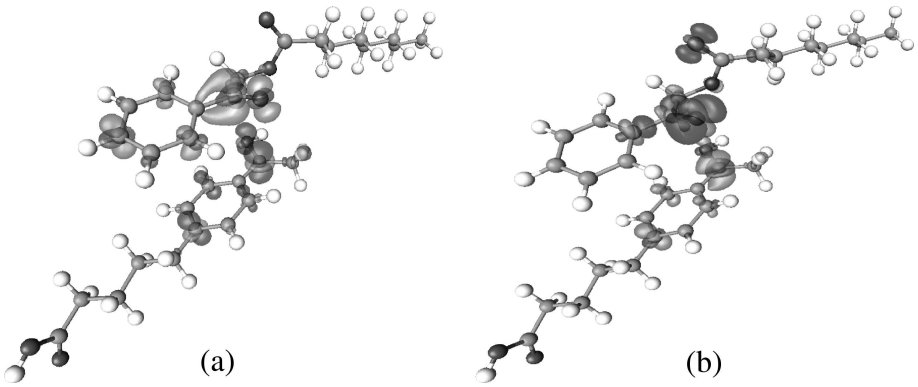

Figure 1: Visualization of the electron spin density tunneling associated with the (a) first and (b) ninth excited state. The transition is from the neutral radical molecule (in the left-bottom) to the pFA molecule (in the top-right). The electron spin density cloud hole is indicated by the dark grey color while the transferred electron cloud location is designated by the grey color. Carbon atoms and their associated covalent bonds are shown as grey sticks, hydrogens are in light grey, oxygens in dark grey.

The shifted electron spin density gives new values of isotropic Fermi coupling according to the algorithms implemented in the supramolecules composed of neutral radical molecules. The non-conventional systems which were designed in our research group include the use of molecular spintronics logic gates to control growth and division of artificial living cells. Longer term goals might be the use these programmable artificial cells for the construction of nanobiorobots for nanomedicine and cleaning of nuclear, chemical and microbial pollutions. The metabolism involves the magnetically controlled photoexcitation of an electron in various neutral radical molecules possessing stable oriented spin in artificial cells. Photosynthetic systems are stabilized by the donation of an electron from non-canonical PNA bases (for example, 8-oxo-guanine). The excited electron is in turn used to cleave a waste organic molecules or tumor cancer cells to yield components of new born artificial cells.

High pressure calculation of the lattice dynamics of the Pb-chalcogenide compounds

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High pressure effects on the lattice dynamics and dielectric properties of the PbS, PbSe and PbTe alloys have been carried out using the density-functional perturbation theory (DFPT) within the local density approximation (LDA) as implemented in the ABINIT code (http://www.abinit.org). We study the variation of the optical phonon frequencies at the high symmetry points Γ, X and L and the dynamic effective charge (Z^*) with the pressure. The obtained values have a quadratic form with pressure. Our results are in good agreement with the available experimental data at null pressure and they allow prediction for the variation of the phonon frequencies with the pressure.

Electron-impact excitation of the $(5p^5 6s^2)\ ^2P_{3/2,1/2}$ autoionizing states in Cs atoms

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The $np^5(n+1)s^2\ ^2P_{3/2,1/2}$ states are the lowest autoionizing states in Na ($n = 2$), K ($n = 3$) and Rb ($n = 4$) atoms. In heavier Cs ($n = 5$) atoms, the large spin-orbit splitting ($\Delta E = 1.76$ eV) results in a situation when the upper $^2P_{1/2}$ component is located in an energy region densely populated by the states from $5p^5 5dnl$ configurations which characterized by the strong excitation efficiency at low impact energies. Recently we reported the results on the near-threshold excitation of the $^2P_{3/2}$ state in cesium in the narrow impact energy region of 12.3–16.6 eV [1]. In the present work, by using the same experimental setup and measuring procedure we have extended these studies for impact energies up to 600 eV and performed similar measurements for the $^2P_{1/2}$ state. The relative experimental cross sections were normalized to the calculated values at 600 eV. The calculations were performed in Born approximation by using our own computer code.

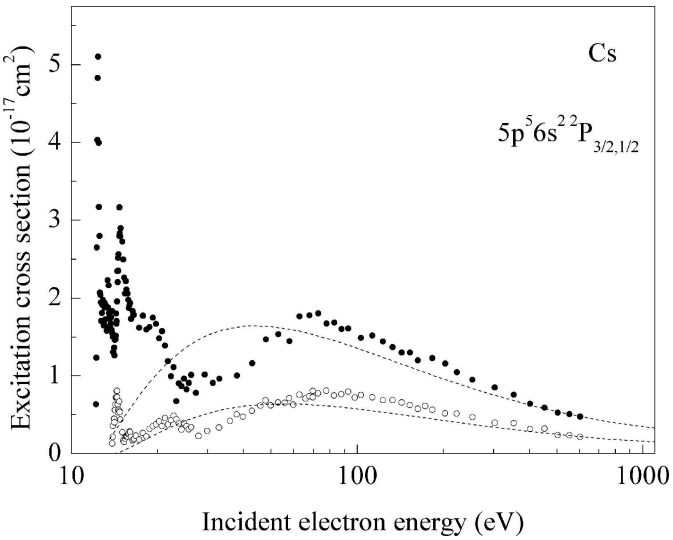

Figure 1. Excitation cross-sections for the $(5p^5 6s^2)\ ^2P_J$ autoionizing states in Cs atoms: •, ∘ present data for $J = 3/2$ and 1/2 states, respectively; dashed lines are calculated data in Born approximation.

As seen from the figure, the cross-sections differ essentially in behavior and magnitude at threshold impact energies. However, above 40 eV both cross sections fit well the dipole character of excitation and their ratio amounts approximately 2:1 at 70 eV impact energy. For the $^2P_{3/2}$ state the cross section reaches the maximum value of $5.1 \cdot 10^{-17}$ cm^2 and that agrees well with the value of $6.0 \cdot 10^{-17}$ cm^2 obtained earlier by normalization to R-matrix calculations [1]. Our preliminary calculations of the cross sections and decay rates for the $5p^5 5dnl$ high-lying doublet levels show that the second resonance at 14.74 eV present in excitation of the $^2P_{3/2}$ state possesses the resonance origin, while a 'shoulder' at 20 eV and the rise of the cross section at 18 eV observed in excitation function of the $^2P_{1/2}$ state reflect the strong cascade transitions from the high-lying doublets.

The work was supported, in part, by the Lithuania-Ukraine project M/78-2009 (AB) and Research Council of Lithuania project TAP-55/2010 (AK).

Reference

[1] A. Borovik, O. Zatsarinny and K. Bartschat, J. Phys. B **42**, 044010 (2009)

Total autoionization cross-section of cesium atoms excited by 12–600 eV electrons

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Autoionizing states increase essentially the ionization cross-section of heavy alkali atoms above p^6 excitation threshold [1]. Such contribution is, in fact, the excitation-ionization or, in other words, autoionization cross-section of atoms [2]. It can be evaluated experimentally by measuring the total intensity of ejected-electron spectra obtained at different impact energies. Earlier, this method was successfully employed for obtaining the data in potassium [3] and cesium [4] atoms. For the latter, the data were obtained only in a narrow impact-energy region of 4 eV above the $5p^6$ excitation threshold. Using the same apparatus and measuring procedure, in the present work we have extended these studies for impact energies up to 600 eV. Figure 1 shows the obtained data together with the single ionization cross-section of cesium atoms [5].

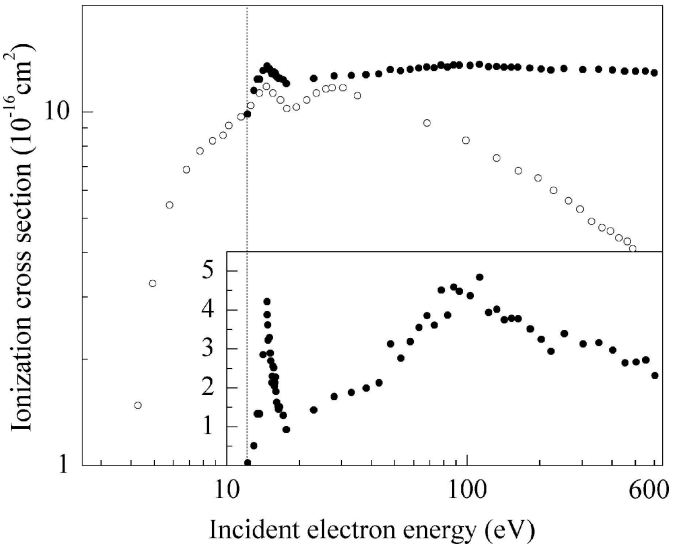

Figure 1. ○ single ionization cross-section of cesium atoms [5]; • autoionization cross-section (present data). Inset shows the present data in a linear Y scale. The vertical line marks the $(5p^5 6s Z^2)$ $^2P_{3/2}$ lowest autoionization threshold at 12.31 eV.

As seen from the figure, there is a good correlation both in position and magnitude of the cross-sections above the lowest autionization threshold at 12.31 eV. Note that the resonance part of the autoionization cross- section is determined exclusively by resonance excitation of levels located between 12.3 and 17 eV [4]. The broad maximum around 100 eV (see inset in figure 1) reflects the high excitation efficiency of doublet levels which belong mainly to the $5p^5 5d6s$ configuration.

This work was supported, in part, by the Lithuania–Ukraine project M/78-2009 (AB) and Research Council of Lithuania project TAP-55/2010 (AK).

References

[1] K. J. Nygaard, Phys. Rev. A **11**, 1475 (1975)

[2] D. Mitnik, P. Mandelbaum, J. Schwob, A. Bar-Shalom, J. Oreg, W. Goldstein, Phys. Rev. A **50**, 4911 (1994)

[3] M.J. Evrij, A. Borovik (Jr), L.L. Shimon, J.E. Kontros, A. Borovik, Nucl. Instr. Methods B **233**, 280 (2005)

[4] A. Borovik and A. Kupliauskiene, J. Phys. B **42**, 165202 (2009)

[5] J.T. Tate and P.T. Smith, Phys. Rev. **46**, 773 (1934)

Electron-impact excitation cross-sections for autoionizing states in cesium

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We present the first results of our joint experimental and theoretical studies of excitation cross-sections for the $5p^5 n_1 l_1 n_2 l_2$ autoionizing states in cesium atoms excited by electrons in a broad impact-energy range from the excitation threshold of levels up to 600 eV. The data were obtained by measuring the ejected-electron spectra at an observation angle of 54.7° for different values of the impact energy. The apparatus, measuring and data processing procedures were described in detail elsewhere [1]. The near-threshold and the high-energy regions were studied at an energy spread of the incident electron beam (FWHM) of 0.3 eV and 0.7 eV, respectively. The relative experimental data were put on an absolute scale by normalizing them to the calculated value at 600 eV. Calculations were performed in Dirac-Fock approximation taking into account superposition of configurations $5p^5 nln'l'$ ($n, n' = 5, \ldots, 11$; $l, l' = 0, \ldots, 4$) [2]. The excitation cross-sections for the lowest autoionizing quartets ^4P_J and two high-lying levels $^4D_{3/2}$ and $(^1P)^2P_{3/2}$ from $5p^5 5d^6 s$ configuration are shown in figure 1. Classification of levels was taken from [3].

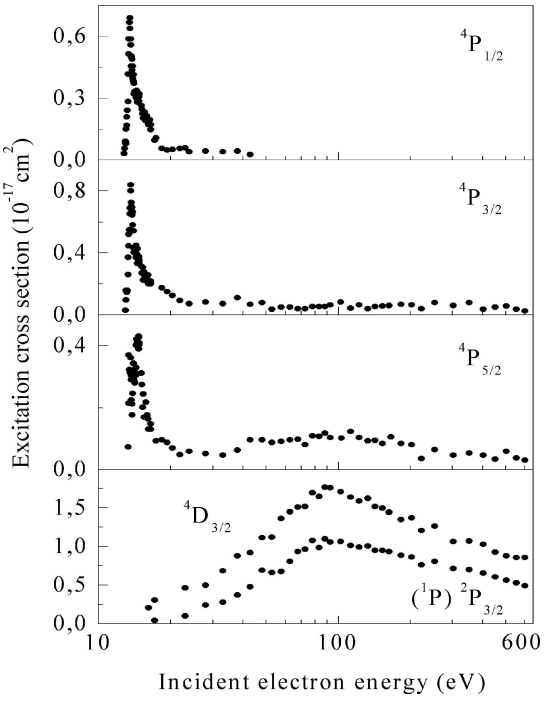

Figure 1. The electron-impact excitation cross sections for $5p^5 5d^6 s$ autoionizing states in cesium atoms.

As seen from the figure, all quartets possess an evident resonance excitation behavior at threshold energies. Single resonances are observed in excitation functions for the $^4P_{1/2,3/2}$ levels whereas for the $^4P_{5/2}$ quasimetastable level an additional strong resonance is observed at 0.4 eV above the excitation threshold. Earlier, a step-like feature at this energy was also observed in electron-impact metastable excitation function [4]. The excitation dynamics for $^4D_{3/2}$ and $(^1P)^2P_{3/2}$ levels points out their clear dipole excitation character. This contradicts the assignment of the $^4D_{3/2}$ level [3] and demands its revision.

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References

[1] Borovik A.A., Grum-Grzhimailo A.N., Bartschat K. and Zatsarinny O., J. Phys. B **38**, 1081 (2005)

[2] M.F. Gu, http://kipac-tree.stanford.edu/fac/

[3] Borovik A. and Kupliauskiene A., J. Phys. B **42**, 165202 (2009)

[4] Feldman P. and Novick R., Phys. Rev. A **160**, 143 (1967)

Large-scale configuration interaction calculations of 4p electron-impact excited Rb states

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The autoionizing levels of Rb atoms excited from the 4p subshell by electron impact were investigated both experimentally [1] and theoretically [2]. For the classification of the measured spectrum [1], Mansfield [2] has calculated the energy of levels in $4p^5 5s^2$, $4p^5 4d5s$, $4p^5 4d^2$, $4p^5 5s6s$, $4p^5 5p^2$, $4p^5 5s5p$, and $4p^5 4d5p$ configurations by using single configuration Hartree-Fock approximation with scaling of the calculated Slater-Condon parameters in comparing calculations with observations. The goal of the present work was to perform ab initio configuration interaction (CI) calculations taking into account both correlation and relativistic effects in multiconfiguration Dirac-Fock approximation. The calculations were made by using FAC computer code [3] in Dirac-Fock approximation taking into account the superposition of configurations $4p^5 nln'l'$ ($n, n' = 4, \ldots, 11$; $l, l' = 0, \ldots, 4$). The total number of states included was 19351. For the classification of measured ejected-electron spectra, the electron-impact excitation cross sections and autoionization probabilities were calculated by using the same CI basis as well. As an example, the results for the lowest strongest lines are presented in Table 1.

Table 1: Energies (E), cross sections (σ) for the energies of 0.09 eV, 3.6 eV and 1.49 eV of the scattered electron and autoionization probabilities (A^a) for autoionizing states in Rb atoms.

State	E_{FAC} (eV)	E_{Exp} (eV) [1]	σ (10^{-18} cm^2)	A^a (10^{12} s^{-1})
$4p^5 5s^2\ {}^2P_{3/2}$	15.21	15.31	20.54, 15.40, 12.24	7.38
$4p^5 5s^2\ {}^2P_{1/2}$	16.08	16.16	10.01, 6.67, 5.09	8.13
$4p^5 5s(^3P)5p\ {}^4D_{5/2}$	16.61	16.69	2.39, 0.97, 0.51	0.31
$4p^5 4d(^3P)5s\ {}^2P_{1/2}$	17.10	17.18	7.33, 2.35, 0.95	6.62
$4p^5 4d(^3F)5s\ {}^4F_{5/2}$	17.19	17.18	7.89, 2.19, 0.73	0.86
$4p^5 4d(^3F)5s\ {}^4D_{7/2}$	17.29	17.21	9.37, 2,77, 1.01	2.34

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References

[1] V. Pejčev, D. Rassi, K.J. Ross, T.W. Ottley. J. Phys. B **10**, 1633 (1977)

[2] M.W.D. Mansfield. Proc. Roy. Soc. Lond. A **364**, 135 (1978)

[3] M.F. Gui, http://kipac-tree,stanford.edu/fac

Electron impact excitation of Al XII

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Emission lines from several ionisation stages of aluminium, including He-like Al XII, have been observed in solar plasmas – see, for example, Landi and Phillips [1]. The $n = 2$ lines of He-like ions in the x-ray region (namely, the resonance w: $1s^2\ ^1S_0$ – $1s2p\ ^1P^o_1$, intercombination x and y: $1s^2\ ^1S_0$ – $1s2p\ ^3P^o_{2;1}$, and forbidden z: $1s^2\ ^1S_0$ – $1s2p\ ^3S_1$) are of particular interest as these are useful for the determination of electron densities and temperatures in the solar corona and transition region. However, to analyse observations, atomic data are required for a variety of parameters, such as energy levels, radiative rates (A- values), and excitation rates or equivalently the effective collision strengths (Υ), which are obtained from the electron impact collision strengths (Ω). Experimentally, only energy levels are available for Al XII (`http://physics.nist.gov/PhysRefData`). Similarly, A- values are also available for many (electric dipole) transitions on the NIST and CHIANTI (`http://www.damtp.cam.ac.uk/user/astro/chianti/`) websites, but collisional atomic data for Al XII are restricted to transitions only from the lowest three levels to higher excited levels [2]. These calculations of Sampson et al. [2] are based on the hydrogenic approximation and do not include the contribution of resonances, which can be important for an ion such as Al XII. Therefore, in this paper we report a complete set of results (namely energy levels, radiative rates, lifetimes, and effective collision strengths) for all transitions among the lowest 49 levels of Al XII. These levels belong to the $1s^2$, $1s2l$, $1s3l$, $1s4l$, and $1s5l$ configurations. Finally, we also report the A- values for four types of transitions, namely electric dipole (E1), electric quadrupole (E2), magnetic dipole (M1), and magnetic quadrupole (M2), because these are also required for plasma modelling.

For the determination of wavefunctions we employ the fully relativistic GRASP code, and for the calculations of Ω, the *Dirac atomic R-matrix code* (DARC) of PH Norrington and IP Grant. Collision strengths and effective collision strengths are calculated for all 1176 transitions among the 49 levels of the $n \leq 5$ configurations over a wide energy (temperature) range up to 340 Ryd (10^7 K), suitable for applications in a variety of plasmas. Additionally, parallel calculations have also been performed with the *Flexible Atomic Code* (FAC) of Gu [3], so that all atomic parameters can be rigorously assessed for accuracy. Detailed data along with comparisons will be presented during the conference.

This work has been financed by the EPSRC and STFC of the UK.

References

[1] E Landi and K J H Phillips, ApJS **160**, 286 (2005)

[2] D H Sampson, S J Goett and R E H Clark, ADNDT **29**, 467 (1983)

[3] M F Gu, ApJ **582**, 1241 (2003)

Differential cross sections and Stokes parameters for electron impact excitations of the 6s6p $^3P_1$ state of mercury

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The traditional physical quantities to describe collision processes are total or differential cross sections. These observables are the results of averages over key variables, such as magnetic quantum numbers or electron spin. The averaging, however, may partly or completely obscure the collision dynamic responsible the process and makes comparison between theory and experiment less valuable. The study of collision Stokes parameters has offered detailed describe of the electron impact processes [1].

In the present work, detailed calculations have been carried out for the direct electron impact excitation differential cross sections and the differential Stokes parameters from the ground state to the excited states 6s6p $^3P_1$ of mercury by using a fully relativistic distorted-wave method. In Fig. 1, the present calculations and the experiments of Sohn and Hanne [2] of the differential Stokes parameter P_3 at the incident energy 8eV are shown. It is can be found that present results in multi-configuration are in good agreement with the experiments.

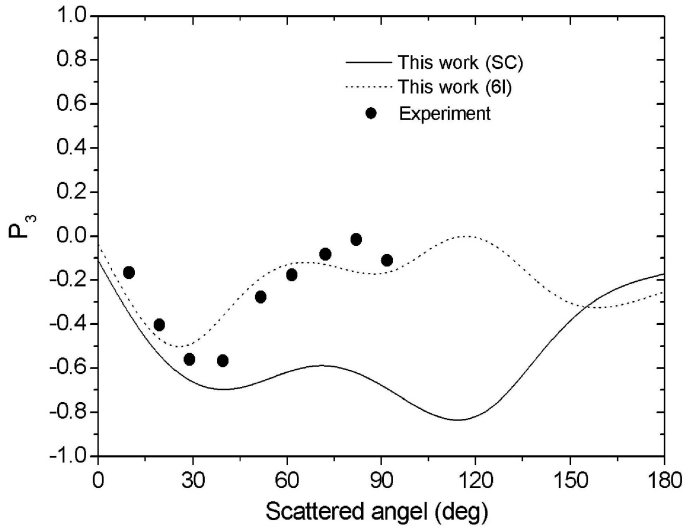

Figure 1: The differential Stokes parameter P_3 of the $6s^2\ ^1S_0$-6s6p $^3P_1$ electron impact excitation. The incident energy is 8 eV. Circles are the experiments of Sohn and Hanne [2]. SC represents single configuration calculations. $6l$ represents multi-configuration calculations including all virtual single and double excitations from the occupied shells into the (unoccupied) $6l$ ($l = \mathrm{s, p, d}$) subshells.

References

[1] Nils Andersen et al., Physics Reports **278**, 107-289 (1997)

[2] M Sohn and G F Hanne,J. Phys. B **25**, 4627 (1992)

Electron impact excitation of singly-ionized chromium

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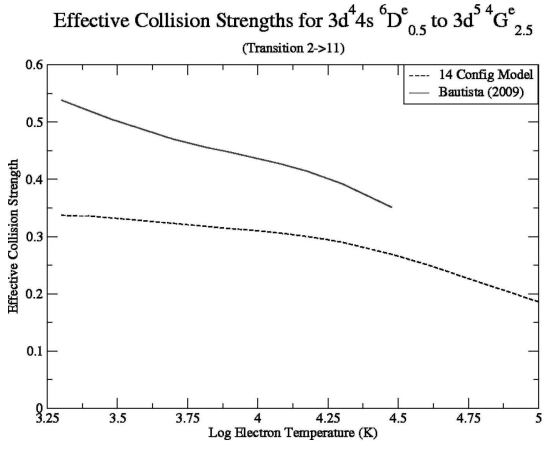
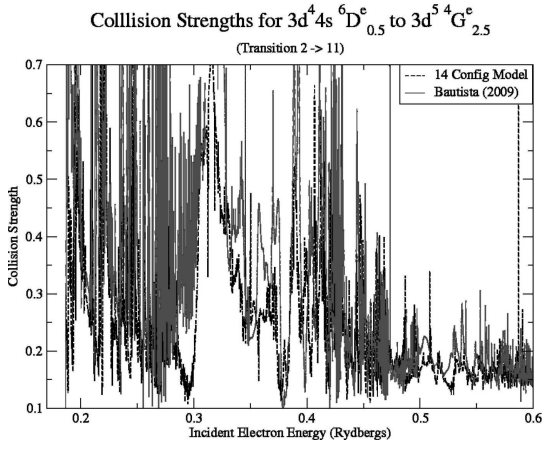
One of the major challenges in atomic physics today is the accurate theoretical evaluation of electron impact excitation collision strengths and effective collision strengths for systems with open d-shells. These ions are known as the Fe-peak elements and are of particular importance to the astrophysics and plasma physics communities. These systems are notoriously difficult to model with calculations typically consisting of 100s of fine structure states and 1000s of closely coupled channels. Numerous publications regularly appear in the literature pertaining to the observation of Cr II emission in the spectra of many astrophysical objects. For example Monier et al [1] have recently reported the first discovery of a damped Lyα System (DLA) using the GALEX Satellite which indicated the presence of unusually strong absorption due to metal lines of Cr II, Zn II, Mn II and Fe II. Significantly, several facets of galaxy formation and evolution can be considered through follow-up studies of the properties of these DLA's. For example, their metal abundances provide an insight into the chemical evolution of the neutral hydrogen gas over cosmic timescales.





We present here the largest and most sophisticated evaluation ever performed for the electron impact excitation of Cr II. It incorporates 280 fine-structure levels, 1932 coupled channels and 39,060 individual transitions, both forbidden and allowed. We have evaluated both the collision strengths and Maxwellian averaged effective collision strengths for all the forbidden and allowed lines for transitions among the $3d^5$, $3d^4 4s$ and $3d^4 4p$ fine-structure levels. Proper delineation of the Rydberg resonance structures has been achieved through the use of very fine mesh of incident electron energies. In addition the effective collision strengths have been evaluated across a wide range of electron temperatures which have particular significance to astrophysical applications. We employ the new parallel suite of R-matrix packages, RMATRX II, which has recently been extended to include relativistic effects and the calculations were carried out on the national HPCx supercomputing facilities.

Comparisons are made with the earlier work of Bautista et al. [3] who adopted a different theoretical approach and model. We find that the effective collision strengths agree well for some transitions but significant discrepancies do exist for others. These disparities will have repercussions on diagnostic applications performed using this data.

References

[1] E.M. Monier, D.A. Turnshek, S.M. Rao, A. Weyant, AJ **138**, 1609 (2009)

[2] http://physics.nist.gov/PhysRefData

[3] M.A. Bautista, C. Ballance, T. R. Gull, H. Hartman, K. Lodders, M. Martínez, M. Meléndez, Mon. Not. R. Astron. Soc. **393**, 1503 (2009)

Excitation and ionization of hydrogen by antiprotons

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We present a theoretical study on the excitation and ionization of hydrogen atom by antiprotons for collision energies from 0.25 to 1000 keV. Taking a semiclassical approximation, we represent the relative motion of the antiproton with respect to the hydrogen atom by a classical trajectory, and calculate the time evolution of electron quantum mechanically by solving the time-dependent Schrödinger equation. The electronic wave function is propagated using the well-known second- order split-operator with the generalized pseudospectral discretization. The obtained ionization and state-selected excitation cross sections are found in good convergent and in good agreement with available experimental results and other theoretical calculations.

Posters, session B

Energies and lifetimes for the lowest 40 levels of Ti X

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Titanium belongs to the iron group of elements and is often an important constituent of fusion reactors. Many of its emission lines, including those from Al-like Ti X, have also been observed in astrophysical plasmas, and hence atomic data for Ti X are important for the modelling of plasmas. There are a number of calculations in the literature, as reviewed by Singh et al [1], but most of these include only a limited number of levels/transitions. To overcome this limitation, Singh et al have performed a very large calculation from the CIV3 code, and have reported lifetimes for 294 levels of Ti X, which belong to the ($1s^2 2s^2 2p^6$) $3s^2 3p$, $3s3p^2$, $3s^2 3d$, $3p^3$, 3s3p3d, $3p^2 3d$, $3s3d^2$, $3p3d^2$, $3d^3$, $3s^2 4l$, $3p^2 4l$, 3s3p4l, $3s^2 5l$, and $3s^2 6l$ configurations. Their calculations are semi- relativistic in LSJ coupling and include extensive CI (configuration interaction) with scores of configurations including up to the $n = 6$ orbitals. However, an important part of any calculation is the assessment of accuracy, for which experimental measurements are very useful. Fortunately, energies as well as lifetimes are available for a majority of the lowest 40 levels of Ti X. Therefore, it is comparatively easier to assess the accuracy of theoretical lifetimes. Since there are significant differences between the lifetimes of Singh et al not only with the measurements but also with other theoretical results, we have performed similar calculations with other independent atomic structure codes.

In the present work we adopt the GRASP (general-purpose relativistic atomic structure package) code, which is fully relativistic and is based on the jj coupling scheme. To make further accuracy assessments of the calculated results, we have also performed parallel calculations with the *Flexible Atomic Code* (FAC). This is also a fully relativistic code which provides a variety of atomic parameters, and yields results comparable to GRASP and CIV3, as demonstrated in many of our earlier papers on a variety of ions – see, for example, Aggarwal et al [2] for Mg-like ions.

With GRASP we have performed a series of calculations with increasing amount of CI and have included up to 1300 levels from 49 configurations involving up to the $n = 6$ orbitals. Similarly, with FAC we have performed 2 sets of calculations, namely FAC1 with the same 1300 levels as in GRASP calculations, and FAC2 which includes all possible combinations of the 3*3, (3*2) 4*1, 5*1 and 6*1, and (3*1) 4*2, 5*2 and 6*2 configurations, generating in total 12139 levels of Ti X. A comparison of our results, from both the GRASP and FAC codes, shows that the lifetimes listed by Singh et al [1] differ by up to 30% for many levels, and hence may not be reliable. Furthermore, the inclusion of extensive CI makes no appreciable contribution to the determination of energies and lifetimes of the lowest 40 levels of Ti X. Since the differences in lifetimes directly arise from the differences in radiative rates, there is a need to reexamine the data for A- values so that results can be applied with confidence in the modelling of plasmas. Detailed data along with comparisons will be presented during the conference.

This work has been financed by the EPSRC and STFC of the UK.

References

[1] J Singh, A K S Jha and M Mohan, J. Phys. B: At. Mol. Opt. Phys. **43**, 11505 (2010)

[2] K M Aggarwal, V Tayal, G P Gupta and F P Keenan, At. Data Nucl. Data Tables **93**, 615 (2007)

Energy levels, transition rates and lifetimes for low-lying levels in Cu-, Zn-, Ga-, and Ge-like ions of iodine

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Intercombination transitions connect level systems of different multiplicity, and therefore they help to establish the absolute position scale of those systems that do not comprise the ground state. Intercombination transition rates serve as sensitive probes of the quality of the wave functions used in atomic structure calculations. Moreover, the relative intensities of resonance and intercombination transitions are useful tools in plasma diagnostics. Resonance and intercombination transitions in few-electron ions are rather well established, but knowledge is much sparser for heavier multicharged ions with many electrons of which only a few are in the valence shell. In the present work, we have calculated the energies of low-lying levels, transition energies, and rates of ground state transitions in Cu- through Ge-like ions of iodine using the GRASP2K package which is based on the multiconfiguration Dirac-Fock method [1]. The wavelength and level lifetime results are employed to interpret prompt and delayed beam-foil spectra in the EUV [2].

References

[1] P. Jönsson, X. He, C. Froese Fischer and I.P. Grant, Comput. Phys. Commun. **177**, 597 (2007)

[2] E. Träbert, J. Phys.: Conf. Ser. (2010) [submitted]

Configuration interaction calculation of allowed and forbidden transitions in Fe II

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Earlier configuration interaction calculations of Fe II E1 transitions by our group (for example, [1, 2]) have been extended in the number of symmetries incorporated as well as the number of configurations used, and also to forbidden (E2 and M1) lines. In the poster we will present a small selection of our results, focusing on transitions which relate to astrophysical observations and laboratory measurements. The work has been completed using the general atomic structure package CIV3 [3, 4]. The A-values of many of the transitions are substantially influenced by CI mixing in the wave functions of one or both of the states of the transition. We will discuss how this mixing can be determined as accurately as possible.

Some of our work has already been published [5]. A sensitive test of the relationship between theory and observation in the study of transitions observed in active galactic nuclei is the [Fe II] $\lambda\,12567/\lambda\,16435$ line ratio. These two transitions have the same upper level ($a\ ^4\mathrm{D}_{7/2}$) so the flux density ratio is related to the ratio of the A-values. The ratio has been studied by a number of different theory groups as well as several observational teams. Our results confirm the earlier values of Nussbaumer and Storey [6] but are somewhat further from those of Quinet *et al* [7]. Of the rather wide range of observational results, we agree closely with unpublished results of Everett and Bautista, but find that those of Smith and Hartigan [8] are somewhat too high, while the majority of the observations of Rodriguez-Ardila *et al* [9] give much smaller values for this ratio.

Amongst comparisons with experimental work, we agree closely with the lifetime of $3\mathrm{d}^6(^3\mathrm{H})4\mathrm{s}\ ^2\mathrm{H}_{11/2}$ measured by Hartman et al [10]. Other comparisons will be presented in the poster.

References

[1] G. Corrégé and A. Hibbert, Astrophys. J. **627**, L157 (2005)
[2] G. Corrégé and A. Hibbert, Astrophys. J. **636**, 1166 (2006)
[3] A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975)
[4] R. Glass, A. Hibbert, Comput. Phys. Commun. **16**, 19 (1978)
[5] N.C. Deb and A. Hibbert, Astrophys. J. **711**, L104 (2010)
[6] H. Nussbaumer and P.J. Storey, Astron. Astrophys. **193**, 327 (1988)
[7] P. Quinet *et al*, Astron. Astrophys. Supp. Ser. **120**, 361 (1996)
[8] N. Smith and P. Hartigan, Astrophys. J. **638**, 1045 (2006)
[9] A. Rodriguez-Ardila *et al*, Astron. Astrophys. **425**, 457 (2004)
[10] H. Hartman *et al*, Astron. Astrophys. **397**, 1143 (2003)

Accurate configuration interaction calculation of transitions in Sn II

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Atomic structure data pertaining to singly-ionised tin is of particular relevance in astrophysical and fusion research applications. The strong 5p $^2P^o_{1/2}$ – 5d $^2D_{3/2}$ transition at 1400.45Å has been adopted by Sofia *et al* [1] in their determination of the interstellar gas-phase abundance of tin, while the transitions found at 5334Å (6p $^2P^o_{1/2}$ – 6d $^2D_{3/2}$), 5563Å (6p $^2P^o_{3/2}$ – 6d $^2D_{5/2}$) and 5591Å (5d $^2D_{3/2}$ – 4f $^2F_{7/2}$) have been highlighted by Foster *et al* [2] as representing suitable candidates for diagnostic purposes in the plasmas found in fusion power plants.

In response to the large inconsistencies that persist among and between previous theoretical and experimental work for these transitions, involving levels of the problematic, heavily-mixed ^{2}D LS term, we have undertaken an extensive configuration-interaction (CI) calculation using the general atomic structure package CIV3 [3, 4]. We will present our sequential determinations of the oscillator strengths (OS), (in the LS coupling scheme), as the complexity of our theoretical model was increased, demonstrating that the consistent inclusion of all important valence and core-valence effects was imperative in achieving results that not only converged, but converged to the 'correct' values. Paying particular attention to the 5s5p^2 – 5s^{2}5d ^{2}D interaction, our *ab initio* calculation has reproduced the experimental ^{2}D energy separations to within 1%, permitting the final minor corrections to the CI coefficients to be made by application of our customary 'fine-tuning' technique.

As expected, our final Breit-Pauli OS exhibit marked discrepancies with previous theoretical models based on limited CI expansions. We would argue that our calculation, being of a much larger scale, corresponds to a major improvement, (a claim validated by the extensive checks to which we have subjected our results, consistent with estimated uncertainties in the region of 5% for the stronger transitions), achieving an accuracy required for the proposed applications. On the experimental front, the consistency between our results and the greater part of the published measurements is a further indication of the reliability of our model, and where larger disparities do exist our calculations are supported by an independent theoretical investigation.

References

[1] U.J. Sofia, D.M. Meyer, J.A. Cardelli, Astrophys. J. **522**, L137 (1999)

[2] A.R. Foster, G.F. Counsell, H.P. Summers, J. Nucl. Mater. **363**, 152 (2007)

[3] A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975)

[4] R. Glass, A. Hibbert, Comput. Phys. Commun. **16**, 19 (1978)

New quasirelativistic approach for *ab initio* calculations of spectral properties of atoms and ions

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The quasirelativistic approach described in [1] and the computer programs based on it are widely known. However the quasirelativistic Hartree-Fock (QRHF) equations implemented there contain certain inaccuracies and substantial difficulties appear when attempting to use their solutions outside the Cowan code. In this context we have developed a new quasirelativistic approach different from the mentioned one. The most essential distinctions of our QRHF equations are the following:

- No statistical potentials are used. There are only conventional self-consistent field direct $V(nl|r)$ and exchange $X(nl|r)$ potentials in QRHF [2, 3].
- The finite size of the nucleus is taken into account in the determination of the electron interaction with a nucleus potential $U(r)$ while solving the quasirelativistic equations [4].
- The mass-velocity term splits into two parts – the direct potential and the exchange one.
- The contact interaction term contains only the nucleus potential $U(r)$ derivative in the numerator. No two-electron potentials are included in the numerator [2, 3].
- Only the direct part of the potential $V(nl|r)$ is included into the denominator of the contact interaction with a nucleus term [2].
- The contact interaction with a nucleus is taken into account not only for s-electrons, but also for p-electrons with some additional corrections made [3].
- The electron contact interaction may be taken into account when calculating the potential functions forming $V(nl|r)$ and $X(nl|r)$ [2].

The methods of calculation of energy spectra are similar to Breit-Pauli approach while performing theoretical investigations based on application of the equations. These methods are described in [5].

In order to take into account the correlation effects within the usual Hartree-Fock approach we widely use the transformed radial orbitals with variable parameters [6]. Their effectiveness is confirmed by numerous calculations. The analogous method is successfully applied by us within the quasirelativistic approach [5].

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References

[1] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, 1981)

[2] P. Bogdanovich and O. Rancova, Phys. Rev. A **74**, 052501 (2006)

[3] P. Bogdanovich and O. Rancova, Phys. Rev. A **76**, 012507 (2007)

[4] P. Bogdanovich and O. Rancova, Lithuanian. J. Phys. **42**, 257 (2002); P. Bogdanovich, V. Jonauskas and O. Rancova, Nucl. Instr. and Meth. B, **235**, 145 (2005)

[5] P. Bogdanovich and O. Rancova, Phys. Scr. **78**, 045301 (2008)

[6] P. Bogdanovich and R. Karpuškienė, Lithuanian J. Phys. **39**, 193 (1999)

The generation and analysis of expansion terms in the atomic stationary perturbation theory

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In present study, we give a brief overview of our recent studies of the atomic stationary many-body perturbation theory (MBPT) for open-shell atoms. The studies are focused on the generation of expansion terms with the arbitrary number of valence electrons and on the angular reduction of obtained terms. For the atoms with more than several valence electrons, hundreds of higher-order expansion terms are generated. Therefore, one must have a tool to produce these numerous deviations. For this purpose, the symbolic computer algebra programs *Mathematica* or *Maple* are widely used. We have developed the package *NCoperators* [1], written on *Mathematica*. The package accommodates a number of mathematical techniques: (i) angular momentum theory (AMT); (ii) second quantization representation (SQR); (iii) Rayleigh-Schrödinger perturbation theory (RSPT). In the effective operator approach, we propose the rules that enable to generate the n-order non-zero terms efficiently.

In this study, we also suggest the angular reduction scheme for the generated expansion terms. The scheme is of versatile disposition. That is, it is applicable to any-order perturbation theory (PT), if some elementary replacements are initiated. The angular reduction is performed for the n-body operators, expressed in a second quantized form, where $n \leq 3$. The reduction scheme also fits the coupled-cluster (CC) approach and it significantly differs from the usual techniques, exploited in other works [2, 3], where each term is represented in parallel with its diagrammatic representation. In contrast, we combine the generated terms in groups related to the different types (valence, core, excited) of one-electron orbitals and examine a couple of possible reduction schemes that were systematically studied in [4].

Table 1: The amount of n-body terms in the third-order MBPT.

n	$(kl\xi)$	d_n^+	d_n^-	n	$(kl\xi)$	d_n^+	d_n^-
1	(111)	13	3	2	(121)	20	10
	(122)	37	18		(211)	13	3
	(212)	14	2		(222)	64	31
	(223)	67	29		(132)	20	10
	(234)	57	18		(233)	75	28
					(244)	25	0

As an example, we demonstrate the number of calculated n-body terms ($n = k + l - \xi = 1, 2$) of the third-order effective Hamiltonian (Table 1). By the definition [5], the solutions of the eigenvalue equation of effective Hamiltonian represent the energy levels of atom. The quantities $(kl\xi)$ denote the ξ-pair contractions between the k-body parts of perturbation and the l-body parts of the wave operator. The $d_n^{\pm}$ denote the number of direct terms that represent the irreducible tensor operators, labeled by the irreducible representations $\Lambda \equiv LS$ or $\Lambda \equiv J$ and by the basis indices $\pm M$.

References

[1] R. Juršėnas and G. Merkelis, Materials Physics and Mechanics **9**, 42 (2010)

[2] H. C. Ho et. al., Phys. Rev. A **74**, 022510 (2006)

[3] S. G. Porsev and A. Derevianko, Phys. Rev. A **73**, 012501 (2006)

[4] R. Juršėnas and G. Merkelis, Cent. Eur. J. Phys. **8**, 480 (2010)

[5] I. Lindgren, J. Morrison, *Atomic Many-Body Theory*, Springer Series in Chemical Physics, vol. 13 (1982)

Characterization of anomalous Zeeman patterns in complex atomic spectra

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The effect of a magnetic field on the broadening of spectral lines and transition arrays in complex atomic spectra is investigated. The anomalous Zeeman pattern is a superposition of many absorption profiles with different Zeeman shifts, widths, asymmetries, sharpnesses and relative strengths [1,2]. The σ and π absorption coefficients can be expanded in powers of the magnetic field, the coefficients being expressed as a function of the moments of the Zeeman components. We discuss different ways of calculating these moments in terms of the quantum numbers and Landé factors of the levels involved in the transition. Using our recently published recursive approach for the numbering of LS-terms of an arbitrary configuration [3], we propose a simple approach to estimate the contribution of a magnetic field to the width (and to the higher-order moments) of a transition array of E1 lines.

References

[1] I.I. Sobelman, *Introduction to the Theory of Atomic Spectra* (Pergamon, New York 1972)

[2] J. Bauche and J. Oreg, J. Physique Colloque C1 **49**, 263 (1988)

[3] F. Gilleron and J.-C. Pain, High Energy Density Phys. **5**, 320 (2009)

Mixing of configurations $3s3p^{N+1}$ and $3s^23p^{N-1}3d$ and its influence on the photoexcitation and emission spectra in isoelectronic sequences

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The transitions $3s^23p^N$ – $(3s3p^{N+1} + 3s^23p^{N-1}3d)$ with the relatively small number of lines in few and multiply charged ions are widely used for the diagnostics and modelling of astrophysical and laboratory plasma. Thus, many experimental and theoretical data of energy levels, oscillator strengths and other characteristics of transitions are published for such atoms at various degrees of ionization. The comprehensive data are collected in the NIST Atomic Spectra Database [1]. The aim of our work was to investigate the general features of such transition arrays in a wide interval of ionization degrees, to establish the regularities of influence of such correlations on the structure of photoexcitation and emission spectra.

We consider the dipole electric excitations from the ground level of $3s^23p^N$ configuration; it corresponds to the photoexcitation or excitation by electron impact in the plain wave Born approximation. The calculations have been performed for the isoelectronic sequences with N =1–5 at ionization stages $5 \leq q \leq 35$. The two configuration quasirelativistic approximation has been used [2], which properly describes the main features of considered spectra. This work continues the investigation of the role of configuration mixing with symmetric exchange of symmetry (SEOS) in atomic spectra [3]. It is shown that the redistribution of intensity from 3s–3p to 3p–3d transitions and its concentration in a narrow interval of wavelengths manifests itself in the photoexcitation and emission spectra for all isoelectronic sequences, but is more expressed for the half-filled and almost-filled $3p^N$ shell. It takes place at the condition that in the single-configuration approximation the energy levels of $3s3p^{N+1}$ configuration, mainly populated by the photoexcitation from the ground level, are situated below such levels of $3s^23p^{N-1}3d$ configuration. This condition is fulfilled for the isoelectronic sequences up to $q = 30$; at larger ionization degrees such levels of both configurations begin to overlap and it causes the widening of spectrum. For $3p^N$ – $3p^{N-1}3d$ transitions at $N = 4$ and 5 another reason of the narrowing of spectrum is the existence of term groups formed by the Coulomb exchange interaction.

The enhancement of transitions in the single-configuration approximation is related with the possibility to introduce the wavefunction basis with the additional selection rule [4]. The cancellation of many lines due to SEOS configuration mixing also indicates the existence of some selection rule.

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References

[1] NIST Atomic Spectra Database, Version 3 (http://www.nist.gov/physlab/data/asd.cfm)

[2] R.D.Cowan, *The Theory of Atomic Structure and Spectra* (Berkeley, CA: University of California Press, 1981)

[3] V.Jonauskas, S.Kučas, and R.Karazija, J. Phys. B: Atom. Mol. Opt. Phys. **40**, 2179 (2007)

[4] A.Bernotas and R.Karazija, J. Phys. B: Atom. Mol. Opt. Phys. **34**, L741 (2001)

Ionization potentials, electron affinities, resonance excitation energies, oscillator strengths and ionic radii of element Uus (Z=117) and Astatine

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Very recently, the discovery of element Uus was announced by the Joint Institute for Nuclear Research in Dubna, Russia [1]. The synthesis of Uus fills the gap on the periodic table up to element 118 and offers more details to study the heaviest known "island of stability".

With the great achievement of synthesis, another aspect of Uus may attract people's interests that the strong relativistic effects may largely influence its atomic structure and further change its physicochemical property. However, chemical investigations for Uus are extremely difficult because of its very short lifetimes (only 14 and 78 milliseconds half-lives for ^{293}Uus and ^{294}Uus, respectively) and yields of a few atoms [1], theoretical calculations therefore can provide useful information for such experiments and may be the only way to investigate a particular aspect of its chemistry.

To provide reliable data for the predictions of some chemical properties of Uus and its homolog At, multi-configuration Dirac-Fock (MCDF) method [2] has been employed to calculate the ionization potentials (IPs), electron affinity (EA), resonance excitation energies (EEs) and ionic radii (IR) for Uus and At. Main valence correlation effects were taken into account. The correction of the Breit interaction with the low frequency approximation and the QED effects including the vacuum polarization and selfenergy correction were also estimated. In this work, the GRASP2K package [3] was used to calculate the wave functions of the atomic and ionic systems and the transition matrix elements. The uncertainties of calculated IPs, EAs and IR for Uus and At resulting from incomplete inclusion of the correlation effects and all other effects were reduced through a widely-used extrapolation procedure [4]. The present results are in good agreement with available experimental and other theoretical values, and can be used for the predictions of some important physicochemical properties of element Uus and At and their compounds in comparison with the lighter homologues. In addition, it was also found that the strong line corresponding to the transition $[7s^2 7p_{1/2}^2 7p_{3/2}^2 8s_{1/2}]_{5/2} \rightarrow [7s^2 7p_{1/2}^2 7p_{3/2}^3]_{3/2}$ at 3.249 eV just lies in the prime energy region, which is suitable for observing low-lying level structure for superheavy atoms using the resonance ionization spectroscopy (RIS) technique [5].

References

[1] Yu. Ts. Oganessian et al., Phys. Rev. Lett. **104**, 044602 (2010)
[2] I. P. Grant, Adv. Phys. **19**, 747 (1970)
[3] P. Jönsson, X. He et al., Comput. Phys. Commun. **177**, 597 (2007)
[4] B. Fricke et al., Radiochim. Acta. **62**, 17-25 (1993)
[5] S. Fritzsche et al.; Eur. Phys. J. D **45**, 107 (2007)

A selection rule and coupling scheme for transitions involving hyperfine structure

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Intercombination transitions, such as transitions between the singlet and triplet states of helium, are strongly suppressed because the dipole transition operator is spin-independent. They can proceed only through the spin-dependent terms in the Breit interaction that mix the singlet and triplet states. It is well known that the strength of these transitions increases rapidly with nuclear charge in proportion to Z^8 due to spin-orbit mixing of the singlet and triplet wave functions. What is not so well known is that hyperfine structure in atoms such as ^{3}He can also induce intercombination transitions, even in neutral helium. The key point is that hyperfine structure comes primarily from the inner $1s$ electron, and so the hyperfine splitting tends to a constant at the series limit for the outer nl electron. On the other hand, fine structure splittings between the singlet and triplet states of the same n decrease in proportion to $1/n^3$. Thus, the two effects become comparable in size for an intermediate value of n. In this region of strong mixing, some normally suppressed transitions are strongly enhanced, and some normally strong transitions are suppressed. As shown in a recent study [1], the patterns of enhancement and suppression can be understood by using an alternative coupling scheme to the usual $(L,S)J,I;F$ scheme in which L and S are coupled to form J, and then J is coupled with the nuclear spin I to form the total angular momentum F. In the alternative scheme, I and S are first coupled to form K, and then K and L are coupled to form F. The advantage is that the dipole transition operator $-e\mathbf{r}$ is independent of both electronic and nuclear spin, and so K does not change in the transition (to a good approximation).

The usefulness of the K selection rule will be illustrated by various examples, and its range of validity will be explored.

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Reference

[1] I.A. Sulai, Qixue Wu, M. Bishof, G.W.F. Drake, Z.-T. Lu, P. Mueller,1 and R. Santra, Phys. Rev. Lett. **101**, 173001 (2008).

Hyperfine structure of low-lying states of ^{14,15}N

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Determination of hyperfine structure constants has various astronomical interests [1]. For ground and metastable states, hyperfine structures can often be determined with good accuracy, providing precious guidelines for *ab initio* calculations. For excited states that are available only through sub-doppler methods in the optical region the experimental values are less reliable, and theoretical evaluations can bring useful information.

In 1943, Holmes [2] measured a surprisingly large variation of the specific mass isotope shifts from one multiplet component to another in some transitions between the configurations $2p^2 3s$ and $2p^2 3p$ of ^{14,15}N. Although this observation was confirmed by sub-doppler spectroscopy experiments [3, 4], Jennerich *et al.* [4] pointed out that the experimental isotope shift values are critically dependent of the interpretation of the hyperfine structures of the ^{14}N and ^{15}N spectra. In the conclusions of their work, they appealed for further theoretical investigation to confirm observations.

Hyperfine structure parameters were calculated recently by Jönsson *et al.* [5] for $2p^2(^3\mathrm{P})3s\ ^4\mathrm{P}_J$, $2p^2(^3\mathrm{P})3p\ ^4\mathrm{P}^o_J$ and $2p^2(^3\mathrm{P})3p\ ^4\mathrm{D}^o_J$ levels, using the *ab initio* multiconfiguration Hartree-Fock method (MCHF) implemented in the ATSP2K package [6]. The resulting theoretical hyperfine coupling constants are in complete disagreement with the experimental values of Jennerich *et al.* [4] deduced from the analysis of the near-infrared Doppler-free saturated absorption spectra. We propose a new interpretation of the recorded weak spectral lines. If the latter are reinterpreted as crossover signals, a new set of experimental hyperfine constants is deduced, in very good agreement with the *ab initio* predictions. The ambiguity in the assignation of the recorded spectra is due to strong line shape perturbation. The present analysis washes out the J-dependency of specific mass shift (SMS) found for $3p\ ^4\mathrm{P}^o$ and $3p\ ^4\mathrm{D}^o$ multiplets. On the contrary, a somewhat large SMS J-dependency is deduced for the even parity $3s\ ^4\mathrm{P}$ multiplet. This effect is enhanced by the strong non-relativistic mixing with the $1s^2 2s 2p^4\ ^4\mathrm{P}$ term, which depends strongly of the total atomic electronic momentum J once relativistic corrections are added.

References

[1] P. Jönsson, Journal of Physics: Conference Series **72**, 012011 (2007)

[2] J.R. Holmes, Phys. Rev. **63**, 41 (1943)

[3] P Cangiano *et al.*, Phys. Rev. A **50**, 1082 (1994)

[4] R.M. Jennerich *et al.*, Eur. Phys. J. D **40**, 81 (2006)

[5] P. Jönsson *et al.*, J. Phys. B: At. Mol. Opt. Phys. **43**, 115006 (2010)

[6] C. Froese Fischer *et al.*, Comp. Phys. Commun. **176**, 559 (2007)

Calculation of the energy levels of the lithium atom using the varying *g*-factor method

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We calculate the energy levels of a lithium atom in the presence of an external magnetic field $B = B\hat{z}$, using the varying g-factor method or diagram method [1] which was first introduced by Saglam et al. [2, 3]. We consider the non-relativistic Hamiltonian [4] with the energy eigenvalues; expression $E(n, l, m_j, B^*) = -C/n^2 - \mu_{\rm B}\, B^*(m_l + g^* m_s)$ corresponding to the eigenstate of $|n, l, m_j\rangle$ hydrogen-like atoms. Here the constant C is determined through the ionization energy, g^* is the effective Lande g-factor, $\mu_{\rm B} = e\hbar/(2mc)$ is the Bohr magneton and B^* is the effective magnetic flux density (effective magnetic field) at the state $|n, l, m_j\rangle$. When an atom is subjected to a laser beam because of the photons magnetic moment [5] and hence the large intrinsic magnetic field, we will have a non-zero magnetic field inside the atom. The plots of $E(n, l, m_j, B^*)$ against g^* gives us a diagram which has crossings at certain g^* values (such as $0, 1, 2, 3, 4, \ldots$). The energies at these crossing points correspond to the energy levels of the lithium atom. We find a complete agreement (within the 1% margin of error) with the previously found experimental energy values. In addition as a result of the present calculations we can also find an guide in producing new laser lights in Lithium atom.

References

[1] Bousiakou L. G., Babsail L. and Saglam M. (2010) [submitted for publication]

[2] Saglam M and Boyacioglu B, Phys. Stat. Sol. (b) **230**(1), 133 (2002)

[3] Saglam M, Physica E, 17,345 (2003)

[4] Drake G W F, *Handbook of Atomic, Molecular and Optical Physics* (Springer, 2006)

[5] Sahin G and Saglam M, XXIV ICPEAC, J. of Physics: Conference Series **194** (IOP Publishing, 2009)

QED corrections for the valence electron in heavy and superheavy atoms

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The first-order electron QED corrections for valence electron are investigated for the neutral Ag, Rg and their neighbors of the Mendeleev Periodic Table within a framework of the Post Dirac-Hartree-Fock method. The including of SE effects in such procedure was done for superheavy atoms. The given results provide the limit of the accuracy for the modern relativistic theoretical calculations for the such superheavy elements and open the discussion for the accuracy of the QED corrections in the superheavy elements itself.

Relativistic mass shift calculations with the GRASP2K package

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The tensorial form of the relativistic mass shift operator (RMS) to the lowest order in m/M [1, 2] (in a.u.)

$$H_{\rm MS} = \frac{1}{2M}\sum_{i,j}^{N}\left[\boldsymbol{p}_i\cdot\boldsymbol{p}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\right)\cdot\boldsymbol{p}_j\right] \tag{1}$$

is derived and implemented in the GRASP2K package [3, 4]. The inclusion of this relativistic operator allows us to investigate more consistently mass shift effects in the full relativistic approach [5].

Multiconfiguration Dirac-Hartree-Fock calculations including single (S), double (D) and triple excitations (T) are performed for Li I (see Table 1). The new results are compared with the corresponding values obtained with the same relativistic wave functions and the uncorrected operator adopted in [6], and with the non relativistic Multiconfiguration Hartree-Fock results [7].

Table 1: Specific mass shift parameter $S_{\rm SMS}$ in a.u. for Li I for $1s^2 2s\ ^2S_{1/2}$.

AS_n	SD		SDT		MCHF [7]
	OLD	NEW	OLD	NEW	
	$1s^2 2s\ ^2S_{1/2}$				
$n=5$	0.3010343291	0.3008225633	0.3013767853	0.3011648528	
$n=6$	0.3010361585	0.3008243666	0.3014579841	0.3012459847	
$n=7$	0.3019544951	0.3017423943	0.3024396569	0.3022273237	
$n=8$	0.3018617523	0.3016497153	0.3024115843	0.3021992791	
$n=9$	0.3017987398	0.3015867742	0.3023512554	0.3021390203	
$n=10$	0.3018561821	0.3016442119	0.3024141615	0.3022019200	
$n=11$	0.3018280421	0.3016160885			0.30205339864

Results for other levels and heavier systems will be presented to illustrate the capability of the present code extension.

References

[1] I.I. Tupitsyn, V.M. Shabaev, J.R. Crespo López-Urrutia, I. Draganic, R. Soria Orts and J. Ullrich, Phys. Rev. A **68**, 022511 (2003)

[2] S.G. Porsev, M.G. Kozlov, D. Reimers, Phys. Rev. A **79**, 032519 (2009)

[3] P. Jönsson, X. He, C. Froese Fischer and I.P. Grant, Comput. Phys. Commun. **177**, 597 (2007)

[4] G. Gaigalas, S. Fritzsche, I.P. Grant, Comput. Phys. Commun. **139**, 263 (2001)

[5] I.P. Grant, Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation (Springer, New York, 2007)

[6] P. Jönsson and C. Froese Fischer, Comput. Phys. Commun. **100**, 81 (1997)

[7] M. Godefroid, C. Froese Fischer, P. Jönsson, J. Phys. B: At. Mol. Opt. Phys. **34**, 1079 (2001)

Origin of high-energy X-ray satellites spectra in the Lβ_2 region

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The X-ray satellite spectra arising due to $2p_{3/2}^{-1}3x^{-1}$–$3x^{-1}4d^{-1}$ ($x \equiv$ s, p, d) transition array, in elements with $Z = 42$ to 90, have been calculated. While the energies of various transitions of the array have been determined by using available Hartree–Fock–Slater (HFS) data on $1s^{-1}$–$2p^{-1}3x^{-1}$ and $2p_{3/2}^{-1}$–$3x^{-1}, 3x'^{-1}$ Auger transition energies, their relative intensities have been estimated by considering cross sections of singly ionized $2x^{-1}$ ($x \equiv$ s, p) states and then of subsequent Coster–Kronig and shake off processes. The calculated spectra have been compared with the measured satellite energies in Lβ_2 spectra. Their intense peaks have been identified as the observed satellite lines. The one to one correspondence between the peaks in calculated spectra and the satellites in measured spectra has been established on the basis of the agreement between the separations in the peak energies and those in the measured satellite energies. It has been established that four satellites observed in the high energy side of the Lβ_2 region of X-ray spectra of various elements and named $\beta_2^{\rm I}$, $\beta_2^{(b)}$, $\beta_2^{\rm II}$ and $\beta_2^{(c)}$ in order of increasing energy are mainly emitted by $2p_{3/2}^{-1}3d^{-1}$–$4d^{-2}$ transitions. In the present study, we report the transition assignments to the satellites $\beta_2^{\rm I}$, $\beta_2^{(b)}$, $\beta_2^{\rm II}$ and $\beta_2^{(c)}$ reported in the spectra of elements with $Z =$ 42 to 90. It is observed that out of these four satellites, $\beta_2^{(b)}$ can be assigned to superposition of $^3F_4$–$^3G_5$ and $^3F_4$–$^3D_3$ transitions and that this must be the most intense of all these satellites in the elements $Z = 42$–50. In the range of elements $Z = 52$ to 77, the satellite $\beta_2^{\rm I}$ is emitted by these transitions. The same transitions have been proved to be the main origin of the satellite $\beta_2^{\rm II}$, reported in the elements $_{79}$Pt to $_{90}$Th. It has been well established that the transitions $^1F_3$–$^1G_4$ and $^3D_3$–$^3D_3$ is the main source of the emission of the satellite $\beta_2^{\rm II}$ in the elements $_{42}$Mo to $_{77}$Ir. Coming to the other two satellites in this region of the spectra, the line $\beta_2^{(c)}$, observed in the spectra $_{42}$Mo to $_{50}$Sn, is mainly assigned to the transition $^3P_1$–$^3D_2$. Lastly, the line $\beta_2^{\rm I}$, observed in the spectra of elements $Z = 42$ to 46, is assigned to the transitions $^3D_3$–$^3F_4$ and $^1D_2$–$^1F_3$, while in the range of elements with $Z = 78$ to 90, $\beta_2^{\rm I}$ has been assigned to these transitions. In the elements $_{48}$Cd and $_{50}$Sn, the line $\beta_2^{\rm I}$ has been associated with transition $^3F_4$–$^3F_4$. Unfortunately, no experimental data are available on the intensities of these satellites. This suggests a need of detailed investigation, both theoretical and experimental, of these spectra.

References

[1] Y. Cauchois and C. Senemaud, *X-ray Wavelength Tables*, 2nd ed. (Pergamon Press, Oxford, 1978) pp. 217–314

[2] S. N. Soni and M. H. Massoud, J. Phys. Chem. Solids **58**(1), 145–151 (1997)

[3] F. Parente, M. H. Chen, B. Crasemann and H. Mark, At. Data Nucl. Data Tables **26**, 383–466 (1981)

[4] M. Vlaicu, T. Tochio, T. Ishizuka, D. Ohsawa, Y. Ito, T. Mukoyama, A. Nisawa, T. Shoji and S. Yoshikado, Phys. Rev. A **58**(5), 3544–3551 (1998)

[5] S. N. Soni and S. Poonia, J. Phys. Chem. Solids **61**(9), 1509–1518 (2000)

[6] S. Poonia and S. N. Soni, J. Phys. Chem. Solids **62**(3), 503–511 (2001)

[7] S. Poonia and S. N. Soni, Indian J. Pure and Appl. Phys. **41**(3), 236–241 (2003)

[8] Surendra Poonia and S.N. Soni, Indian J. Pure and Appl. Phys. **45**(2), 119–126 (2007)

[9] Surendra Poonia and S.N. Soni, Indian J. Physics **83**(3), 325–337 (2009)

Atomic data: Photon absorption, electron scattering, vacancy decay

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We present calculation data for different characteristics of atomic processes with participation of photons and electrons: photoabsorption and electron scattering cross-sections, and probabilities of decay of vacancies formed in these processes for a big number of atoms and ions. Some attention is given also to photoionization and vacancy decay in endohedrals and to positron–atom scattering.

The calculations are performed in the frames of the best one-electron Hartree–Fock and with account of multi-electron correlations in the Random Phase Approximation with Exchange. The influence of correlations usually is very important. We use the version of it that is based on technique of Feynman diagrams. The theoretical description of the processes is given briefly, but includes formulation of the basic ideas, and also key formulas.

The collected data and the methods used in their derivations can be useful for the theoretical description of already performed experiments, and in suggesting of new ones.

These Data are required in a number of scientific domains connected to investigation of electronic structure and of physical processes in solids and liquids, molecules and clusters, astronomical objects, solar and planet atmospheres, atomic nucleus and so on. Deep understanding of chemical reactions and processes is impossible without clear, deep and accurate knowledge of atomic structure and processes with participation of atoms.

One should not forget also that all atoms but hydrogen and, perhaps, helium, are relatively complex systems by itself. They are still objects of intensive theoretical and experimental studies, in which rather sophisticated methods are applied. For planning corresponding experiments, for estimating the value of very sophisticated new theoretical approaches one needs data that are reasonably accurate, sufficiently general and relatively easy to obtain. Our data with also serve this aim.

The role, played by atoms in macrophysics, chemistry, biology, some domains of engineering and the entire macro world is similar to the role played by elementary particles in micro world. Indeed, atoms are the bricks, the main building elements of which all the macroscopic world is constructed. The "glue" that keeps together the macroscopic bodies is the inter-atomic interaction that is modified to some extend, in many cases considerably, when many atoms are bound together.

In spite of obvious demand, there is no such a data available. Usually, if it is data on experiment, the main focus is on the results of measurements, which are compared to available theoretical results. If a data are theoretical, it concentrates on details of the presented theoretical approaches, illustrating their achievements by comparing with experimental data. In both cases the main interest is information on considered physical process. Our aim is to concentrate on the calculation data itself. To obtain the data, we will use theoretical methods, which open the possibility of extensive calculations and at the same time are as accurate as possible. Of course, it would be best of all to have simple analytic formulas to calculate all necessary atomic characteristics and probabilities. Alas, the atomic structure is complicated enough. So, the analytical formulae are too crude. On the other hand, rapid development of computing facilities, PC in particular, permits to perform relatively accurate calculations, using rather complicated theoretical approaches. The result of such an approach is the subject of data collection. Main attention will be given to presenting the results of calculations. As to the theoretical methods employed, they will be described briefly in order to clarify how the presented results are obtained.

Dielectronic recombination of W^{37+} ions

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Tungsten will be used for a certain plasma-facing components in the divertor region of the International Thermonuclear Experimental Reactor (ITER), and will also be used for the diagnostics of the erosion of heavy species into the plasma. In order to consider the inuence of DR on the ionization balance of tungsten ions in divertor plasma modeling and radiative plasma cooling, we calculate the dielectronic recombination rate coeficients of W^{37+} ions by using the Flexible Atomic Code (FAC) [1].

The calculated DR rate coeficients are given in Fig. 1(a). It can be seen that the contribution from 4p subshell excitation dominates in the whole energy region and it is larger than 4d subshell excitation near one order of magnitude. DR rate coeficients from 4s, 4p and 4d subshell excitations increase with the decreasing electron temperature in the low temperature. The contribution from 3d shell excitation play an additional important role in the total DR rate coeficients at high temperature, and the relative contributions from 3s, 3p and 3d subshell excitations increase smoothly with the increasing temperature.

The radiative recombination (RR) rate coeficient and three-body recombination (TBR) rate coefficient, which are also two important recombination processes in plasmas, are estimated simply [2] in Fig. 1(b). The number of free electrons density is assumed as 10^{14} cm^{-3} [3]. It can be seen that the DR rate coeficients are great than the RR rate coeficients and TBR rate coeficients for the whole energy region. Clearly, DR is predominate the ionization balance. This conclusion is similar to the case of Sn^{10+} ions [4].

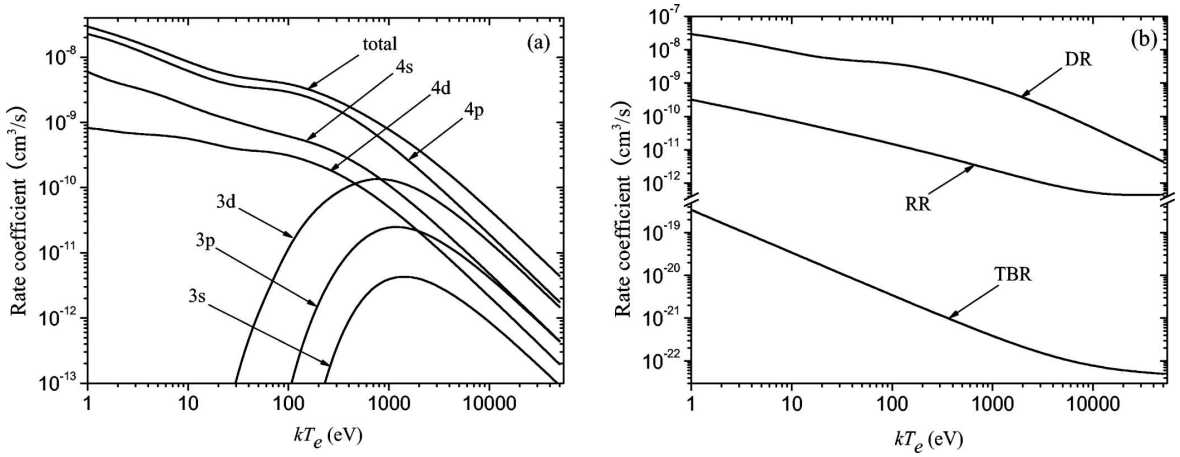

Figure 1: (a) The DR rate coeficients of the W^{37+}ions. (b) DR, RR and TBR rate coeficients of W^{37+} ions.

References

[1] M. F. Gu, Can. J. Phys. **86**, 675 (2008)

[2] N. J. Peacock and R. S. Pease, J. Phys. D: Appl. Phys. **2**, 1705 (1969)

[3] C. H. Skinner, Can. J. Phys. **86**, 285 (2008)

[4] Y. B. Fu, C. Z. Dong, M. G. Su and G. O'Sullivan, Chin. Phys. Lett. **25**, 927 (2008)

Analysis of visible light emissions of highly charged tungsten ions in electron beam ion trap

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In recent decades, a strong interest has been focused by many authors on the properties of atomic or ionic tungsten, which is one of the desirable candidates for wall or divertor materials of magnetic confinement fusion (MCF) reactor. Spectroscopic measurements for wide range of the wavelengths of photo-line emissions are desired for various charge states of tungsten ions. Among them, visible lights emitted from highly charged tungsten ions are of special interest; they are mainly realized by magnetic dipole transitions between the fine structure levels of ions and therefore they suffer less self-absorption by surrounding plasmas providing us with a great advantage for the diagnostics of core plasmas.

In recent years, Nakamura and his coworkers made a systematic measurement, using two EBITs (Electron Beam Ion Traps) in Tokyo [1, 2], of the light emissions from highly charged tungsten ions. They have reported new spectral data of visible line emission spectra [3, 4] and found a number of new emission lines that are ranging 350 nm to 410 nm for ions ranging tungsten 12+ to 30+.

In the present report, we study the source of these visible line emissions in terms of accurate non-empirical atomic structure calculations and of population kinematics analyses. In the EBIT ion source, the tungsten ion plasma always receives the impact of energetic electrons that are confined by a coaxial external magnetic field. The ions are normally believed to be in ground state configurations for each ionic charge state, and in this consequence, the visible line emissions may be supposed to be due to magnetic dipole transitions between fine structure terms of the ground state. We, firstly, examine the hypothesis by performing line by line assignment to the experimental spectra. The GRASP package [5] for multi-configuration Dirac-Fock atomic structure calculation provides us with the transition energies that are accurate enough to discriminate if the emission lines are from the ground state configurations or from any excited state configurations. We, secondly, try to reproduce the emission spectra by modifying a population kinetics code that has been used for the analysis of boron like ion plasmas [6].

We have assignd new visible emission lines. We have compared our synthesized spectra to the experimental spectra [3, 4]. We may be suggested that the spectroscopy of the visible line emissions of tungsten ions gives a reliable tool for the diagnostics of the MCF plasmas.

References

[1] N. Nakamura et al., Phys. Scr. T **73**, 362 (1997)

[2] N. Nakamura et al., Rev. Sci. Instrum. **79**, 063104 (2008)

[3] H. A. Sakaue, Invited Talk of EBIST2010 (April 7 to 10, 2010, Stockholm)

[4] A. Komatsu et al., Abstract Book of HCI2010 (August 31 to September 3, 2010, Shanghai)

[5] P. Jönsson et al., Comp. Phys. Communications **177**, 597-622 (2007)

[6] I. Murakami et al., Annual Report of NIFS, April 2005 to March 2006, 425 (2006).

Lowest 977 energy levels, E1 transition probabilities and lifetimes for W^{24+}

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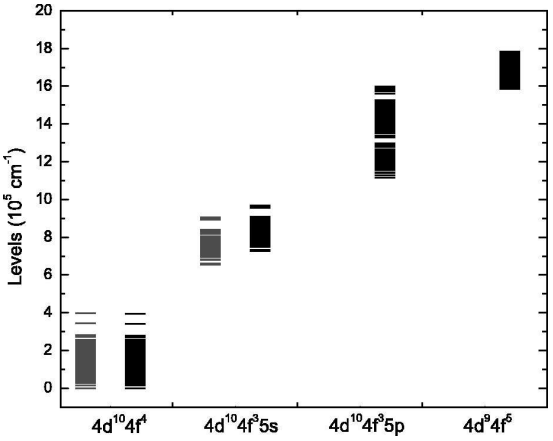
Tungsten (W) is used as a wall material in tokamaks. For detailed analysis of the thermonuclear plasma spectra, impurities in it, a large number of its spectroscopic parameters is needed. Therefore, it is important to perform a theoretical modelling of the atomic structure of various tungsten ions. Such ions, having simple electronic configurations of open shells, are studied widely both experimentally and theoretically, but this is not the case for ions, having open f-shell, due to the large number of the energy levels. The use of the second quantization method in coupled tensorial form combined with quasispin technique, described in [1], opens the real possibilities to efficiently consider such configurations, as well. The goal of this paper is to illustrate these possibilities.

We have performed the large-scale multiconfiguration Hartree-Fock and Dirac-Fock calculations for the lowest 977 energy levels of W^{24+} ion in different approaches (MCHF+BP in grey (left) and MCDF+B+QED in black (right) on the Figure below).



All these levels correspond to [Kr]$4d^{10}4f4$, [Kr]$4d^{10}4f^35s$, [Kr]$4d^{10}4f^35p$ and [Kr]$4d^94f^5$ configurations. The relativistic corrections were taken into account in the Breit-Pauli and Breit (without and with QED corrections) approximations with the help of ATSP [2] and GRASP2 packages[3,4]. The role of correlation, relativistic and QED correctons is discussed. Transition probabilities, line strengths in Coulomb and Babushkin gauges are obtained for the electric dipole (E1) transitions among these levels. The agreement between two gauges is within 2.5 % for the strong transitions. The lifetimes of the levels, belonging to the configuration [Kr]$4d^{10}4f^35p$, are also calculated in Coulomb and Babushkin gauges. The analysis of the role of electric and magnetic electronic transitions of higher multipolarities has been performed, as well.

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References

[1] Z. Rudzikas, *Theoretical Atomic Spectroscopy* (Cambridge University Press, 1997, 2nd ed. 2007) p. 427

[2] C. Froese Fischer, G. Tachiev, G. Gaigalas, M.R. Godefroid, Comput. Phys. Commun. **176**, 559 (2007)

[3] P. Jönsson, X. He, C. Froese Fischer, I.P. Grant, Comput. Phys. Commun. **177**, 597 (2007)

[4] C. Froese Fischer, G. Gaigalas, Y. Ralchenko, Comput. Phys. Commun. **175**, 738 (2006)

Quasirelativistic treatment of spectral characteristic of W^{37+}, W^{36+} and W^{35+}

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Recently a scientific interest in spectral characteristics of tungsten and its ions has grown noticeably. It is caused by the fact that tungsten as a heat-resistant material is planned to use while building a new fusion reactor within ITER project. Tungsten atoms can penetrate into the plasma and be ionised to very high degrees when the thermonuclear plasma interacts with the walls of the reactor. Seeking to take into account an influence of the tungsten ions on the thermonuclear plasma it is necessary to accumulate a large amount of information on spectral characteristics of tungsten ions in databases. In spite of all this theoretical investigations play an important role.

In present work a possibility to employ the quasirelativistic approach [1-3] for calculations of energy spectra, characteristics of E1, E2, M1 electron transitions and radiative lifetimes of W^{37+}, W^{36+} and W^{35+} ions is investigated. The ground configurations of these ions contain an open $4d^N$-shell ($N = 1$, 2 and 3) and two first excited configurations $4p^5 4d^{N+1}$ and $4p^6 4d^{N-1} 4f$ are strongly mixed.

The energy spectra are calculated: a) within a simplest approach (a single-configuration approximation for a ground state and mixing of two excited configurations); b) taking into account mixing of all quasidegenerate configurations (when virtual excitations do not change the main quantum number) of the same parity; c) within the multiconfiguration approach (the transformed radial orbitals [4] have been used to describe virtual excitations into shells with $n \geq 5$) with different numbers of the admixed configurations. A comparison of the obtained energy spectra and wavelengths with the experimental data available [5] has revealed, that it is possible to achieve a coincidence of the first two significant digits. Usually such accuracy is sufficient for employment of the wavelengths obtained into calculations of the transition characteristics and radiative lifetimes.

Acknowledgement. This work is partially supported by the European Communities under the FP7 contract of Association between EURATOM/LEI FU07-CT-2007-00063.

References

[1] P. Bogdanovich and O. Rancova, Lithuanian. J. Phys. **42**, 257 (2002);
P. Bogdanovich, V. Jonauskas and O. Rancova, Nucl. Instr. and Meth. B, **235**, 145 (2005)
[2] P. Bogdanovich and O. Rancova, Phys. Rev. A **74**, 052501 (2006)
[3] P. Bogdanovich and O. Rancova, Phys. Rev. A **76**, 012507 (2007)
[4] P. Bogdanovich and O. Rancova, Phys. Scr. **78**, 045301 (2008)
[5] A.E. Kramida, T. Shirai, At. Data Nucl. Data Tables **95**, 305 (2009)

Magnetic dipole lines in highly-charged ions of tungsten

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A significant portion of the research being carried out on the EBIT at NIST is directed toward production of data that will be of importance for diagnostics of plasmas such as will be found in ITER. Since tungsten will be used as a plasma facing wall material in the divertor region of ITER, its spectral properties are of special interest. In earlier experiments we observed spectra of W at beam energies 2.0-4.3 keV [1] and 8.8-25 keV [2]. In this work the EUV spectra of highly ionized W were measured at intermediate beam energies varying from 4.5 to 7.0 keV. We observed the region from 10 to 20 nm with a flat-field grazing-incidence spectrometer. At these beam energies the W ions range from Cu-like W^{45+} to Cl-like W^{57+}. The allowed electric-dipole transitions between the ground and excited configurations are primarily located below 10 nm, while the majority of the spectral lines observed in the 10-20 nm region are due to magnetic-dipole (M1) transitions. The measured spectra from the non-Maxwellian EBIT plasma are analyzed using the collisional-radiative code NOMAD [3] with atomic data generated with the flexible atomic code [4]. Altogether, we identified 37 M1 lines in this region; almost all are due to transitions within the $3d^n$ ground configurations. The intensities of the M1 lines are highly sensitive to electron densities in various plasmas and thus can be used for density diagnostics in many types of plasmas, including ITER. Further experiments are planned to observe similar spectra in neighboring ions of Hf, Ta, and Au.

Acknowledgement. This work is supported in part by the Office of Fusion Energy Sciences of the U.S. Department of Energy.

References

[1] Yu. Ralchenko et al., Spectra of W^{39+}-W^{47+} in the 12-20 nm region observed with an EBIT light source, J. Phys. B: At. Mol. Opt. Phys. **40**, 3861 (2007)

[2] Yu. Ralchenko et al., EUV spectra of highly-charged ions W^{54+}-W^{63+} relevant to ITER diagnostics, J. Phys. B: At. Mol. Opt. Phys. **41**, 021003 (2008)

[3] Yu.V. Ralchenko and Y. Maron, Accelerated recombination due to resonant deexcitation of metastable states, J. Quant. Spectr. Rad. Transf. **71**, 609 (2001)

[4] M.F. Gu, Flexible Atomic Code, Can. J. Phys. **86**, 675 (2008)

Spectra of moderately charged tungsten ions and isoelectronic ions of Hf, Ta and Re

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In relation with the ITER project and some other tokamaks using tungsten as material for divertor, the determination of radiative properties of moderately charged ions of this atom is of current interest. The recent compilation of existing data [1] shows that the spectra of W III – W VII are not complete whereas W VIII – W X spectra are fully unknown. In the last case only observation of low resolution (5 Å) tokamak spectrum in the region 150–300 Å attributed to W VIII was published [2].

For observation of resonance lines of W VI – W X, a set of spectra was produced in the wavelength region of 150–350 Å using a triggered spark source and recorded on photographic plates with a grazing incidence spectrograph (resolution ∼0.015 Å) in the Institute of Spectroscopy of Troitsk. The vacuum spark spectrum in this region consists of about 3000 lines. Most of the intense lines are located in two regions centred at about 220 and 250 Å. They are composed, apart from known W VII lines [3], predominantly by the unknown ($4f^{14}5s^25p^k$ + $4f^{13}5s^25p^{k+1}$) – [$4f^{14}5s5p^{k+1}$ + $4f^{14}5s^25p^{k-1}$(5d+6s) + $4f^{13}5s^25p^k$(5d+6s)] transitions in W VIII – W X spectra (k = 5–3, respectively). A comparison with the tokamak spectrum [2] is made. For reliable identification of such complex spectra the analysis of isoelectronic ions of neighbouring chemical elements which are completely unknown is nesessary. The spectra of Hf, Ta and Re were also recorded and compared with W spectrum.

Theoretical calculations have been performed by means of the Cowan codes, predicting level energies and transition probabilities that take into account configuration interactions. Parametric study allows the continuous improvement of these predictions by least squares fit of radial integrals against experimental level energies. Calculated spectra are compared with the experimental spectra and some preliminary identifications are made.

For longer wavelength region (500–1650 Å) where transitions between excited states occur, data are provided by spectra produced using sliding spark and triggered spark sources and recorded on the 10 m normal incidence spectrograph (resolution ∼0.008 Å) of the Meudon Observatory. Photographic plates are used for precise wavelength measurements while image plates are used for intensity measurements.

This work is partly supported by RFBR grant 00390-02-100, by the French CNRS and by a PPF grant of Univ. UPMC. It is part of the IAEA Coordinated Research Project "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV".

References

[1] A.E. Kramida, T. Shirai, At. Data Nucl. Data Tab. **95**, 305-474 (2009)

[2] J. Veres, J.S. Bakos, B. Kardon, JQSRT **56**, 295 (1996)

[3] J. Sugar, V. Kaufman, Phys. Rev. A **12**, 994–1012 (1975)

Photoionization of tungsten ions with synchrotron radiation

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Tungsten is used on the interior walls of nuclear fusion reactors. By erosion processes tungsten atoms enter the plasma and are ionized to high charge states. Profound knowledge of atomic collision processes involving tungsten atoms in all possible charge states is therefore required for a quantitative understanding of the radiation losses from the plasma that are associated with this heavy impurity element. Consequently, tungsten has received much attention in recent research efforts (see e.g. references [1–4]). Because of the complexity of the tungsten atomic structure, theoretical calculations of atomic cross sections are challenging and guidance by experiments is vital. Photoionization measurements are a particularly sensitive spectroscopic tool for investigating the role of intermediate multiply excited states in photon-ion interactions with implications also for electron-ion recombination and ionization processes.

The present measurements were performed using a photon-ion merged-beams setup [5] at the Advanced Light Source. Cross sections for photoionization of W^{q+} ions (q=1,2,3,5) have been explored in the energy range 20–65 eV. Figure 1 shows our preliminary results for single ionization of W^{3+} ions. The cross section is dominated by resonance features probably involving excitation of the $5p$ and $4f$ shells. Similarly strong resonances have been observed for the other tungsten charge states as well.

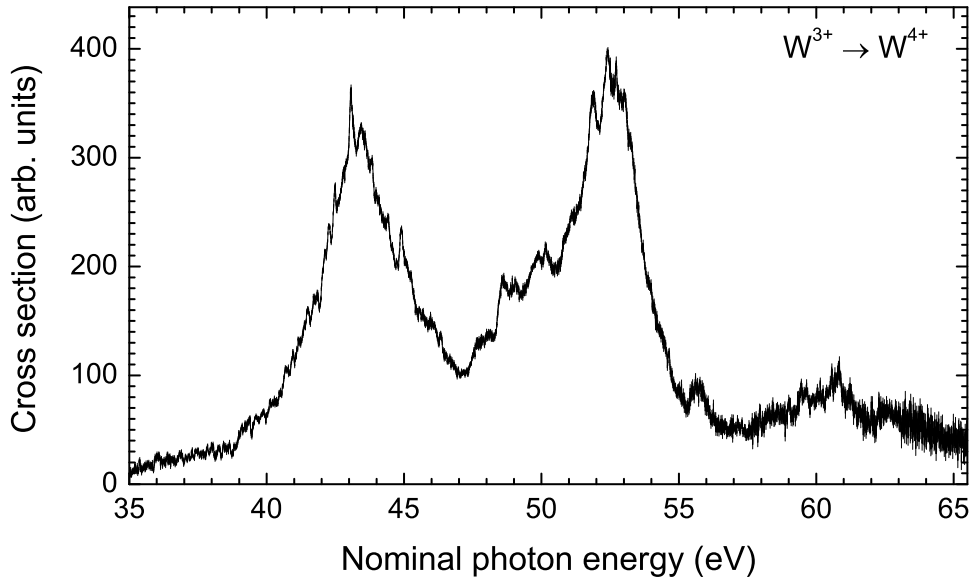

Figure 1: Experimental cross section for single photoionization of W^{3+}([Xe] $4f^{14}\,5d^3$) ions. The nominal experimental photon energy spread is 100 meV.

References

[1] A.E. Kramida and T. Shirai, At. Data Nucl. Data Tab. **95**, 305 (2009); **95**, 1051 (2009)

[2] M. Trzhaskovskaya, V. Nikulin, and R. Clark, At. Data Nucl. Data Tab. **96**, 1 (2010)

[3] C. Biedermann, R. Radtke, R. Seidel, and E. Behar, J. Phys.: Conf. Ser. **163** 012034 (2009)

[4] Y. Podpaly, J. Clementson, P. Beiersdorfer, J. Williamson, G. V. Brown, and M. F. Gu, Phys. Rev. A **80**, 052504 (2009)

[5] A. Covington et al., Phys. Rev. A **66**, 062710 (2002)

Collision data calculation for highly-charged open $n = 4$ shell tungsten ions using analogues of relativistic integrals

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In order to obtain emission-line spectra or energy losses due to plasma impurities, one needs to solve the balance equation which determines level populations for the ions of different ionization stages. On its turn, the balance equation requires a detailed knowledge of accurate atomic data, describing atomic structure (energy levels, radiative transition probabilities, Auger transition rates) and photon/charged particle scattering from ionized atoms. Both the theoretical and experimental methods for obtaining scattering parameters are very complicated, especially when exploring heavy and/or highly-charged ions. Consequently, there is a real need for the sophisticated theoretical methods allowing to simplify or to reduce calculations required for a large scale scattering data generation and data basis production.

There exist several theoretical methods to calculate the cross sections required for practical applications. One of the most accurate and suitable technique to solve the scattering problem is the R-matrix method. The method includes nearly all of the physical effects that contribute to cross sections and is applicable to all kinds of atoms, from neutral to highly ionized stages.

We have developed an approach based on the analogues of the relativistic integrals (ARI) which enables one to utilize relativistic wave functions obtained in the Dirac-Fock approximation [1]. By this both the direct and indirect relativistic effects are included in the final result. The direct effects arrise when the masses of electrons increase due to the speed of electrons, and the electrons are pushed closer to the nucleus. The indirect relativistic effects are caused by the inner electrons screenning the charge of centrally-placed nucleus.

The goal of present work is to assess different methods implementing the relativistic R-matrix approach in the calculation of atomic data for electron scattering from the highly-charged tungsten ions and to estimate the importance of correlation and relativistic effects for heavy ions. The collision strengths Ω and the effective collision strengths Υ for the electron- impact excitation of relativistic levels of the configurations with electron in the outer 4p, 4d, 4f shells from the ground state $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4l^N$ ($l = 0, 1, 2, 3$) are being determined when the different approaches for the inclusion of the relativistic effects are implemented.

We calculate electron-impact collision strengths using different R-matrix code versions for the $4l^N$ configurations of tungsten ions. We investigate the influence of relativistic effects to the bound-continuum and continuum-continuum integrals of the collision strength in quasirelativistic and relativistic approximations. A suitability of relativistic integrals method for highly charged ions is cross-checked by comparing calculation results.

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Reference

[1] V. Jonauskas, F.P. Keenan, R. Kisielius, P.A.H. van Hoof, M.E. Foord, R.F. Heeter, S.J. Rose, G.J. Ferland, P.N. Norrington, Journal of Physics B: Atomic, Molecular and Optical Physics **38**, L79 (2005)

Plasma diagnostics with magnetic-dipole lines from $3d^n$ ions of W

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Recent work [1] reports measurements and identification of about 40 new M1 lines in highly-charged ions of tungsten, from Co-like W^{47+} to K-like W^{55+}. The M1 lines within the $3d^n$ (n = 1–9) ground configurations were measured in a narrow EUV range of spectra, from 10 nm to 20 nm. We present analysis of diagnostic application of these lines in fusion research. While plasma temperature can be inferred from different ionization stages to which the lines belong, the electron density analysis requires detailed collisional-radiative (CR) modeling. The CR simulations for tokamak plasmas were performed with the population kinetics code NOMAD [2] using atomic data generated with FAC [3]. It was found that about 20 intensity ratios for the M1 lines identified in [1] can be used to determine electron density between 10^{13} and 10^{16} cm^{-3}. Examples of intensity ratio dependencies on electron density is shown in Fig. 1.

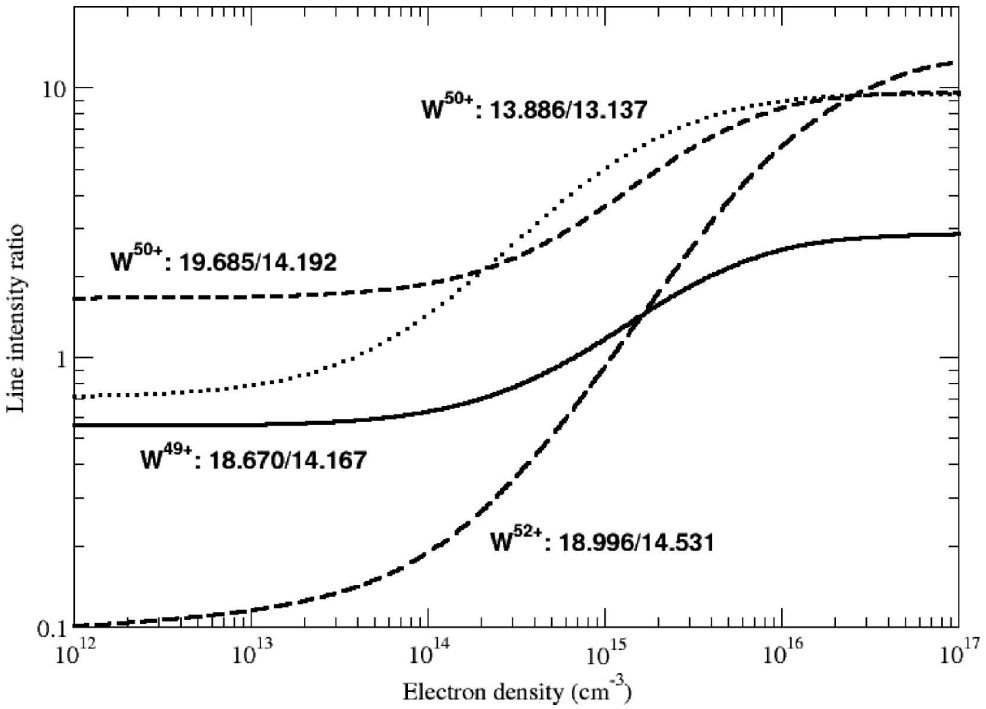

Figure 1: Line intensity ratios for several lines from W^{49+}, W^{50+} and W^{52+}. Wavelengths are given in nm.

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References

[1] J. Reader et al, ICAMDATA-2010 poster B-21

[2] Yu. V. Ralchenko and Y. Maron, J. Quant. Spectr. Rad. Transf. **71**, 609 (2001)

[3] M.F. Gu, Can. J. Phys. **86**, 675 (2008)

Mass-spectrometric studies of electron-impact dissociative ionization of the methionine molecule

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Present paper deals with the experimental and theoretical studies on the methionine molecule fragmentation under the low-energy electron impact. Using the specially designed mass-spectrometric apparatus based on the magnetic mass-analyzer, we have studied the dissociative ionization of one of the members of the amino acid group with a special emphasis given to the determination of the appearance energies for the ionized fragments. Such data are of specific interest in view of tracing the possible consequences of the live tissue interaction with ionizing radiation. Note that amino acids, which methionine belongs to, are one of the basic building blocks of the live body.

Our experiment was carried out using a crossed-beam technique combined with the mass separation of electron-molecule interaction products. Measuring procedure was fully automated using the PC control. Besides measuring the mass-spectra of the initial molecule (see figure), we have determined the energy dependences of the ionized fragment yield with the 0.1 eV energy step and the <0.5 eV (FWHM) energy resolution in the energy range from the threshold up to 100 eV. Application of a special least-square fitting procedure enabled the absolute values of the appearance potentials for the fragments under study to be found. Since the initial molecule may undergo strong fragmentation due to the thermal processes, the special studies of possible temperature-induced destruction of the methionine molecule were carried out.

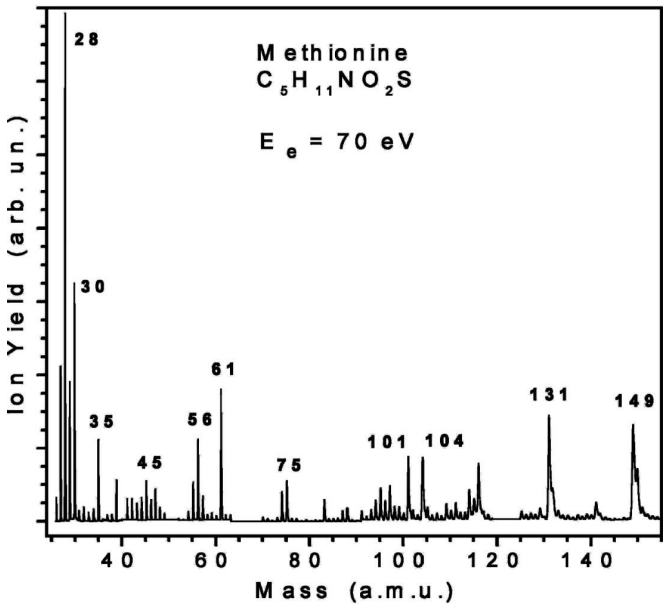

Figure 1: Mass-spectrum of the methionine molecule.

The theoretical investigations were performed by using the generalized gradient approximation for the exchange-correlation potential in the density functional theory (DFT) as it is described by Becke's three-parameter hybrid functional, using the nonlocal correlation provided by Lee, Yang, and Parr (B3LYP method). The ccpVTZ basis set has been used as well.

Based on the theoretical results obtained it has been predicted that the ionic fragments of the initial $C_5H_{11}NO_2S$ molecule are $C_4H_{10}SN^+$ ($m = 104$ a.m.u.) and $C_2H_5S^+$ ($m = 61$ a.m.u.). These fragments should be the ionic fragments of the initial $C_5H_{11}NO_2S^+$ (multiplicity=2) molecule cation too exactly like a $C_3H_7S^+$ ($m = 75$ a.m.u.) fragment. An experiment investigation proved that among the main ionic fragments of the initial $C_5H_{11}NO_2S$ molecule one may be note $C_2H_5S^+$ ($m = 61$ a.m.u.). The appearance potentials for the above ionic fragment of 12.5±0.1 eV is determined.

Total electron scattering cross-section for POPOP molecules

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Up today the total electron scattering cross-section is one of the very important processes in atomic and molecular physics [1]. Experiments of this type however, are associated with difficulties: high temperatures and densities are required to produce atomic and molecular beams or one needs a gas-filled cell and well-collimated momochromatic intense electron beams. Our modernized electron spectrometer with a gas-filled cell (Fig. 1(a)) comprises two serially mounted hypocycloidal electron energy analyzers [2]. The whole spectrometer is immersed into the homogenous magnetic field.

The POPOP molecules were produced using a compact reservoir made of stainless steel. Inside of this reservoir a quartz ampula with molecules is placed. The reservoir is connected with the gas-filled cell by a tube with inner diameter 4 mm. The temperature of the gas-filled cell was taken about 50 K higher than that of the molecular vapour in the heated reservoir.

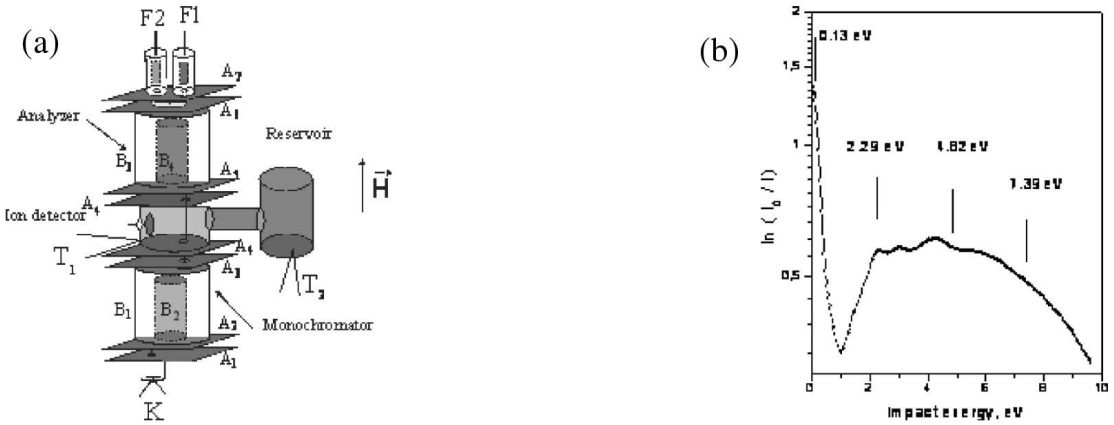

Figure 1: (a) Experimental layout. (b) Total electron scattering cross-section.

A typical value of the electron energy spread was 0.15 eV (FWHM) in the 0.1–15 eV energy range. The primary electron beam current was equal to $\sim 10^7$ A. The energy scale was calibrated with the accuracy of ± 0.05 eV.The relative uncertainties of the cross-section lie within 2 % interval. In Fig. 1(b) the energy dependence of the total electron scattering cross-section is shown being obtained in the transmission experiment. First we measured the transmitted current I_0 without POPOP vapour in the cell, then after resistive heating the reservoir up to 128 °C the electron current I was measured. Four distinct resonance features are revealed in this dependence in the 0–10 eV energy region. These resonances are attributed to the temporary anion states of the POPOP molecule.

The work was supported, in part, by the Lithuania–Ukraine projects M/782009 (ICh, JK) and Research Council of Lithuania TAP55/ 2010 (JT).

References

[1] M.A. Morrison, Aust. J. Phys. **36**, 239 (1983)

[2] Kontros J.E. et al. J. Phys. B **35**, 2195 (2002)

Low-energy electron collisions with gas-phase thymine molecule

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The total crosssections for low-energy (0–9 eV) electron scattering and electron attachment to the DNA base thymine (T) molecule in the gas-phase have been studied. The above studies were carried out using a gas-filled cell. The controlledenergy electron beam ($\Delta E_{1/2}$ = 0.15 eV) was formed using a hypocycloidal electron monochromator [1]. An effusion source of molecular beam heated to 390 K was employed, that is considerably below the parent molecule decomposition temperature of about 590 K. Negative ions were extracted from the interaction region by a small voltage (sim1.5 V) applied to the ion collector. The electron energy scale was calibrated using the position of the maximum of the first derivative of the electron beam current in the initial area of the voltage-to-current characteristic. Additionally, the ionization cross section has been calculated using binary-encounter–Bethe model applying B3LYP/ccpVTZ approach.

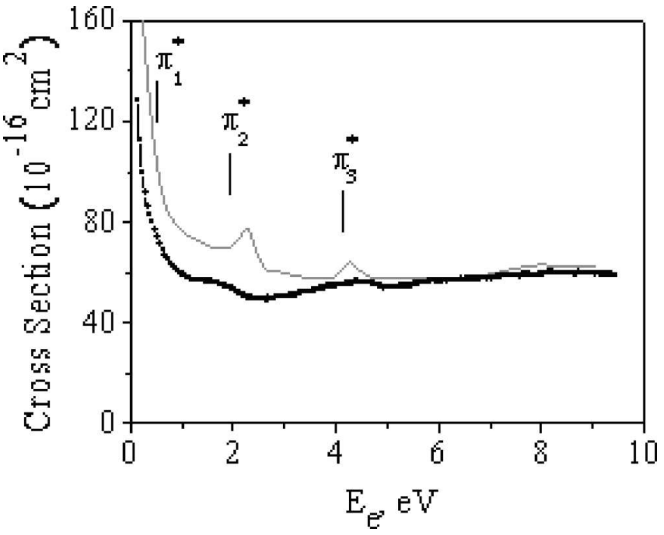

Figure 1: Total cross-section for electron scattering by thymine molecules. • our results, — calculations.

There exist some features (at E = 0.27, 1.70 and 4.08 eV) appearing in the total scattering cross-section. They were observed earlier in [2] and were identified as the π_1^*-, π_2^*- and π_3^*-shape resonances. The absolute cross-sections were determined by normalizing our data to the theoretical calculations [3], showing a good agreement with our results (see Fig. 1). However, distinct resonant-like peaks are not observed in the total ionization cross section for the thymine molecule. It allows us to conclude that short-lived negative-ion state is not formed effectively. It leads to that the total cross section of electron attachment to the T molecules in the energy range 0–3 eV reveal a prominent structure attributed to the formation of the $(T–H)^-$ negative ion.

The work was supported, in part, by the LithuaniaUkraine projects M/782009 (ICh, JK) and Research Council of Lithuania TAP55/2010 (JT).

References

[1] N.I. Romanyk, O.B. Shpenik, I.A. Mandy, F.F. Papp, I.V. Chernyshova, Tech. Phys. **38**, 599 (1993)

[2] K. Aflatooni, G.A. Gallup, P.D. Burrow, J. Phys. Chem. A **102**, 6205 (1998)

[3] C. Winstead, V. McKoy, S. Sanchez, J. Chem. Phys. **127**, 085105 (2007)

Resonances in the total low-energy electron scattering cross-section for cytosine molecule

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The studies of the energy dependence of the total slow (0–9 eV) electron scattering cross-section for the cytosine (C) molecules have been carried out. The experiment was performed using the vaporfilled cell apparatus. The controlled-energy electron beam ($\Delta E_{1/2} = 0.15$ eV) produced using the hypocycloidal electron monochromator [1]. The effusion source heated up to 390 K (that is much below the molecule melting point, 593 K) was applied to produce the molecular beam. Thus, the original structure of the C molecules in the gas phase left undamaged. Electrons scattered by the molecules were detected at the collision chamber walls. The energy scale was calibrated with respect to the position of the maximum of the first derivative of the initial area of the current-to-voltage characteristic of the primary electron beam. The ionization cross-section has been calculated using binary-encounter–Bethe model applying B3LYP/ccpVTZ approach too.

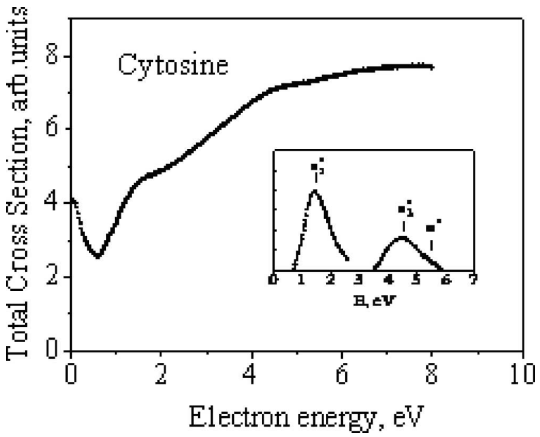

Figure 1: Energy dependence of total electron scattering cross-section for the cytosine molecule.

The energy dependence of the total electron scattering cross-section for the C molecule is shown in Fig. 1. It reveals a deep minimum and the pronounced maxima at $E = 1.53$, 4.52 and 5.62 eV shown in the inset in Fig. 1. The first two of them were observed earlier in [2] and identified as the π_2^*- and π_3^*-shape resonances. The feature at 5.62 eV could be related to the σ^*-shape resonance. Such resonances have small lifetimes as compared to the π^*-shape resonances and are revealed in a form of the broad features of less intensity. They are not clearly revealed in the total cross-section since they overlap with the more intense π^*-shape resonances [3].

Distinct resonant-like peaks are not observed in the calculated total ionization cross-section for the cytosine molecule, i.e. short-lived negative-ion state is not formed. It allows us to conclude that free electron attachment to cytosine yields the $(C–H)^-$ as a major fragment anion.

The work was supported, in part, by the Lithuania–Ukraine projects M/782009 (ICh, JK) and Research Council of Lithuania TAP55/2010 (JT).

References

[1] N.I. Romanyk, O.B. Shpenik, I.A. Mandy, F.F. Papp, I.V. Chernyshova, Tech. Phys. **38**, 599 (1993)
[2] K. Aflatooni, G.A. Gallup, P.D. Burrow, J. Phys. Chem. A **102**, 6205 (1998)
[3] P D. Burrow, G.A. Gallup, A M. Scheer, S. Denifl et al., J. Chem. Phys. **124**, 124310 (2006)

Method based on reduced density matrices and molecular data generation for haloalkanes

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The method based both on reduced density matrix (RDM) method and quantum mechanical calculations for generation of molecular data needed for determination of relative conformational energies in haloalkanes is presented. The main idea of data generation is based on additivity rule for conformational energies obtained analytically using perturbation theory for 1-RDM [1]:

$$E^{\mathrm{conf}} = E - E^{\mathrm{T}} = n_G^{XY} E_G^{XY} + n_{GG}^{XY} E_{GG}^{XY} + n_{GT}^{XY} E_{GT}^{XY} + n_{GG'}^{XY} E_{GG'}^{XY} + \dots , \tag{1}$$

where E denotes total energy of the molecule in the given conformation; E^{T} total energy of the molecule in the conformation having the lowest energy; E_G^{XY}, E_{GG}^{XY}, E_{GT}^{XY}, $E_{GG'}^{XY}$ ($X, Y = \mathrm{CH_3}$, Cl, F, Br, etc.) are energy increments; n denotes the number of corresponding increments in the molecule; G and T denotes correspondingly *gauche* and *trans* conformational segments.

Consequently the additivity rule expresses the conformational energy of any saturated molecule as a sum of energy increments corresponding to the conformational segments and their sequences of different lengths. For obtaining values of additivity increments both the additivity rule and quantum mechanical methods have been used. It has been shown that the evaluated magnitudes of additivity increments are sensitive to the method and the basis set used. However applying special criteria proposed in [2, 3] it was possible to achieve the optimal concert of calculation recourses allowing describing correctly increments values of different length for halogenated alkanes. The generated molecular data for evaluation of relative conformational energies in haloalkanes is presented and analyzed in the contribution. In passing it was shown that additivity increments concerned with sequences of conformational segments are closely related with long range interactions between terminal atoms of mentioned sequences and reflect their peculiarities. The additivity series representing conformational energy of the molecule converge with properly good accuracy when including five-segmental increments. It allowed optimize the number of increments needed to determinate relative conformational energies in haloalkanes with sufficient accuracy. Thus, it can be concluded that the proposed method reveals itself as appropriate for generating molecular data for haloalkanes.

References

[1] D. Šatkovskienė, Int. J. Quantum Chem. **91**, 5 (2003)

[2] D. Šatkovskienė, R. Jankauskas, P. Pipiraitė, J. Šulskus, J. Mol. Struct. (Theochem) **816**, 43 (2007)

[3] R. Jankauskas, P. Pipiraitė, D. Šatkovskienė, Lith. J. Phys. **47**, 143 (2007)

Full-dimensional potential energy surfaces for molecular collisions and spectroscopy

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Analytical fitted potential energy surfaces are a valuable tool for study of reaction dynamics and molecular spectroscopy. In full generality the surface depends on $3N-6$ independent coordinates, where N is the number of nuclei. Already for small systems, say of $5-9$ atoms, the construction of such surfaces is a problem of high-dimensional approximation. In recent years we have used computational invariant theory and the MAGMA computer algebra system as an aid to develop representations for the potential energy and dipole moment surfaces that are fully invariant under permutations of like nuclei [1]. We express the potential energy in terms of internuclear distances using basis functions that are manifestly invariant, with coefficients fitted to the results of ab initio calculations. The resulting full-dimensional surface is then used for quasiclassical trajectory calculations, for diffusion Monte Carlo or path integral calculations, or for quantum mechanical calculations of a rovibrational spectrum. Applications have been made to a wide variety of systems of interest in combustion science, astrophysics, plasma physics, and molecular spectroscopy [2]. Larger systems are accessible through a many-body expansion. The presentation will describe the mathematical background and will highlight some recent applications.

References

[1] B. J. Braams and J. M. Bowman, Int. Rev. Phys. Chem. **28**, 577 (2009)

[2] J. M. Bowman, B. J. Braams, S. Carter, C. Chen, G. Czakó, B. Fu, X. Hung, E. Kamarchik, A. R. Sharma, B. C. Shepler, Y. Wang and Z. Xie, J. Phys. Chem. Lett. **1**, 1866 (2010)

Some spectroscopic studies on the photo physical characteristics of 4-methyl-7-hydroxy coumarin

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This is in continuation to our earlier work regarding the effect of solvents, susbstituents, and temperature on various photo physical properties of coumarin derivatives [1–3]. It has been established that the nature of solvents and susbstituents, brings about a change in the values of fluorescence wavelength maxima, quantum yield, life time, polarization and excited state dipole moment of the coumarins. In the present case we have studied the spectroscopic characteristics of 4-methyl-7-hydroxy coumarin by recording its uv-absorption and fluorescence emission spectra in various polar and non polar organic solvents. Spectral shifts occurred due to change in solvents are interpreted in terms of neutral (N), hydrogen bonded (HB), and phototautomer (PT) species of the coumarin derivative likely to exist in the excited state. Further the occurrence of these three species of coumarin derivative have been established by studying the uv-absorption and fluorescence spectra of coumarin derivative in benzene – a non polar solvent and also in methanol–benzene solution, in which concentration of methanol is increased in regular steps. Using absorption and fluorescence emission spectra the values of various spectral parameters namely, half band width, extinction coefficient, relative quantum yield, and radiative life time are calculated (see Table) and discussed in detail.

The effect of temperature on fluorescence emission of 4-methyl-7-hydroxy coumarin is also studied and it is observed that there is a decrease in emission intensity with the rise in temperature. It is explained in terms of intramolecular charge transfer (ICT) and twisted intramolecular charge transfer (TICT) processes.

Solvent	Absorption max. (nm)	Fluorescence max. (nm)	Half band width (cm)	Extinction coeff. (mol. cm)	Radiative life time (ns)	Relative quantum yield	Fluorescence life time (ns)
Benzene	321	383	27	105	3.18	0.05	0.16
Hexane	324	ND	28	125	3.20	ND	–
Heptane	324	383	27	114	3.50	0.06	0.21
Cyclohexane	325	ND	26	104	3.70	ND	–
Dioxane	321	380	27	97	3.70	ND	–
Dichloromethane	321	385	24	119	3.40	0.04	0.14
Toluene	323	382	26	106	3.40	0.03	0.10
Methanol	389, 323	485	28	107	3.91	0.33	1.29
n-butanol	388, 325	486	26	115	3.44	0.36	1.23
n-propanol	388, 324	486	26	99	4.06	0.36	1.50
Ethanol	387, 324	495	26	106	3.97	0.33	1.31
Water	322	451	31	76	4.82	0.96	4.63

References

[1] Rajesh Giri, Spectroscopic Acta A **60**, 757 (2004)

[2] S. Kumar, R. Giri, M.K. Machwe, Ind. J. Pure & Appl. Phys. **36**, 622 (1998)

[3] R. Giri, Spectroscopic Acta A **48**, 843 (1992)

Experimental double differential cross sections for electrons ejected by MeV He^{q+} impacts on gaseous adenine molecules

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Study of atomic and molecular ionization by energetic charged particles is of great importance in a wide range of research fields such as plasma physics, astrophysics and radiation therapy. This is because ionization is the predominant energy loss process of an incident particle penetrating through matter. In particular, experimental double differential cross sections (DDCSs) with respect to energy and angule of electrons ejected in collisions between MeV ions and polyatomic molecules are highly required in applications for e.g., charged particle cancer therapy. Also, the data may be practically useful to find the theoretical formula of ionization concerning larger molecules like biomolecules.

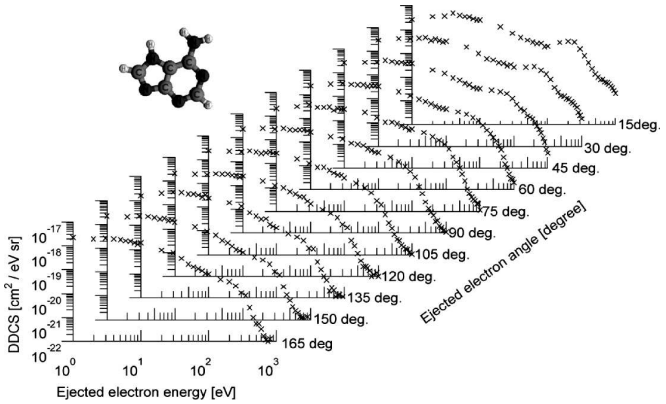

Figure 1: Energy and angular distributions of electrons measured for 2 MeV He^+ impact on gaseous Adenine.

In this work, we measured DDCSs in collisions of 2 MeV He^+ with a gaseous Adenine ($C_5N_5H_5$) target. The experiment was performed at the QSEC heavy ion accelerator facility of Kyoto University. Experimental apparatus consists of an oven of a vapor target, a 45-degrees parallel plate electrostatic spectrometer [1] for energy analysis of electrons ejected from the vapor target and a passivated implanted planar silicon (PIPS) detector which was used to determine a target density from a number of projectile ions forwardly scattered by target molecules. To reduce residual magnetic fields, the collision chamber had double parmalloy magnetic sheilds inside.

Absolute data of DDCSs for Adenine molecules are presented in Fig. 1. We also measured ionization cross sections of Ar and the result was excellently in good agreement with those of Toburen et al [2]. It was found that our data are larger than Ar by about three. It should be pointed out that ionization cross section may be proportional to the number of outer electrons (total number of electrons minus inner shell electrons) as suggested by Wilson et al [3]. Thus, we compared our data with those of Isoleucine [4] and found that the Bragg's additivity rule holds successfully. Measurement will be extended to He^{2+} projectile ions and more detaild analysis will be given in the conference.

References

[1] N. Stolterfoht, Z. Phys. A **248**, 81 (1971)

[2] L. H. Toburen and W. E. Willson, Phys. Rev. A **19**, 2214 (1979)

[3] L. H. Toburen and W. E. Willson, Phys. Rev. A **11**, 1303 (1975)

[4] Y. Iriki et al., J. Phys.: Conf. Ser. **194**, 102036 (2009)

Variational pair-correlation functions for atomic properties

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It is possible to make good use of the variational method to target specific correlation effects in a many-electron system by tailoring the configuration expansion. In this line, the multiconfiguration Hartree-Fock method [1] (MCHF) is used to produce independent variational pair-correlation functions (PCFs), each one dedicated to a given electron pair. These nonorthogonal PCFs are coupled to each other by solving the generalised eigenvalue problem associated with a low dimension pair-correlation function interaction (PCFI) matrix. The Hamiltonian and overlap matrices are calculated using biorthonormal orbital transformations and efficient counter-transformations of the configuration interaction eigenvectors [2]. This methodology is shown to be efficient for the ground state energy of the beryllium atom [3]. In the present work, we investigate it for the $2s2p\ ^1P^o$ and $2s2p\ ^3P^o$ excited states, not only through the total energy convergence but also through the expectation values of the specific mass shift operator and the hyperfine structure parameters for measuring the impact of the mixing coefficient contraction.

The beryllium atom constitutes a perfect benchmark for the PCFI method since reference calculations based on complete active space expansions with a single common orthonormal basis remain possible to describe simultaneously all pair-correlation effects. For larger systems, it becomes hopeless to saturate a single orbital basis for describing different types of correlation contributing to the total energy, or different type of operators, and the PCFI approach should constitute an interesting alternative. The present study is supported by current developments of both the ATSP2K [1] and GRASP2K [4] packages.

References

[1] C. Froese Fischer *et al.*, Comp. Phys. Commun. **176**, 559 (2007)

[2] J. Olsen *et al.*, Phys. Rev. E **52**, 4499 4 (1995)

[3] S. Verdebout *et al.*, J. Phys. B: At. Mol. Opt. Phys. **43**, 074017 (2010)

[4] P. Jönsson *et al.*, Comp. Phys. Commun. **176**, 597 (2007)

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