INDC International Nuclear Data Committee

Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

20-22 March 2013

Prepared by

Hyun-Kyung Chung and Bastiaan J. Braams

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Abstract

The third and final research coordination meeting of the Coordinated Research Project (CRP) "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" was held 20–22 March 2013 at IAEA headquarters, bringing together 17 experts representing 15 institutions. Participants reviewed their work done in the course of the CRP and the current state of knowledge, and made plans for a final CRP report. Presentations, discussions and recommendations of the research coordination meeting are summarized here.

May 2013

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1. Introduction

All light elements H–O are of interest for fusion experiments: hydrogen as the main plasma constituent, helium as the product of fusion, lithium and boron as wall coating materials, beryllium and carbon as primary wall materials, nitrogen as a deliberately introduced radiating gas and oxygen as a ubiquitous impurity. In the edge and divertor region of fusion plasma devices these impurities may be introduced as molecules or may form molecules (including hydrides, hydrocarbons and N_2 and O_2) and a wide variety of collision processes need to be considered for modelling and for interpretation of spectroscopic diagnostics. The Coordinated Research Project (CRP) on "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" was established in order to improve the database on processes of the light element impurities in fusion plasma. Fourteen research projects in the area of experimental and computational atomic physics are represented in the CRP. Participants met in November 2009 for the first Research Coordination Meeting (RCM) (see report INDC(NDS)-0564), in May 2011 for the second RCM (report INDC(NDS)-0604) and the third and concluding RCM was held 20-22 March 2013. Seventeen participants presented overviews on their research in the scope of the CRP and discussed the current status of the knowledge and made recommendations for future activities. The presentations are available on the A+M Data Unit web pages at http://www-amdis.iaea.org/CRP/.

Brief summaries of the presentations are given in Section 2 and discussions and recommendations in Section 3. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2. The long summary of each presentation is collected in the Appendix 3 and relevant publications by participants during the period of the CRP are listed in Appendix 4.

2. Summary of Presentations

Dr R. Forrest (Section Head, Nuclear Data Section) opened the meeting and welcomed the participants. He emphasized the importance of atomic and molecular data sets of light elements for current fusion activities, and reviewed specific tasks to be done in the final Research Coordination Meeting. After brief introductions of participants, the proposed agenda was reviewed and adopted without change. The meeting was attended by representatives of all the institutions participating in the CRP and by Dr J. Reader of the Atomic Spectroscopy Group at NIST, USA, plus several guests who participated fully in the meeting. The work of lead investigator Dr Janev was presented by Dr Jakimovski and that of lead investigator Dr J. G. Wang by Dr Y. Wu.

Presentations are briefly described below and more detailed summary of each presentation is given in Appendix 3. Presentation slides are available through the A+M Unit web pages for this CRP (http://www-amdis.iaea.org/CRP/LightElement/) for more information including most current data in tables and figures, citations and literature information. The subject matter of the CRP includes data for atomic transitions and electron-atom collisions ("atom" understood to include ions), data for heavy-particle collisions, and data for electron-molecule collisions ("molecule" likewise understood to include molecular ions).

2.1 Atomic Processes

Prof S. Loch presented the recent work at Auburn University on generalized collisional radiative (GCR) modeling for light elements relevant for fusion. The GCR theory and results for Li and O were presented with an emphasis on the treatment of excited state ionization, which can increase the effective ionization of near neutral ions by up to a factor of ten. It was noted that the perturbative approaches would overestimate the cross-section of excited state ionization while the non-perturbative methods cannot be extend to high-lying excited states. He demonstrated an approach to extend the non-perturbative methods to high n states for B, B^+, and B^{2+}. The new B data should be available shortly for use by the modeling community.

Prof I. Bray presented the convergent close-coupling (CCC) method for electron scattering extended to quasi-one-electron targets and quasi-two-electron targets, such as beryllium and all of its positive ions. The complete Laguerre basis is used to diagonalise the target Hamiltonian, for each angular momentum l, basis size N_l and exponential fall-off parameter $\lambda_l/2$. Presently, for the Be^{q+} targets, they set $\lambda_l/2 = q+1$ for all target orbital angular momentum $l \leq 4$. For the H-like Be^{3+}, 85-state CCC calculations were performed and for He-like Be^{2+}, 284 state calculations were used. The Li-like Be^+ target wave functions were expanded in much the same way as for Be^{3+}, except that the 1s state was obtained in the Hartree-Fock approximation. Consequently the number of states included in the electron-scattering calculations was 84. Lastly, electron scattering on neutral beryllium is similar to the e-Be^{2+} case, and was performed by expanding the total wave function with 292 target states. These were required to give a good representation of the target discrete singlet and triplet states, as well as the continuum.

Dr J. Reader summarized the work at NIST on the spectra of light atoms. Critical compilations of transition probabilities for F^{4+}-F^{7+} and Ne^{5+}-Ne^{8+} were recently completed and the data are disseminated through the online databases found on the NIST Physical Measurement Laboratory website, http://www.nist.gov/pml/. The current version of the NIST Atomic Spectra Database (ASD) contains data for more than 194,000 transitions in about 1000 spectra. Online tools include production of Grotrian diagrams and Saha equilibrium plots. Bibliographic databases are updated on an approximately biweekly basis. A new database within ASD provides ionization energies for all atoms and ions. It is noted that an estimated uncertainty is provided for almost every value. The NIST website also provides access to online collisional-radiative modeling with the FLYCHK code and to the plasma population kinetics database from the non-LTE calculation workshops. Dr Reader briefly described the work on tungsten and other highly charged ions at NIST.

Dr V. Stancalie presented collision strength and cross sections for low-energy inelastic scattering of electrons by atomic systems calculated using the R-matrix method. In C I the calculation is more difficult due to the low-energy electron scattering dominated by a resonance due to the $1s^2 2s^2 2p^3\ ^3P^0$ state of C^-. The theoretical prediction of the location of this resonance, and of the $1s^2 2s^2 2p^3\ ^4S^0$ and $^2D^0$ bound states of C^-, depends on a balance between short-range correlation and long range polarization effects. The importance of configuration interaction wave functions was investigated both in the target-state expansion and in the (N+1)-electron quadratically integrable function expansion. Calculations of fine structure splitting in Ar III using the R-matrix method were also presented.

Dr Y. Qi discussed plasma effects in atomic structure, photo-excitation and ionization and electron-impact excitation processes. The first Born approximation is applied to investigate plasma effects on the high energy electron-impact ionization process of hydrogen-like ions embedded in weakly coupled plasmas. The screening of Coulomb interactions decreases ionization energies and changes the behaviour of the wave function. Multiple shapes and virtual-state resonances appear in the single differential cross sections as the plasma screening parameter passes through a certain critical value. Fewer angular-momentum states are included in the generalized oscillator strength density calculation and hence the contribution from the lower-angular-momentum states dominates the generalized oscillator strength densities.

Prof D. Schultz summarized the work in the Controlled Fusion Atomic Data Centre (ORNL) and later at University of North Texas during the time span of the CRP. The previous work regarding elastic and transport cross-sections was extended to H^+ + O processes. Collisions of highly charged ions with H, H_2 and He are relevant for neutral beam studies and charge exchange recombination spectroscopy. For charge transfer processes (C^{5+}, N^{6+}, O^{6+}, O^{7+}) + H, (C^{5+}, C^{6+}, O^{7+}, O^{8+}) + He and C^{6+} + (H, H_2) a database of recommended state-selective and total cross sections has been created by combining results from the various methods (MOCC, AOCC, CTMC, results from the literature) within their overlapping ranges of applicability and the results have been published. Cross sections and density matrix elements for a large number of impact energies are provided as inputs to a collisional-radiative model for excitation of atomic hydrogen by protons, injected alphas, fusion alphas, Be^{4+}, and C^{6+}. For

proton-impact processes results show the importance of consideration of non-statistical populations for interpreting these beam diagnostics.

Dr Y. Wu presented the work on collision processes between basic edge/divertor plasma constituents (H, He, H_2^+) and light element plasma impurities (Ne^{q+}, O^{q+}), as well as collisions between Ar and He^{2+}. The Molecular Orbital Close-Coupling (MOCC) and Atomic Orbital Close-Coupling (AOCC) methods have been applied to investigate charge transfer and excitation process in ion-atom and ion-molecule collisions. The time-dependent density functional theory (TDDFT) method has been recently developed to treat charge transfer and electron loss processes in ion-atom collisions. Results were presented for the following processes: (1) Collisions of bare and hydrogen-like ions of Ne and O with H and He; (2) charge transfer and excitation processes in H_2^+-He collisions; (3) electron capture and electron loss in H_2^+-Ar collisions.

2.2 Molecular Processes

Dr B. Wei described the establishment of a new cold target recoil-ion momentum spectroscopy (COLTRIMS) facility at Fudan University. As a first test the dissociative ionization of methane (CH_4) by electron impact was studied with COLTRIMS. The relative cross sections between different dissociation channels were measured for electron energy ranging from 20 eV to 200 eV, and the measurements agree well with previous studies. From time-of-flight (TOF) and position information of the fragments the kinetic energies of the fragment ions was deduced. The mean kinetic energy released (KER) during dissociation processes was estimated from the average kinetic energy of ionic fragments and the agreement with previous theoretical data is good.

Prof P. Defrance described electron impact experiments performed using a crossed electron-ion beam set-up. Absolute inclusive cross sections were measured for the process of electron impact dissociation to individual ionic fragments from the energy threshold up to 2.5 keV. The contributions from the different reaction channels were separately obtained for single ionization (SI), dissociative excitation (DE) and dissociative ionization (DI). Kinetic energy release distributions (KERD) of the fragment ions were determined at selected incident electron energies, which allowed the determination of groups of electronically excited states that contribute to the process considered. Energy threshold determination allowed identification of target initial ground and excited states. (See the summary in Appendix 3 for the detailed list of processes and elements)

Prof J. B. A. Mitchell presented an overview of experimental studies on dissociative recombination processes, which have increased significantly in recent years. Experiments provide information concerning not only reaction cross sections but also product branching ratios. Many studies have been performed using the merged beams technique at heavy ion storage rings (CRYRING in Sweden, ASTRID in Denmark, TSR in Heidelberg, TARN II in Japan). Recent research highlights include the theoretical examination of the sharp fall-off of the cross section observed at super-thermal energies, the measurement of internal temperatures of ions used in storage ring experiments and the importance of knowing true branching ratios on the subsequent chemistry of plasmas. More experiments are underway at the new heavy ion storage ring in Langzhou, China, and at the electrostatic storage ring at KACST in Saudi Arabia.

Dr. Å. Larson presented electron scattering calculations combined with structure calculations which produce molecular potential energy curves, couplings and autoionization widths. Both quantum *ab initio* as well as semi-classical calculations on reactions involving the H_2, HeH and BeH molecular systems were performed. Studies were presented of electron-molecular ion collisions leading to dissociative recombination, vibrational excitation (or de-excitation) or dissociative excitation. Mutual neutralization reactions between H^- and light atomic cations and in collisions of H^+ and H^- were investigated. A very small isotope effect was observed in the neutralization cross sections for collisions between different isotopes of the hydrogen ions. Both the resonant and direct processes of dissociative excitation of HeH^+ were studied. Calculations on the non-adiabatic couplings between

resonant states of HeH are under the way. Investigations on the direct and indirect mechanisms of dissociative recombination of BeH^+ were presented.

Prof M. Larsson described the current status of the double electrostatic ion storage DESIREE, which is now in the commissioning phase. It has been cooled down to 15 K and the storage in the symmetric ring has been demonstrated. The anion C_2^- has been stored for several minutes, which is extremely promising taking into account how easily an anion is destroyed in collisions with residual gas molecules. The next step is to store ions also in the asymmetric ring. Once this is accomplished, the first mutual neutralization experiments can start.

Prof I. Schneider and Dr Z. Mezei presented rate coefficients of reactive collisional and radiative elementary processes calculated with multichannel-quantum-defect theory methods, and partly measured in merged-beam (storage ring) and crossed-beam experiments. The reaction mechanisms were described and output data were presented in a form ready to be used. For electron collisions, HD^+ and H_2^+, BeH^+, H_3^+ and H_2 targets were studied for dissociative recombination, dissociative excitation and vibrational transitions. For photoionization processes, the cross sections for the Q(N) (N = 1 − 4) photoionization of H_2 in $X^1\Sigma^+g$ ground (v″ = 0) and vibrationally excited (v″ = 1, ..., 10) states have been computed and resolved with respect to the vibrational level (v^+) of the resulting H_2^+ ion. It is found that the temporary captures into npπ $^1\Pi^-_u$ (v′ = 0, . . .; n=2-6) H_2 Rydberg states strongly drive the ionization process.

Dr D. Jakimovski presented the work by Dr. R. Janev as well as his own work. Cross sections for dissociative electron attachment on vibrationally excited H_2 molecules taking place via Rydberg-excited resonant states were calculated using the local complex potential model for resonant collisions from selected initial vibrational levels of the neutral molecule. State-resolved cross sections and rate coefficients for electron-impact-induced excitations in BeH^+ and BeH molecules were presented for a broad energy range as well as analytic fit expressions. Electron impact ionization cross sections for Be and some of its hydrides, from the ionization threshold to 1 keV are in good agreement with results from earlier calculations when available.

Prof H. Takagi discussed collision processes of electrons with H_2^+, HeH^+, and their isotopes, that is, dissociative recombination (DR), dissociative excitation (DE), and vibrational and rotational transition by electron impact. Using adiabatic scattering states the dynamical processes are solved as scattering problems induced by the configuration interaction (CI) and the non-adiabatic interaction (NAI). The NAI in the Rydberg and ionizing states is well represented by multi-channel quantum defect theory (MQDT). The calculated DR cross-sections of HD^+ below 1 eV and of H_2^+ agree well with experiments. At low energies, only the NAI is found to induce the DR process of HeH^+.

Dr L. Mendez presented calculated cross sections for electron capture (EC), excitation and ionization in ion-atom and ion-molecule collisions in a wide energy range. The Classical Trajectory Monte Carlo (CTMC) treatment was applied to evaluate ionization and nl-resolved EC cross sections for collisions of fully stripped ions (B^{5+}, C^{6+} and N^{7+}) with H (n=1,2) at high impact energies and the combined approach of semi-classical close-coupling and CTMC calculations for excitation up to n=6 in Li^{3+} + H collisions. For low energy ion-atom collisions, EC total cross sections in H^+ (D^+, T^+) + $Be(1s^2\ 2s^2)$ collisions and isotope effects were discussed. These cross sections were evaluated by employing a quantal treatment of the nuclear motion. For ion-molecule collisions, semi-classical calculations of $H^+ + N_2 \rightarrow H + N_2^+$ and quantal and semi-classical treatments with a vibronic close-coupling expansion of H^+ (D^+) + $H_2 \rightarrow H$ (D) + H_2^+ were presented.

2.3 Data Evaluation Activities

Dr H. Chung summarized the most recent meetings of the IAEA atomic and molecular data unit on the critical assessment of atomic, molecular and plasma-surface interaction data for fusion applications. In the 2nd technical meeting of code centre network meeting in 2010 and the 21st technical meeting of data centre network meeting in 2011 the importance of evaluated and recommended data and the

international collaboration on the topic was raised and the unit has organized three meetings in 2012 to address these issues. The short-term plans and long-term roadmap of the unit were presented on various aspects of internationally coordinated data evaluation activities.

Dr B. Braams summarized activities of the IAEA atomic and molecular data unit on data centre network, code centre network and coordinated research projects (CRP). The nature and history of ALADDIN and AMBDAS databases were described and a knowledge base of a wiki style was introduced. The ALADDIN database has started as a database of evaluated and recommended data, however, in recent years it has become a depository of old evaluated data sets and new contributed data sets. The unit would like to renew the effort to make ALADDIN a host for evaluated and recommended data sets. The bibliographical database AMBDAS for atomic, molecular and plasma-surface interaction data needs a new provider of bibliographical data on collisional processes since the main contributor, the Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge National Laboratory, has closed closed. A new database is planned for data sets on dust particles collected in fusion reactors, a product of the CRP on "Characterization of Size, Composition and Origins of Dust in Fusion Devices". The unit will promote activities to obtain high quality data sets from code capabilities instead of emphasizing the availability of on-line codes. The present and planned CRPs were described in the context of ITER and DEMO activities.

Dr S. Loch, in a second presentation, described the propagation of uncertainties in atomic data through collisional-radiative models. He demonstrated its significance through the example of helium-like line ratio diagnostics for temperature interpretation of a young star where inferred temperatures differ hugely depending on the choice of element (O VII, Ne IX or Mg XI) used in the diagnostic. Theoretical line ratios of three elements obtained with collisional-radiative models can be sensitive to the uncertainties of certain types of atomic data sets. The Auburn group explored propagation of atomic data to the population distributions and line ratios by employing Monte Carlo CR models with two tiered approaches: 1) baseline uncertainties (a generous estimate using the difference between R-matrix and distorted wave (DW) calculations) and 2) method sensitivities (a tighter constraint due to the variation by key input parameters within a chosen method). Errors and correlation in emissivities, effective ionization and recombination rate coefficients were investigated by using baseline uncertainties of atomic data.

3. Discussions and Recommendations

Participants reviewed the current status of atomic and molecular (A+M) data sets of light elements and discussed prospects for uncertainty estimates of theoretical data sets. Critical data needs of the fusion community were identified and future work to address the needs was recommended. Finally, publications and final databases from the CRP participants were discussed.

It was emphasized that a direct and continuous relationship between atomic physicists and fusion modelers is crucial to advance the field of A+M data for fusion applications. For example, atomic physicists normally produce total cross-sections, but these are not as useful as expected since modelers need coupling coefficients or differential cross-sections. More often than not it is unclear to the A+M physicist for which transitions the most effort should be invested to obtain the best values. In general, the smaller a cross-section is, the larger is the scale of its calculation. Interactions between the two communities will help them to identify interesting physics problem that are also useful. An example of such a continuous collaboration that benefits both parties is the one between Auburn University and DIII-D researchers.

Plasma diagnostics and modeling have improved to a stage where results can be highly sensitive to input A+M data. This led to the latest proposal from the IAEA atomic and molecular data unit to establish the internationally agreed reference data for AM/PSI data. (See reports INDC(NDS)-0627 and INDC(NDS)-0622).

The fusion community and other plasma physics communities have benefited from work by the atomic, molecular and optical (AMO) physics community without much direct funding for AMO data research. In recent years the funding for AMO data development has declined markedly and the production of high quality data is at risk. It is crucial that national funding agencies and also ITER recognize the current situation and support the AMO research projects that are important to fusion energy research.

3.1 Status of Data for Light Element Electron-Atom (Ion), Ion-Atom and Radiative Processes

Atomic data sets of electron-atom (ion) collisions are in a relatively good position in providing high quality data for systems having one or two electrons outside the closed shell. With more electrons, however, it is difficult to provide data sets for neutral or almost neutral systems since electron correlation effects require a large size of calculations. Some fusion relevant applications require state resolved data and this increases volume of needed data sets.

For one- or two-electron systems (H, He, Li and Be) theoretical data sets exist for electron impact processes from ground and excited states and for state resolved processes. On the other hand, very few experimental data sets exist especially for transitions from excited states. Uncertainties of the available theoretical data sets are not well known. Comparisons between CCC (convergent close-coupling) and RMPS (R-matrix with pseudo-states) results are expected to provide uncertainties in ionization rate coefficients of neutral Li despite the complexity in both methods,

For electron impact ionization from neutral He various total ionization cross-section calculations agree well with each other and with experiment (by S. Buckman). However, recent calculations of cross sections for excitation to metastable states and ionization from metastable states agree with each other, but the calculated cross sections are lower than the experimental ones by up to a factor two. On the other hand, new experimental results of He-like Li ions (by A. Müller) agree with theories within 3% for both ground and metastable contributions together for total ionization. A new experiment of neutral He is recommended to understand the discrepancies.

In addition to H and He data, Li data are important for edge diagnostics. In the edge region, not only protons and electrons but also B and C exist and comprehensive data sets for interaction between Li and the constituents are needed including charge exchange interaction of neutral Li.

Highly excited states play an important role in both charge exchange and electron collision rates and reasonably good data sets are available by R-matrix methods up to n=4 or n=5 states. Data for higher lying states are obtained by scaling laws.

Generalized Collisional Radiative (GCR) coefficients are evaluated with independent assessments on individual data. Energy levels and transition probabilities are benchmarked against the NIST database. Self-consistency is checked and the propagation of uncertainties of individual data to the uncertainties of final GCR coefficients is explored. Experiments to benchmark GCR coefficients are greatly needed, particularly for the dielectronic recombination and stepwise excitation and ionization rate coefficients.

Very few benchmark experiments of atomic data exist and the number has decreased in recent years. It may be possible to designate benchmark calculations for one or two electron target, though not for many electron targets such as carbon. It will be also feasible for Ne-like or Cu-like tungsten targets to designate benchmark calculations.

For charge exchange processes in ion-atom collisions, data for one and two electron systems are well managed. The structures of heavy particles in these processes are not in general a difficult issue. Data for charge exchange between neutral He and any combination of charged ions are readily available.

3.2 Status of Data for Light Element Molecular Processes

Beryllium hydrides: BeH and BeH₂

Beryllium is of interest as a wall material in fusion experiments. It is foreseen as the main wall material for ITER (tungsten will be used in the regions of highest load) and since 2011 the JET experiment operates with an ITER-Like Wall of beryllium and tungsten. Beryllium erodes rather easily under plasma exposure due to physical and chemical sputtering, which release Be, Be^+, BeH and BeH_2 into the plasma. The erosion mechanism itself is not studied in this CRP, but we are interested in data to support diagnosing beryllium in the plasma.
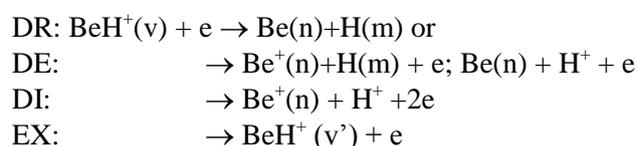
In principle the rate of erosion can be measured by spectroscopy of the lowest charge states of the atoms and molecules (source terms spectroscopy), so primarily of Be, Be^+, Be^{2+}, BeH, BeH^+, BeH_2 and BeH_2^+. In order to make quantitative sense of such spectroscopic measurements one needs a complete set of rate coefficients for excitation, ionization and the various molecular break-up channels, for relevant plasma conditions. The relevant plasma temperature is anywhere from 1 eV to 100 eV. In experiments the relevant isotope is most often deuterium; we generally use "H" to denote any isotope.

In fusion experiments molecules are diagnosed via spectroscopy of electronic transitions. (The molecular vibrational spectrum is in the IR and there is too much background.) The spectrum depends on the vibrational state population, so these electronic transitions can serve also as a measurement of vibrational excitations. It implies that one needs data for joint electronic and vibrational excitations of the molecule. The principal experiments in which beryllium is exposed to plasma are the linear plasma device PISCES at UCSD and the JET tokamak in the UK.

Information about spectroscopic measurements of BeH and BeH_2 was refined after the meeting through email correspondence with D. Nishijima at UCSD and S. Brezinsek at JET. It was learned that on both experiments neutral BeH is measured via the A–X electronic transition ($\Delta v = 0$, $\lambda \sim 497.3$–499.2 nm), but there is no documented measurement of BeH^+. There is no direct measurement of BeH_2 or its ion, but it is speculated that a vibrational line for BeH_2 (strict protonium this time) could be measured in the PISCES laboratory environment. The corresponding line in BeD_2 would be too far into the IR in any case.

The molecular breakup of BeH is likely to proceed via ionization to BeH^+ and then dissociation to Be and H^+ or to Be^+ and H, but dissociative recombination to Be and H is also possible and at high enough energy also dissociation to $Be^+ + H^+$. For the case of BeH_2 the dissociation chains would most likely proceed via either BeH or BeH^+.

The required data therefore include vibrationally resolved dissociative recombination (DR), dissociative excitation (DE) and ionization (DI) of BeH^+ (BeD^+, BeT^+) as well as excitation:

$$\text{DR: } BeH^+(v) + e \rightarrow Be(n)+H(m) \text{ or}$$
$$\text{DE: } \rightarrow Be^+(n)+H(m) + e; Be(n) + H^+ + e$$
$$\text{DI: } \rightarrow Be^+(n) + H^+ +2e$$
$$\text{EX: } \rightarrow BeH^+ (v') + e$$

where n and m refer to electronic states and v and v' refer to vibronic states. For neutral BeH one needs cross sections for excitation and ionization and also for DE and DI.

These data for electron impact processes on BeH and BeH^+ have the highest priority. Similar data for BeH_2 are relevant as well, but interest is somewhat lower so long as BeH_2 isn't being measured. Probably the most important piece of information for molecular processes of BeH_2 is the fraction of BeH_2 that dissociates via BeH versus the fraction that bypasses neutral BeH. This information is needed in order to interpret measurements of BeH and relate those measurements to an erosion rate.

For this process some data is available for low collision energy (below a few eV). At higher energies, more channels and states are needed and the data is not currently available. At higher energy also dissociative ionization break-up should be important.

In addition to being formed on the wall BeH can also be formed by exchange reactions in the plasma volume: $Be^+ + H_2 \rightarrow BeH + H^+$; this is an important process to make sense of measurements of BeH in the divertor plasma when the temperature is below ~3 eV

All elastic and inelastic atomic collisions Be+H can be done with multiple combination of theoretical methods. It is a ripe field and data are available for elastic, inelastic, and n-resolved processes for:

$$Be + H^+,$$
$$Be^+ + H(*),$$
$$Be^{2+} + H.$$
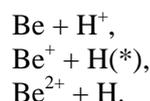
BeH (v) + proton process is less important, but not unimportant in the energy ranges of 10-200 eV:

$$BeH(v)+H^+ \rightarrow BeH(v') + H^+$$
$$\rightarrow Be + H + H^+$$
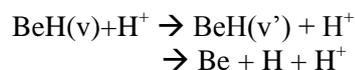
Lithium hydride, LiH

Lithium wall coating and lithium diagnostic beams have long been used on fusion experiments. At present the most intense interest in lithium is probably due to the NSTX experiment at Princeton Plasma Physics Laboratory, which is devoted to the development of lithium wall technology.

The relevant molecular processes are similar to those for BeH: excitation, ionization and DE and DI by electron impact on neutral LiH; DR, DE and DI by electron impact on LiH^+, formation of the molecule in collisions $Li^+ + H_2$; all vibrationally resolved and distinguishing H, D, T.

N_2 in edge plasmas

N_2 gas injection is used for edge plasma radiative cooling as well as rare gases such as Ne and Ar. We have seen modeling of N_2 gas injection in which the molecular aspect is ignored so that the source term is treated as atomic N and rate coefficients (from ADAS) for ionization, excitation and recombination of N^{q+} are used. In order to include the molecular contribution, data for excitation, ionization and breakup of N_2 are needed. The relevant temperature is in the range from 1eV to 100eV.

A good diagnostic scheme for gas temperature is $N_2 + e \rightarrow N_2^+(*) + e + e$ where the rotational state is frozen so that rotational T can be inferred. This diagnostics has been used in the supersonic jet expansion with the strongest intensity from v=0 $\rightarrow$ v'=0 transition. It has been widely used and relevant data must be available in a tabulated form.

The dissociative ionization process is important for E > 20 eV:
$$N_2^+(v) + e \rightarrow N^+ + N^+ + e + e.$$
Data for dissociative recombination has been produced by S. L. Guberman.

Miscellaneous remarks

Precise experimental studies of collision processes are more difficult for neutrals than for ions. In the incoming channel it is difficult to prepare a neutral beam and in the outgoing channel it is difficult to detect and characterize the neutrals. On the other hand, computational studies are often motivated by the availability of measured data. As a result there are gaps in the data sets for electron collisions with neutral molecules. (Note work by Celiberto et al, for example).

R-matrix calculations can be performed for electron impact process of BeH (B. McLaughlin and J. Tennyson), however, the difficulty lies in molecular structure calculations. Å. Larson may perform calculations on electron collisions with neutral molecules (such as BeH) using the complex-Kohn variational method.

3.3 Prospects for Uncertainty Estimates

Provision of an internationally agreed reference data library of AM/PSI data for fusion applications is an ambitious project initiated by the IAEA A+M data unit. In order to achieve this goal it is crucial to obtain evaluated data from community. Until recently, a data evaluation project was not highly valued in the competition so that it was not a promising career move to specialize in data evaluation. A review paper may become highly cited, but original research is most sought after. For these reasons it is difficult to motivate researchers to be involved in data evaluation.

In spite of these obstacles the problem is already starting to be solved in the astrophysics community by embedding data evaluation activities into collaborative research involving applications. Similarly, a paper on AM/PSI data within fusion modeling is considered as an original paper in the plasma physics field if not in the AMO field. A paper on new temperature diagnostics or data analysis with plasma modelers can become highly cited. Atomic and molecular data work leading to a reduction of error bars in temperature diagnostics will be viewed as valuable original work in plasma physics.

Data evaluation depends essentially on the uncertainties of reported (measured or calculated) values. However, it is difficult to assess the uncertainty of theoretical data. It will require multi-dimensional analysis of small and non-linear variations over many parameters and enumeration of all the assumptions, both physical and numerical, in the calculation. However, asking everyone to do it for every calculated data point is unrealistic. It would be logical to proceed as a community to perform sensitivity analysis and obtain quantitative information on the multi-dimensional variations. How uncertainties arise should be characterized and documented. Researchers should be encouraged to provide such information in their publications and reports.

Structure and scattering calculations should be understood together for their uncertainty evaluations. Uncertainties of structure data do not propagate linearly and automatic scripts may be used in exploring uncertainties of collisional strengths resulting from the uncertainties of atomic structures. But the funding for such projects is difficult to find. In general collisional strengths of resonance transitions are reasonable even with less accurate structures. Scattering calculations will be too big to tackle if one tries to reproduce spectroscopically accurate structure. Others, typically of small values such as transitions involving double excited states may be affected by better structures.

Z-scaling laws for uncertainties of atomic data were shown in the Monte Carlo exploration of uncertainty propagation. The scaling law for uncertainties of R-matrix collisional strengths (S. Loch) gave a good agreement within 10% for allowed transitions but 40% for forbidden transitions when compared with Monte Carlo results. Such information will be useful in defining uncertainty estimates of theoretical data.

Regarding molecular scattering data, vibrational constants are one of the biggest uncertainties in input parameters. Electronic structures are required to perform nuclear dynamics calculations for dielectronic recombination data. Even for a given electronic structure, reaction calculations are so complicated that one struggles with simple systems like H_2 or HeH. Quantum defects used in R-matix calculations should be examined for their accuracies. R-matrix codes widely available in the community should be checked for the reported bugs from collaborators.

The accurate treatments of resonance states are important for reliable results. Individual resonances have large uncertainties which are sensitive to quantum-defects or coupling constants. However, it is not clear how much each resonance affects the averaged data eventually to be used by modeling, or if it is possible to quantify uncertainties of the averaged data. The importance of resonances depends on

the systems: Some Rydberg resonances do not contribute much or others dominate. In the example of H_3^+, there is no DR without Rydberg resonances. It's a question of mechanism more than precision, that is, it matters more to include resonances in calculations than how accurately they are specified.

Highly excited vibrational states are interesting, but experimental data are rarely available. Calculations depend on the Hamiltonian which is rather suitable for low lying vibrational states. For better results, coupling constants, Hamiltonian interaction, quantum defects need to be reviewed and improved. Simpler methods can be introduced to test approximations of Hamiltonians.

The IAEA A+M data unit supported two code comparison workshops to help theoretical physicists understand uncertainties of their codes: the 7th non-local thermodynamic equilibrium (NLTE) code comparison workshop and the first spectral line shapes in plasmas (SLSP) code comparison workshop. In these workshops participants submit their results of pre-defined cases beforehand, and compare them at the workshop to identify sources of discrepancies and most significant assumptions in the codes. The unit is interested in supporting workshop proposals to understand the assumptions and uncertainties underlying theoretical atomic and molecular data sets.

3.4 Comprehensive Review; Data and Remaining Data Needs for Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

The importance of hydrocarbon data was deemphasized since ITER is moving towards a decision not to use graphite in the divertor. Currently data with Be and BeH are most urgent, however, experimental data is sparse due to toxicity of Be material.

The role of Li in the context of flowing blanket design was raised. A few tokamaks have heavy Li coating and LiH can be important. Liquid metal Li has been proposed to be used for wall protection though it is a questionable concept for the time being. Boron is discussed in the context of the wall coating and oxygen is hard to avoid as an impurity in the present machines.

There are observations of light elements in fusion devices: spectroscopic data of BeH, BeD are measured in tokamak (JET, PISCES) of X-A decay without any rotational resolution. Spectroscopic measurements of BeD^+ and of BeD_2 would be of interest if they are possible.

There are too few AM/PSI experiments to support the tokamak studies. Dissociative recombination of BeH_2^+ may be done (Stokholm) but it needs a motivation. In early days in JET there used to be a laboratory for electron-impact ionization to support the fusion relevant data. There needs to be an action to increase experimental activities in support of ITER program, such as a laboratory to produce Be data. It would be helpful if the need for standard recommended and evaluated AM/PSI data is acknowledged by ITER and ITPA. A document that lists the current needs and status could help to bring this about. A technical general meeting to produce a detailed list of processes is desired.

3.5 Follow-ups of the CRP: Final Report and Recommended Database

Final Report

The report of the CRP project will be published in the Journal of Physics: Conference Series (J. Phys. Conf. Ser.). The IAEA AM data unit has published final reports of CRP projects in the book of atomic and plasma-material interaction data for fusion (APID, also known as the Green books) since 1989. The APID volume was provided as a supplement to the Nuclear Fusion journal at its inception. Since volume 7, however, the association to the journal was lost and APID became less recognized. Contributions to APID volume are hardly citable and are not considered as a proper publication. The IFRC (International Fusion Research Council) subcommittee on A+M data agreed with a new proposal to use J. Phys. Conf. Ser as a medium to publish the CRP final report.

The manuscript should be submitted by June and refereed by September for a special volume of J. Phys. Conf. Ser. devoted to this CRP. The content of report may include data or a summary of work during the period of CRP. There will be one referee inside the group and the other outside the group. There is no limit in pages for this electronic journal and it is a good place to publish data sets unfit for traditional journals as a source of a new and recent reference.

An alternative of a review report of current status and progress in the CRP topic is a possibility. It was successfully demonstrated by the group of the CRP on the "Tritium Inventory in Fusion Reactors". C. Skinner coordinated and published a joint paper (~ 7-8 groups) in 2008 two years after the conclusion of the CRP. The scope of the joint publication was not a review of the whole field, but a coherent story based on the CRP. As more authors are included in the publication, more citations benefit the groups in the CRP. Participants in the tritium CRP also produced an APID green book. The possibility to produce a few review publications of atomic and molecular work based on the present CRP was discussed, but in the end this was not favoured.

Various citation measures are increasingly being used for evaluation of researchers and research groups by funding agencies. Although the current proposal is a huge improvement over the non-citable APID volume, there was a concern raised that a publication at J. Phys. Conf. Ser. would adversely affect the evaluation of one's work since no impact factor is assigned to journals of conference papers. The situation is unfortunate for the data community. Data is usually generated using well-established methods that are already published, possibly with small modifications, and the work that produced the data will not be published in high impact factor journals since it is not new or original. If the most up-to-date data are cited by data user with the old paper where the method was published, it is simply incorrect and any changes done for the new data will not be reported.

It is strongly suggested that data centers and databases should provide references for individual data so that the contributor can get the credit for the data. Citation will be a good payback for data contributors and data used and cited will help data research projects getting the support to continue the work.

Recommended databases

After the completion of this rather broad CRP there are possibilities of smaller follow-up meetings on special topics. One topic that comes to mind is assembly, evaluation and recommendation of data for beryllium in fusion plasma, focused on processes of Be, BeH and BeH_2 and their ions in the near-wall region. Another topic is data for neutral beams spectroscopy, which would be concerned with H, He, Li and possibly Na neutral beams.

A combined dataset for atomic Be from CCC (I. Bray) and R-matrix (S. Loch) to provide differential and integrated electron-impact cross-sections of Be, Be^+, Be^{2+}, Be^{3+} was discussed. R-matrix results are known to present resonances at low energies while CCC results work well for high energies. Comparisons will be done for near ionization energies and overlapping energy regions and the two data sets will be combined to represent a wide range of energies. A comparison between R-matrix and CCC results will lead to an improved understanding of uncertainties of theoretical data.

Some fusion applications require unprocessed data sets such as differential cross-sections or resonance structures. ADAS only stores the limited size of processed data sets and it will be useful to store the raw data sets at available sites such as IAEA A+M data unit page.

A database for molecular processes involving BeH is urgent in the impurity diagnostics of the ITER-like wall fusion devices. For the core plasma the most important light element data are those related to neutral beam charge transfer processes and associated spectroscopy.

4. Conclusion

IAEA's coordinated research activities are designed to stimulate and coordinate research by scientists in IAEA Member States towards development and application of atomic energy, including fusion energy, and to foster collaborations among scientists and the exchange of scientific and technical information. Coordinated research projects of the Nuclear Data Section encourage cooperation in the development of fundamental nuclear and atomic data to support peaceful nuclear applications.

The contributions at the third and final research coordination meeting of the CRP on data for light elements in fusion plasma cover a wide range of atomic and molecular processes of light element impurities and the results demonstrate the continued importance of atomic and molecular physics for fusion energy research. New data produced in the course of the CRP has been entered into the ALADDIN database and it is expected that more data will follow. The meeting discussions also clarified in what areas further data development is needed; primarily this is the area of combined electronic and rovibrational excitations of light element molecules in edge plasma conditions. More work is also needed to obtain uncertainty estimates and provide expert recommendations for comprehensive light element datasets to be used in plasma modelling.

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Agenda

Wednesday 20 March   **Meeting room: F0811**

09:30:   Robin Forrest / Bas Braams: Welcome, adoption of the agenda, introductions

Session I   ***Chair: David Schultz***

09:50:   **Stuart Loch:** "Generalized collisional radiative model for light elements: C: Data for the boron isonuclear sequence"

10:25:   **Igor Bray:** "Electron scattering on beryllium and its ions"

11:00:   *Break*

11:20:   **Joseph Reader:** NIST database work on spectra of light elements and brief update for tungsten

11:55:   **Viorica Stancalie:** The low-energy inelastic scattering of electrons by atomic systems

12:30:   *Lunch*

Session II   ***Chair: Baoren Wei***

14:00:   **Yueying Qi:** Impact-ionization process of high-energy electrons on hydrogen-like ions in Debye plasmas

14:35:   **David Schultz:** Update on light ion calculations

15:10:   **Yong Wu:** Theoretical investigations on ion-atom collisions

15:45:   *Break*

16:10:   **Hyun Chung:** Coordinated activities on data evaluation

16:30   **All:** Status of data for light element electron-atom (ion), ion-atom and radiative processes

19:30:   Social dinner (outside VIC)

Thursday 21 March   **Meeting room: F0811**

Session III   ***Chair: Luis Mendez***

09:00:   **Baoren Wei:** The dissociation process of hydrocarbon molecules by low energy electron impact

09:35:   **Pierre Defrance:** Electron impact fragmentation of molecular ions

10:10: **Brian Mitchell:** Dissociative recombination: recent development in theory and future experimental facilities

10:45 *Break*

11:10: **Åsa Larson, Mats Larsson:** Recombination reactions and commissioning of DESIREE

11:50: **Ioan Schneider, Zsolt Mezei:** Electronic and photonic reactive collisions: application to H_2, BeH and H_3 systems

12:30: *Lunch*

Session IV   ***Chair: Pierre Defrance***

14:00: **Dragan Jakimovski:** 1) Dissociative electron attachment to H_2 molecules and 2) electron impact processes of plasma impurities: BeH^+ and BeH

14:40: **Hidekazu Takagi:** Processes of electron and molecular ion collisions relevant to divertor plasma: H_2^+, HeH^+, and their isotopes

15:15: **Luis Mendez:** Recent calculations of total and state-selective electron capture cross sections

15:50: *Break*

16:20: **All:** Status of data for light element molecular processes

Friday 22 March   **Meeting room: F0811**

Session V   ***Chair: Hyun Chung***

09:00: **Bas Braams:** Data Centres Network and Code Centres Network activities

09:20 **All:** Prospects for uncertainty estimates; spectroscopic and collisional data for beryllium and its hydrides

10:45: *Break*

11:10 **All:** Comprehensive review; data and remaining data needs for light element atom, molecule and radical behaviour in the divertor and edge plasma regions

12:30: *Lunch*

Session VI   ***Chair: Bas Braams***

14:00: **Bas Braams:** Procedures for Journal of Physics Conference Series

14:15: **All:** Outline and schedule for final report of the CRP

15:00: *Close of meeting; opportunity for informal work and discussion*

Summary of Presentations

Summaries are given below for the meeting presentations available at http://www-amdis.iaea.org/ .

Electron collisions with beryllium and its ions

Igor Bray

The original convergent close-coupling (CCC) method for electron scattering on atomic hydrogen [1] was extended to quasi one-electron targets [2] and quasi two-electron targets [3]. This allows CCC to be applied to electron collisions with beryllium and all of its positive ions. The foundation of the method is the complete Laguerre basis, used to diagonalise the target Hamiltonian, for each angular momentum l, basis size N_l and exponential fall-off parameter $\lambda_l/2$. Presently, for the Be^{q+} targets, we set $\lambda_l/2 = q + 1$ for all target orbital angular momentum $l \leq 4$.

Beginning with the H-like Be^{3+}, 85-state CCC calculations were performed to determine the electron-impact cross sections. The 85 states were generated by taking $N_l = N_0 - l$ Lagurre basis functions, with N0 = 20.

Electron-impact excitation and ionization on the He-like Be^{2+} was calculated using the CCC method with a total 284 states. Here the two-electron target states were generated using two Laguerre bases, one for the "inner", and another for the "outer" electron. The size of the calculations was primarily determined by the "outer" basis, where $N_l = N_0 - l$ with $N_0 = 25$, for both singlet and triplet states.

The Li-like Be^+ target wave functions were expanded in much the same way as for Be^{3+}, except that the 1s state was obtained in the Hartree-Fock approximation. Consequently the number of states included in the electron-scattering calculations was 84.

Lastly, electron scattering on neutral beryllium is similar to the e-Be^{2+} case, and was performed by expanding the total wave function with 292 target states. These were required to give a good representation of the target discrete singlet and triplet states, as well as the continuum.

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[1] Bray I and Stelbovics A T 1992 Phys. Rev. A 46 6995–7011
[2] Bray I 1994 Phys. Rev. A 49 1066–1082
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Electron Impact Dissociation of Molecular Ions

Pierre Defrance

Electron impact experiments were performed by means of our crossed electron-ion beam set-up. Singly and/or multiply charged ions that results from molecular ion fragmentation are detected individually. Cross-sections for their production are determined from their respective thresholds up to 2.5 keV.

The animated crossed beams method is applied to measure:
- Absolute inclusive cross sections for electron impact dissociation to individual ionic fragments from the energy threshold up to 2.5 keV.

- The contributions from the different reaction channels are separated: single ionization (SI), dissociative excitation (DE) and dissociative ionization (DI).
- Kinetic energy release distributions (KERD) of the fragment ions are determined at selected incident electron energies. It allows determination of groups of electronically excited states that contribute to the process considered.
- Energy threshold determination allows identification of target initial ground and excited states.

Monohydride	HeH^+ To be published	CH^+ (2007)	NH^+ (2010-11)	OH^+ (2012)	NeH^+ (2008)
Polyhydride		CH_2^+, CH_3^+, CH_4^+ (2008-9)	NH_2^+, NH_3^+ To be published	OH_2^+, OH_3^+ To be published	
		C_2D^+, $C_2D_2^+$ (2010) $C_2D_3^+$, $C_2D_4^+$ To be published	N_2D^+ In progress		
Diatomic	H_2^+ (2004)	C_2^+ To be published	N_2^+ (2001)	O_2^+ (2006)	
Others:	D_3^+ (2009) D_2H^+ (2011)				

1. Monohydride ions: HeH^+, NH^+, OH^+, and isotopologues XD^+
For HeH^+, experimental results are available for the production of He^+ and He^{2+}. They were analysed taking into account the vibrational population measured in a separate charge transfer experiment (paper in preparation).

2. Polyhydride ions: NH_2^+, NH_3^+, OH_2^+, OH_3^+ and isotopologues *(unpublished)*

3. Hydro(deutero)-carbon ions: $C_2D_3^+$, $C_2D_4^+$ and isotopologues $C_2D_3H^+$, $C_2D_2H_2^+$
(unpublished) Experimental results have been obtained for $C_2D_3^+$ and $C_2D_4^+$. The collected data were analysed in detail.

4. Others: C_2^+ *(unpublished)*
The full analysis of data for electron impact dissociation of C_2^+ yielding the C^+ fragment was performed. These data now need to be published.
N_2H^+, in progress.
D_3^+, D_2H^+
Dissociation of H_3^+ isotopologues have recently discussed comprehensively, especially as regards isotope effects in the fragmentation.

Dissociative electron attachment to H_2 molecules and electron impact processes of plasma impurities: BeH^+ and BeH

D. Jakimovski

This presentation encompasses four published papers of other authors, devoted to following themes:

1) Calculation of cross sections for dissociative electron attachment on vibrationally excited H_2 molecule taking place via Rydberg-excited resonant state, studied using the local complex potential model for resonant collisions, from selected initial vibrational levels of the neutral molecule. The results of corresponding rate coefficients for all included levels, calculated in the 0.5–1000 eV energy range are also presented.

2) The results for cross sections and rate coefficients for electron-impact-induced excitations in BeH^+ molecules, occurring between vibrational levels of different electronic states (vibro-electronic transitions) have been presented for a broad energy range. Accurate analytic fit expressions have been also presented.

3) The results for electron-impact cross sections for transitions between selected vibrational electronic states of the BeH molecule, using R-matrix method have been presented. Rate coefficients were also presented for these same transitions as well as scaling relationships in simple analytic form.

4) The results for electron impact ionization cross sections for Be and some of its hydrides, from the ionization threshold to 1 keV, have been presented, with good agreement with results from earlier calculations (convergent close-coupling, R matrix, distorted-wave and plane-wave Born approximation in the low energy region. The data for various beryllium hydrides are presented without such comparisons for the authors are not aware of other available data.

Recombination reactions and commissioning of DESIREE

Åsa Larson and Mats Larsson
Department of Physics, Stockholm University, Sweden

By combining electron scattering calculations with structure calculations molecular potential energy curves, couplings and autoionization widths are obtained. Using this molecular data the cross sections of different recombination reactions relevant for the fusion plasma of the Divertor can be calculated. Here electron-molecular ion collisions leading to either dissociative recombination, vibrational excitation (or de-excitation) or dissociative excitation have been studied. Furthermore, the believed presence of H^- in the plasma is a motivation for the study of mutual neutralization in collisions between H^- and light atomic cations (H^+, He^+, Be^+).

We have performed both quantum *ab initio* as well as semi-classical calculations on reactions involving the H_2, HeH and BeH molecular systems.

On H_2, the focus has been on the mutual neutralization reaction in collisions of H^+ and H^-. An fully quantum *ab initio* study [1] of the reaction produce total cross section and final state distributions in good agreement with experimental studies. Additionally, the neutralization cross sections are computed for collisions between different isotopes of the hydrogen ions and a very small isotope effects are observed. Furthermore, the differential cross section of the reaction is calculated. A semi-classical Landau-Zener model is used to study the reaction. Different methods to obtain the electronic coupling elements between ionic and covalent states are examined by comparing the semiclassical results with those obtained quantum mechanically.

Theoretical studies of dissociative excitation of HeH^+ are performed where both the resonant and direct processes are investigated. Calculations on the non-adiabatic couplings between resonant states of HeH are under the way and goal is to perform a fully quantum *ab intio* study of mutual neutralization in $He^+ + H^-$ collisions as well dissociative recombination and resonant ion-pair formation.

The direct mechanism of dissociative recombination of BeH^+ has previously been studied [2] and now the indirect capture through bound Rydberg states are included in the model [3]. The cross section for mutual neutralization in collisions of $Be^+ + H^-$ is computed using the semi-classical Landau-Zener model.

The double electrostatic ion storage DESIREE [4] is now in the commissioning phase. It has been cooled down to 15 K and storage in the symmetric ring has been demonstrated. The anion C_2^- has been stored for several minutes, which is extremely promising taking into account how easily an anion is

destroyed in collisions with residual gas molecules. The next step is to store ions also in the asymmetric ring. Once this is accomplished, the first mutual neutralization experiments can start.

References
[1] M. Stenrup, Å. Larson and N. Elander, Phys. Rev. A, **79** 012713 (2009).
[2] J. B. Roos, *et al.,* Phys. Rev. A **80**, 012501 (2009).
[3] S. Niyonzima *et al.* Phys. Rev. A **87**, 022713 (2013).
[4] R. D. Thomas *et al.* Rev. Sci. Instr. **82**, 065112 (2011).

Generalized collisional radiative model for light elements: C: Data for the boron isonuclear sequence

S. D. Loch

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In this talk, the recent work on generalized collisional-radiative (GCR) modeling for light fusion relevant elements was summarized. GCR theory was presented, along with some illustrative examples from previous calculations on Li and O. A particular focus was placed on the importance of excited state ionization, which can increase the effective ionization of near neutral charge states by up to a factor of ten.

The problem of excited state ionization was then discussed for near neutral systems. Perturbative approaches will overestimate the cross section, while non-perturbative methods cannot be extended to very high n-shells. Recent work on B was presented as a example of how one might proceed. If one first isolates the direct ionization contribution, and calculates it for successive n-shells with a non-perturbative approach, it may be possible to calculate high enough in n that a classical n-scaling emerges. This was shown to work well for B, B^+, and B^{2+}. This allows the high quality ionization data to be extrapolated to much greater n-shells.

A summary was then given of the data used in recent boron GCR calculations. Some brief results from the GCR calculations were then shown, again showing the importance of excited state ionization. The new B data should be available shortly for use by the modeling community. Finally, a quick description of the fundamental atomic data remaining for carbon GCR calculations was presented.

Recent calculations of total and state-selective electron capture cross sections

L. Méndez

Departamento de Química, Unversidad Autónoma de Madrid

The group of the Universidad Autónoma de Madrid has performed calculations of cross sections for electron capture (EC), excitation and ionization in ion-atom and ion-molecule collisions in a wide energy range. At high impact energies, $1<E<500$keV/amu, we have applied the Classical Trajectory Monte Carlo (CTMC) treatment (see [1] and references therein) to evaluate ionization and *nl*-resolved EC cross sections for collisions of fully stripped ions (B^{5+}, C^{6+} and N^{7+}) with H(n=1,2). The EC cross sections show general good agreement with recent calculations of Igenbergs *et al.* [2]. We have also considered H excitation in ion collisions. In particular we present new cross sections for excitation up to n=6 in Li^{3+} + H collisions, obtained by combining semiclassical close-coupling and CTMC calculations.

With respect to low energy ion-atom collisions, we present EC total cross sections in H^+ (D^+, T^+) + $Be(1s^2 2s^2)$ collisions, evaluated by employing a quantal treatment, where we explain the or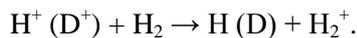igin of the huge isotope effect [3] found for this system at energies of about 25 eV/amu with $\sigma_H/\sigma_D \approx 20$ and $\sigma_H/\sigma_T \approx 200$. However, it is found that $\sigma_T > \sigma_D > \sigma_H$ for the inverse (endothermic) reaction:

$$Be^+(1s^2 2p) + H(1s) \rightarrow H^+ + Be(1s^2 2s^2) .$$
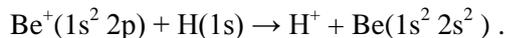
We have studied EC in ion-molecule collisions. Two reactions have been considered:

$$H^+ + N_2 \rightarrow H + N_2^+$$

and

$$H^+ (D^+) + H_2 \rightarrow H (D) + H_2^+.$$
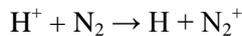
In the former system we have carried out semiclassical calculations [4] for $0.1 < E < 10 keV$, and compared the ensuing total cross sections with previous calculations and experiments. In the later system we have considered collision energies between 10eV and 1 keV, in order to study the variation of the vibrational distribution of H_2^+ with the collision energy. In this case we have employed quantal and semiclassical treatments with a vibronic close-coupling expansion.

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Electronic and photonic reactive collisions: application to H_2, BeH and H_3 systems

J. Zs. Mezei and I. F. Schneider

Reactive collisional and radiative elementary processes rate coefficients have been computed using multichannel-quantum-defect theory methods [1], and partly measured in merged-beam (storage ring) and crossed-beam experiments. The reaction mechanisms are explained and output data are displayed in ready-to-be-used form.

1. Electronic collisions

a) $\underline{HD^+$ and H_2^+ targets.}$ At low energy (below the ion dissociation limit), the dissociative recombination (DR) is dominated by the resonant captures into Rydberg series of states converging to numerous ro-vibrational thresholds [2]. Above the dissociation limit, these resonances disappear, and other states, built on the vibrational continuum of the molecular ion, play an essential role in the DR, through the dissociative excitation (DE) [3].

b) $\underline{BeH^+}$ target. Low-energy DR and vibrational transitions (VT) have been studied [4], based on previous extensive molecular structure data calculations [5]. The first results on the high-energy computations, including the DE, are shown.

c) $\underline{H_3^+}$ target. An analytical method to estimate the DR average rate is presented [6]. It is based on a three-channel MQDT-based approach and on previous experimental determination of the H_3 Rydberg-states autoionization width.

d) $\underline{H_2}$ target. The first results on the production of fast metastable $H(2^2S)$ atoms obtained in coincidence experiments of electron/molecule impact dissociation [7] in Laboratoire Aimé Cotton are displayed and discussed.

2. Photoionization

The cross sections for the Q(N) (N = 1 − 4) photoionization of H_2 in $X^1\Sigma^+g$ ground ($v'' = 0$) and vibrationally excited ($v'' = 1,...,10$) states have been computed [8] and resolved with respect to the vibrational level (v^+) of the resulting H_2^+ ion. The temporary captures into $np\pi\ ^1\Pi^-_u$ ($v' = 0, . . .;$ n=2-6) H_2 Rydberg states strongly drive the ionization process.

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Dissociative recombination: Recent Developments in Theory and Future Experimental Facilities

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Dissociative recombination is a critical reaction in fusion edge and divertor plasmas as it governs the state of ionization in molecular systems as well as leading to reactive and stable products that can be detected and that can continue to play a role in the chemistry of the environment. The last two decades have seen an explosive growth in the experimental study of this process and this has provided much information concerning not only reaction cross sections but also product branching ratios. Much of this work has been performed using the merged beams technique at heavy ion storage rings (CRYRING in Sweden, ASTRID in Denmark, TSR in Heidelberg, TARN II in Japan). At this time however, only TSR is still operating in this mode (ASTRID operates exclusively as a synchrotron radiation source).

Some recent research highlights will be discussed in the talk. These will include:
- The theoretical examination of the sharp fall-off of the cross section observed at super-thermal energies [1].
- The measurement internal temperatures of ions used in storage ring experiments [2].
- The importance of knowing true branching ratios on the subsequent chemistry of plasmas [3].

Future prospects for experimental work at the new Heavy Ion Storage Ring in Langzhou, China and at the electrostatic storage ring at KACST in Saudi Arabia.
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NIST database work on spectra of light elements and brief update for tungsten

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Work at NIST on the spectra of light atoms is concentrated mainly on critical compilations of papers that have appeared in the literature and dissemination of the data through online databases. We are currently completing work on transition probabilities for F^{4+}-F^{7+} and Ne^{5+}-Ne^{8+}. We have also carried out theoretical calculations to interpret intensities of Balmer alpha lines of atomic hydrogen split by motional Stark effect. Some of our recent papers include:

1. Transition probability measurements for some strong and weak lines of N I, J. M. Bridges, and W. L. Wiese, Phys. Rev. **A** 82, 024502 (2010).
2. Energies and E1, M1, E2, M2 transitions rates for states of the $2s^22p$, $2s2p^2$, and $2p^3$ configurations in boron-like ions between N III and Zn XXVI, P. Rynkun, P. Jonsson, G. Gaigalas, and C. Froese Fischer, At. Data Nucl. Data Tables **98**, 481 (2012).
3. Non-Statistical Population Distributions for Hydrogen Beams in Fusion Plasmas, O. Marchuk, Yu. Ralchenko, and D. R. Schultz, Plasma Phys. Contr. Fusion **54**, 095010 (2012).

Our online databases are found on the NIST Physical Measurement Laboratory website. http://www.nist.gov/pml/ The current version of our Atomic Spectra Database (ASD) contains data for more than 194,000 transitions in about 1000 spectra. Online tools include production of Grotrian diagrams and Saha equilibrium plots. Our bibliographic databases are kept current on an approximately biweekly basis. A search for papers on light elements of fusion interest yields references for about 45 recent papers. A new database within ASD provides ionization energies for all atoms and ions. Almost every value has an estimated uncertainty. This database can be queried by specifying either element and ion stage or by isoelectronic sequence. The NIST website also provides for online collisional-radiative modeling with the FLYCHK code and the plasma population kinetics database from the most recent non-LTE calculation workshop NLTE4.

Recent spectroscopic work on tungsten has been reviewed by Kramida.[1] A search for papers on W in the NIST Bibliographic Database provides references for about 65 papers on W since 2010.

With the NIST electron beam ion trap (EBIT), we continue to observe spectra of W and related heavy elements. We observed ~130 new M1 lines in $3d^n$ configurations of highly ionized Hf, Ta, and Au.[2] In other recent work[3] we observed 50 strong n=3-3 transitions for Xe^{26+}-Xe^{43+}. Surprisingly, of these 50 lines, 30 were new. In work with Kr, we found that the relative intensities of the three lines of the $3s^23p$-$3s^23d$ resonance multiplet differed greatly from what would be expected based on statistical populations of the levels. We interpreted this as being due to the presence of an M1 transition within the $3s^23p$ term, which depletes the $3s^23p\ ^2P_{3/2}$ level and in turn reduces population of $3s^23d\ ^2D_{5/2}$. This is confirmed by collisional radiative modeling of the EBIT plasma both with and without the M1 transition. This now provides a convenient method to determine electron densities in tokamaks containing injected Kr gas by comparing the observed relative intensities to those obtained by modeling with varying electron densities.

In further studies of W, we use the ratio of the intensity of an M1 line in Ca-like W to that of a close M1 line of K-like W to analyze the modifications of the ionization balance in the plasma due to dielectronic recombination. Our modeling shows the importance of anisotropic effects encountered in the EBIT plasma compared to the isotropic environment found in tokamaks.

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2. D. Osin et al., Eur. Phys. J. D **66**, 286 (2012).

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Update on light-ion calculations

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During the time span of the CRP, calculations were (1) initiated extending previous work regarding elastic and transport cross sections relevant to light-species impurity-ion transport modeling, (2) completed for total and state-selective charge transfer (C^{5+}, N^{6+}, O^{6+}, O^{7+} + H; C^{5+}, C^{6+}, O^{7+}, O^{8+} + He; and C^{6+} + H, H_2) for diagnostics such as charge exchange recombination spectroscopy, and (3) completed for excitation of atomic hydrogen by ion impact (H^+, He^{2+}, Be^{4+}, C^{6+}) for diagnostics including beam emission spectroscopy and motional Stark effect spectroscopy.

The first calculations undertaken were to continue work begun more than a decade ago providing plasma modelers with elastic total and differential cross sections, and related transport cross sections, used to model transport of hydrogen ions, atoms, and molecules as well as other species including intrinsic and extrinsic impurities. This body of work was reviewed in the course of reporting recent new calculations in a recent paper (P.S. Krstić and D.R. Schultz, Physics of Plasmas, 16, 053503 (2009)). After initial calculations for H^+ + O were completed, work was discontinued in light of other priorities.

Charge transfer data for diagnostics provide important knowledge about the state of the plasma from the edge to the core and are therefore of significant interest to continually evaluate and improve. Further motivation for such calculations comes from recent and ongoing benchmark measurements of the total charge transfer cross section being made at Oak Ridge National Laboratory by C.C. Havener and collaborators. We have undertaken calculations using a variety of theoretical approaches, each applicable within a range of impact energies, that have led to the creation of a database of recommended state-selective and total cross sections composed of results from the various methods (MOCC, AOCC, CTMC, results from the literature) within their overlapping ranges of applicability. Results for all systems enumerated in item (2) above are complete and the following papers reporting them have been published so far: Y. Wu et al. , "Theoretical investigation of charge transfer between N^{6+} and atomic hydrogen," Phys. Rev. A 84, 022711 (2011); Y. Wu et al., "Theoretical investigation of total and state-dependent charge exchange in O^{6+} collisions with atomic hydrogen," J. Phys. B 45, 235201 (2012); and J.L. Nolte et al., "Final-state resolved charge exchange in C^{5+} collisions with H," J. Phys. B 45, 245202 (2012); with the rest in preparation.

Other important diagnostics depending on a large database of atomic physics are those based on the motional Stark effect and beam emission spectroscopy. In collaboration with Y. Ralchenko and O. Marchuk, we have computed the cross sections and density matrix elements for a large number of impact energies to follow their variation as input to a collisional-radiative model for protons, injected or fusion alphas, Be^{4+}, and C^{6+} exciting atomic hydrogen. Results have been published for proton-impact (O. Marchuk et al., "Non-statistical population distributions for hydrogen beams in fusion plasmas," Plasma Phys. Control. Fusion 54, 095011 (2012)) showing, for example, the importance of consideration of non-statistical populations in interpreting these diagnostics. Work to complete the collisional-radiative models and perform simulations of relevant plasmas (such as those for ITER) is underway for the higher charged ions.

The low-energy inelastic scattering of electrons by atomic systems

V. Stancalie

The R-matrix method is used to calculate collision strength and cross sections for low-energy inelastic scattering of electrons by atomic systems. Application refers to the carbon neutral atoms, and to the C IV and Ar III atomic ions.

Since the collision models applied are very closed, the differences in the resulting cross sections and collisions strengths reflect the differences in the target description. In C I the calculation is made more difficult by the fact that low-energy electron scattering is dominated by a resonance due to the $1s^2 2s^2 2p^3\ ^3P^0$ state of C^-. The theoretical prediction of the location of this resonance, and of the $1s^2 2s^2 2p^3\ ^4S^0$ and $^2D^0$ bound states of C^-, depends on a balance between short-range correlation and long range polarization effects. In our work the importance of including configuration interaction wave functions both in the target-state expansion and in the (N+1)-electron quadratically, integrable function expansion was investigated. Results are compared with the existing reported data.

We have calculated fine structure splitting in the Ar III using the R-matrix method. Two independent atomic structure calculations have been performed. Results from the Breit-Pauli –and the Dirac-Atomic –R matrix relativistic calculations are analysed comparatively. Cross sections and collision strengths are provided for selected weak and intercombination transitions allowing explicitly for resonance effects. Convergence of the partial wave expansion is ensured by examining the partial collision strengths at collision energy up to 20Ry.

Processes of Electron and Molecular Ion Collisions Relevant to Divertor Plasma: H_2^+, HeH^+, and their isotopes

H. Takagi

Collision processes of electrons with H_2^+, HeH^+, and their isotopes are discussed on the evaluation of theoretical calculation. The focused processes are dissociative recombination (DR), dissociative excitation (DE), vibrational and rotational transition by electron impact. Those cross sections (CSs) depend on the initial and final states of vibrational, rotational, and electronic states. Theoretical calculation is indispensable compiling such state specific CS.

Theoretical calculation is based on the scattering of electrons by molecular ions of which nuclei are fixed. Using these adiabatic scattering states, the dynamical processes are solved as scattering problems induced by the configuration interaction (CI) and the non-adiabatic interaction (NAI). The NAI in the Rydberg and ionizing states is well represented by the multi-channel quantum defect theory (MQDT). The accuracy of the theoretical calculation deeply depends on the electronic states included in the calculation. There are two types of electronic states: one is partial waves of incident electrons, and another is excited states of a molecular ion. The present calculation is limited below the collision energy of 11 eV because of the employed electronic states of a molecular ion. [1] The calculated DR CS of HD^+ below 1 eV shows rational convergence according to the accuracy of treatment of the CI and the NAI.[2] That converges to the experimental CS of vibrationally ground state. The calculated DR CS of H_2^+ agrees with experiment within the difference of a few tens % for the ions of rotationally and vibrationally ground state, which is the only state-specific CS measured by experiment. Since any number of the rotational and vibrational states can be included in the calculation, various vibrational and rotational state-specific CSs can be calculated with the same accuracy as the CS of the ground state. Furthermore, if an accuracy is verified for a certain molecule, the same accuracy is guaranteed for its various isotopes.

Only the NAI induces the DR of HeH^+ at low energies. That CS is so large as the DR by the CI. The NAI is represented by inter-nuclear dependence of quantum defects in the MQDT. The value of

quantum defect depends the position of center of partial wave according to the R-matrix calculation by M. Tashiro (IMS). When we choose the center on the H atom, the quantum defect quickly becomes small as the angular momentum increases. If we choose the center on the midpoint of molecule, the CS hardly converges with increasing the partial waves.

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Plasma Effect on Ionization Process of Fast-Electron and Hydrogen

Yueying Qi

Plasma effects can't be neglectful in the atomic structures, photo-excitation and ionizations and electron-impact excitation process, which are shown in the our previous works and other researcher's papers. In the present work, plasma effects on the high energy electron-impact ionization process of Hydrogen-like ions embedded in weakly coupled plasmas are investigated in the first Born approximation. The screening of Coulomb interactions decreases the ionization energies and changes the behaviors of the wave functions, and then the multiple shapes and the virtual-state resonances appear in the single differential cross sections when the plasma screening parameter passes through a certain critical value. The number of the summation for the angular-momentum states in the generalized oscillator strength densities is reduced for the same ratio between the ejecting energy and the ionization energy for the different plasma condition; the contributions from the lower-angular-momentum states dominates the generalized oscillator strength densities, the accessional minima and the outstanding enhancement emerge in the generalized oscillator strength densities in a certain energy region, whose position and width are related to the plasma screening effect. The local maximum exists in a smaller scattering angle for the double differential cross section, which is dependent of the plasma effect on the incident electron.

The dissociation process of hydrocarbon molecules by low energy electron impact

B. Wei

During the CRP project, a cold target recoil-ion momentum spectroscopy (COLTRIMS) has been established and tested at Fudan University. In our COLTRIMS, a full Titanium collision chamber is employed to reduce the residual magnetic. The earth magnetic has also been carefully shield by a pair of coils, and now the incident electron beam can work at the ionization threshold of the molecules. The low energy electron beam, produced from an electron gun, was pulsed by ultra-fast gate generator and the pulse width is about 1 ns with a repetition rate of 10 kHz. To accurately measure the interaction of a low energy electron with a molecule, the resolution of the TOF and detector had been optimized.

The dissociative ionization of methane (CH4) impacted by electron was studied experimentally with COLTRIMS. The relative cross sections between different dissociation channels were measured for electron energy ranging from 20eV to 200eV and a good agreement was achieved with previous studies. From time-of-flight (TOF) and position information of the fragments, the kinetic energies of fragmental ions can be deduced. Taking advantages of supersonic jet expansion, the thermal contribution to the kinetic energy distribution of the fragmental ion is reduced. In the present work, the mean kinetic energy released (KER) during dissociation process was estimated from the average kinetic energy of ionic fragments and the result agreed with the previous theoretical data.

Theoretical investigations on ion-atom collisions

Y. Wu, L. Liu, C.H. Liu, J.G. Wang

In this talk, I will present the main progresses of our work achieved or initiated in 2012, which focused on the collision processes between basic edge/divertor plasma constituents (H, He, H_2^+) and the light element atomic plasma impurities (Ne^{q+}, O^{q+}), as well as the collisions between Ar and He^{2+}, which exists in the neutral beam injection processes in the magnetic confinement fusion.

In our work, the MOCC and AOCC methods have been applied to investigate the charge transfer and excitation process between ion-atom or ion-molecule collisions. Especially, the time-dependent density functional theory method has been recently developed to treat the charge transfer and electron loss processes in ion-atom collisions. The main results of the following processes will be presented in my talk: (1) Bare and hydrogen-like ions of Neon and Oxygen collisions with H and He; (2) Charge transfer and excitation processes in H_2^+-He collisions; (3) Electron capture and electron loss in H_2^+- Ar collisions.

For processes (1), by using AOCC method, accurate charge transfer cross sections have been computed for a large collision energy range and compared with the available theoretical calculations and measurements. The emission spectra following charge transfer processes have also been simulated and excellent agreements with the available measurements have been achieved. For processes (2), the MOCC method has been applied to investigate the dynamic processes in H_2^+-He collisions, in which the collision-induced dissociation (CID) processes are found to be dominant. It is also found that the rotational couplings play an important role in CID process and the dissociation cross sections sensitively depend on the molecular alignment, especially for low energy collisions. For processes (3), accurate charge transfer and electron loss cross sections have been computed by using the TDDFT method. Note that the accurate cross sections for multi-electron processes have also been obtained, including multi-electron loss and multi-electron charge transfer cross sections.

In summary, the AOCC and MOCC methods have been applied to treat the highly charged ion collisions with atomic hydrogen and helium, as well as the ion-molecule collisions. The TDDFT method has been developed to effectively treat the multi-electron processes in ion-atom collisions. Accurate total cross sections, n-, and l- resolved cross sections have been obtained for the collisions systems studied, which are important parameters required in the magnetic confinement fusion researches.

List of Publications

[Publications since 2009 by participants in the CRP and their close associates and related to the subject matter of the CRP.]

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