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

Summary Report of the Second Research Coordination Meeting

IAEA Headquarters, Vienna, Austria
23-25 May 2011

Prepared by
B. J. Braams and H.-K. Chung

August 2012

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

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Abstract

The second Research Coordination Meeting (RCM) of the Coordinated Research Project (CRP) "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" was held 23-25 May 2011 at IAEA headquarters, bringing together experts representing 14 institutions and the IAEA. Participants summarized their recent and ongoing work on atomic and molecular processes involving light elements in plasma and reviewed progress made since the first RCM. Gaps in knowledge were identified and a plan of work for the remainder of the CRP was developed. The presentations, discussions and recommendations of the meeting are summarized in this report.

August 2012

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1. Introduction

Light elements H, He, Li, Be, B, C, N and O are the dominant plasma constituents and impurities in fusion research devices. Hydrogen isotopes constitute the fuel of fusion reactors, helium is the product of the fusion reaction, lithium is used as a beam diagnostic material and also as wall coating, beryllium is a wall material for some fusion vessels, boron is used as a coating material, carbon is used in divertor target plates, nitrogen may be used as a buffer gas and oxygen is a ubiquitous impurity from water vapour that is absorbed in the walls. The CRP on "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" was created in order to generate new data on processes including excitation, ionization, recombination and heavy particle collisions for ions of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen and molecules of these atoms. Data for many of these processes are either poorly known or non-existent, particularly when excited states of atoms or molecules are involved.

At the second RCM participants described their ongoing research pertinent to the CRP and discussed plans for the remainder of the CRP. The available presentations are collected on the A+M Data Unit web pages below the CRP link at http://www-amdis.iaea.org/.

Section 2 of this report provides a summary of the presentations. Section 3 presents the discussion and work plan. The list of participants is provided in Appendix 1, the meeting agenda in Appendix 2 and participants' summaries in Appendix 3.

2. Presentations and Proceedings

2.1 Opening

Dr D. Abriola, deputy Section Head of the Nuclear Data Section at the IAEA, welcomed the participants to the meeting and to Vienna. He noted that the core mission of the Nuclear Data Section and of the Atomic and Molecular Data Unit is to develop and maintain internationally recognized databases for fundamental nuclear, atomic, molecular and materials processes that are important for nuclear applications including nuclear fusion. The objectives of the 2nd research coordination meeting of this CRP are to review the work that was done since the first RCM in November 2009, to inventorize available data and remaining data needs and to update the CRP work plans for the remainder of the CRP.

Dr B. J. Braams, head of the Atomic and Molecular Data Unit of the Nuclear Data Section and scientific secretary of the meeting extended his welcome. The meeting participants briefly introduced themselves. There are two new participants in the CRP since the first RCM: Dr Viorica Stancalie of the National Institute for Laser, Plasma and Radiation Physics (INFLPR) in Magurele, Romania, and Dr Ioan F. Schneider (represented at the present meeting by Dr Zsolt Mezei) of the Laboratory of Waves and Complex Media at Le Havre University in France. The work in the group on Theory of Atomic and Molecular Collisions (TCAM) at Universidad Autónoma de Madrid was represented at this meeting by Dr Ismanuel Rabadán instead of by Dr Luis Méndez and the work in the Atomic Spectroscopy Group at National Institute of Standards and Technology, USA, by Dr Joseph Reader instead of by Dr John Curry.

2.2 Atomic Data and Electron-atom Collisions

V. Stancalie: Atomic data for plasma modeling: research projects at INFLPR

Dr Stancalie described computational studies at INFLPR to provide accurate atomic data for plasma spectroscopy. The Laser Department at INFLPR [http://atomic.inflpr.ro/] is devoted to the study of atomic processes in a laser field and to atomic and ionic spectroscopy of laboratory and astrophysical plasma. The Department seeks to provide accurate atomic data with applications in fusion research and astrophysics. The work involves collaborations through the EFDA Integrated Tokamak Modelling task force (ITM-TF) for atomic, molecular, nuclear and surface data (many participants), with the R-Matrix groups at Queens' University Belfast and Daresbury Laboratory, with the Laboratory for Interaction of X-Rays with Matter (LIXAM) at Paris-Sud/CNRS and with the Atomic Data Analysis Structure (ADAS) project.

Atomic processes under investigation include electron impact excitation with special interest for forbidden transitions, dielectronic recombination (DR) and proton impact excitation. Theoretical methods and numerical codes employed are: 1) Plane wave Born (PWB) from generalized oscillator strength (GOS), 2) Perturbative method (the Coulomb-Green's function for excited states), 3) Non-perturbative methods (non-relativistic RMATXI and RMATXII, semi-relativistic BPRM and full relativistic DARC codes), 4) Non-perturbative R-matrix Floquet (RMF) method and 5) Cowan's suite of codes. Collisional radiative calculations are carried out in connection with the ADAS project.

A detailed semi-classical analysis of dielectronic recombination of Li-like into Be-like ions has been done in order to compare the efficiencies of different recombination pathways according to the electron temperature in the plasma. A new formalism has been developed that retains the essential ingredients of the full R-matrix Floquet theory, namely a bound state coupled non-perturbatively by the field to an autoionizing state and to the continuum. Results from the calculation of the autoionization probability and the radiative width, taking full account of the electron collision and radiative processes in a consistent way, show a Z-dependence over the isoelectronic lithium sequence.

The influence of plasma opacity effects on hydrogen (H-α and Ly-β) and Li-like oxygen emission lines from the RFP EXTRAP T2R plasma has been studied and also simulations of total radiated power have been performed. The research plan for this CRP includes a detailed study of electron excitation of neutral carbon over an energy range from threshold to 150 eV.

I. Bray: Benchmark calculations for electron scattering on atomic hydrogen and helium

Dr Bray reported on the progress in the development of the Convergent Close-Coupling (CCC) theory for electron, positron, photon, proton and anti-proton collisions with atoms, ions and molecules. This is joint work with D. V. Fursa at the ARC Centre for Antimatter-Matter Studies at Curtin University. The primary objective is to provide accurate atomic collisional data. The approach relies on a surface integral formalism that is valid for short and long-range potentials [Kadyrov et al., PRL 101, 230405 (2008) and Annals of Physics 324, 1516 (2009)].

The details of atomic target structure and electron atom scattering in the nonrelativistic CCC theory were presented as well as benchmark calculations of electron-hydrogen scattering and electron-helium scattering. The comparison with measurements shows that there are almost no substantial discrepancies for electron-impact excitation or ionization of quasi one- and two-electron targets and for photon-impact single and double ionization of He. The theory are extended to positron collisions with quasi one- and two-electron targets, (anti)proton collisions with H and He including ionization, and more complicated targets such as inert gases and molecules.

T.-G. Lee: Atomic collision data for light atoms and ions

Dr Lee presented the work by the Auburn group (Mitch Pindzola, Stuart Loch, Connor Ballance, John Ludlow, Mike Fogle, Teck-Ghee Lee) on atomic collision data for light elements. Theoretical methods were outlined and the previous application to atomic data sets for H, He, Li and Be were briefly reviewed and then the presentation focused on the current work on the boron and carbon isonuclear sequences.

Theoretical methods include distorted-wave calculations for perturbation theory and non-perturbative methods such as R-matrix close-coupling (RM, RMPS), time-dependent close-coupling (TDCC), convergent close coupling (CCC) and exterior complex scaling (ECS). The cross-sections and rate coefficients are applied to yield generalized collisional-radiative (GCR) coefficients directly applicable to plasma modeling.

Excitation cross-sections ($n \leq 5$) for H, He, He^+, and Li, Be, B isonuclear sequences were obtained with RMPS method and the results are in good shape in agreement with CCC and TDCC calculations. Ionization ($n \leq 2$) cross-sections are calculated by TDCC, RMPS and CCC methods. For radiative recombination and dielectronic recombination, distorted wave calculations are applied and the results compare well with experiments.

The processed GCR data were presented for H, He, Li and Be and it is shown that for moderate density plasmas, ionization from excited states can be significant. While the direct ionization can scale up to higher n shells, it is important to note that the excitation autoionization (EA) contributions should be carefully investigated in the scaling. The EA contributions could be much larger for heavier atoms and ions.

J. Reader: NIST database work on spectra of light elements and brief update for tungsten

Dr Reader presented an overview of research projects on the spectra of light elements by the NIST atomic spectroscopy group which consists of experimental research, theoretical research, database development, data assessment and compilation. He also gave a brief update on the Tungsten research at NIST.

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. Compilations were done for H, D, T, He and Li, and more recently for Be and B. Other elements such as Na, Mg, Cl and Ar are in progress. The compilations involve spectral lines, energy levels and transition probabilities. Current work on transition probabilities for F and Ne were presented. Because of advances in the theoretical calculations, it is possible to compile many more lines with accurately calculated values. Dr Reader used calculated and measured lifetimes of F V and Ne VI to illustrate that theoretical transition probabilities are currently about as good as the experimental ones in cased where experimental lifetimes are available.

The online databases are found on the NIST Physical Measurement Laboratory website. http://www.nist.gov/pml/. The current version of our Atomic Spectra Database contains data for 950 spectra and over 180,000 transition wavelengths. Online tools include production of Saha equilibrium plots of spectra and Grotrian diagrams. The bibliographic databases are kept current on an approximately biweekly basis. A search for papers on light elements of fusion interest yields references for about 50 recent papers.

2.3 Experimental Studies

P. Defrance: Electron impact fragmentation of molecular ions

Dr Defrance presented the crossed electron-ion beam method to study electron induced fragmentation of molecules. Singly and/or multiply charged ions that results from molecular ion fragmentation are detected individually and the 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: 1) absolute inclusive cross sections for electron impact dissociation to individual ionic fragments, 2) different reaction channels of single ionization (SI), dissociative excitation (DE) and dissociative ionization (DI), 3) Kinetic energy release distributions (KERD) of the fragment ions and 4) energy threshold.

For this CRP it is proposed to study 5 different systems: 1. Light ions: H_2^+, D_2^+ and D_3^+, D_2H^+; 2. Hydride ions: HeH^+, NeD^+, OH^+, OH_2^+, OH_3^+ and isotopologues; 3. Hydro(deutero)-carbon ions: CH_n^+, CD_n^+(n=1-4), C_2D^+, $C_2D_2^+$, $C_2D_3^+$, $C_2D_4^+$ and isotopologues $C_2D_3H^+$, $C_2D_2H_2^+$; 4. CO^+, CO_2^+, O_2^+, C_2^+; and 5. Nitrogen: NH^+, ND^+ and N_2^+.

Isotopes are equivalent with respect to the electronic energy of the molecular system, but they are not equivalent with respect to the dynamics. The isotope effects on DE and DI processes are studied. In addition, the theoretical ionization cross-sections are compared with the measurement.

J. Lecointre: Nitrogen hydrides, dissociation of NH^+ and ND^+

Nitrogen exists as an impurity in plasma experiments and it is important to understand the formation of nitrogen hydrides. Dr Lecointre presented the absolute cross-section measurements of the molecular activated processes involving the nitrogen hydrides. Three types of molecular activated processes coexist: 1. dissociative recombination (MAR), 2. dissociative excitation (MAD) and 3. dissociative ionization (MAI).

Absolute cross-sections of direct and indirect dissociative excitation of NH^+ were presented. The indirect dissociative excitation (IDE) via the electron capture into a doubly excited electronic state of NH is observed below the threshold of direct dissociative excitation (DDE) at 8.0 eV. For ionization of

NH^+, the dissociative ionization to N^++H^+ and the asymmetric dissociative ionization to N^{2+}+H are observed. Absolute cross-sections of ND^+ are presented as well.

B. Wei: Progress of the interaction between e^- and molecules at Fudan University

Dr Wei introduced the experimental study using the Recoil Ion and Electron Momentum Spectrometer (RIMS) at Fudan University to study the interaction between low energy electrons and methane molecules. The plan is to study electron impact ionization and DI (dissociation ionization) for H_2 and CH_4, later also for N_2 and O_2. By measuring the momenta (and thus angle and energy) of all particles involved in a collision in coincidence, the excitation, ionization and fragmentation of e.g. a molecule hit by an electron can be studied.

The advantage of the RIMS is that is allows one to measure the time of flight, TOF, and the impact position on the detector of the all fragments produced in the collision. A super-sonic gas jet target has been employed here to produce the cold molecular beam. The collision system was tested through studies of the interaction of ns laser pulses with methane molecules in 2010. Singly charged ions of CH_3^+, CH_2^+ , CH^+, C^+, H^+ and H_2^+ were observed in the TOF spectra. The liberation of an H_2 molecule from CH_4 was also observed in our experiment. Cross-section measurements of ionization and dissociation of molecules of (C_xH_y, N_2) by electron impact are planned in the future.

J.B. Mitchell: Dissociative recombination: recent results and developments

Dr Mitchell outlined a number of recent developments in dissociative recombination (DR) research, primarily experimental and modelling issues. Firstly, the interesting data on a range of cyclic ions containing C, N, O as well as their dimers are observed in the flowing afterglow experiments that their rate coefficients fall at 300 K in the range from $3x10^{-7}$ to $4x10^{-6}$ cm^3s. Secondly, modeling studies demonstrated that the yields of individual neutral species in ion chemistry model are sensitive to the branching ratios, in some cases up to 5 orders of magnitude.

A recent analysis explains why the DR cross-sections for polyatomic species are observed to sharply fall off above 0.1 eV. It is attributed to the indirect process (initial capture into a vibrationally excited, neutral Rydberg state) in which propensity rule ($+\Delta v=1$) dominates the capture. As the electron energy exceeds the excitation energy between the v'=0 and v'=1 levels of the ion, the capture involving $\Delta v=2$ transition will be much less effective and so the cross section drops precipitously. H_3^+ continues to be an active subject of research and a very recent experiment at the TSR ring in Heidelberg has examined the influence of rotational excitation on the rate of the recombination. Finally, there will be a new storage ring facility for dissociative recombination research in Langzhou in China. This machine will have a higher magnetic rigidity that previous rings used for DR and so heavier ions and higher mass resolution experiments can be performed there.

2.4 Electron-molecule Collisions

J.Z. Mezei: Reactive collisions of diatomic systems with electrons, atoms and photons: recombination, excitation, ionization and dissociation

Dr Mezei reported on reactive radiative and collisional processes involving neutrals - H_2, HD, OH CN, He - and molecular cations - H_2^+, HD^+. The processes include photoabsorption, spontaneous emission, photoionization, dissociative excitation, dissociative recombination, reactive molecular collision, and atom-diatom excitation processes.

Energy levels, the wave functions and the spontaneous emission Einstein coefficients are computed using a method based on the multichannel quantum defect theory (MQDT), where the radiative transitions are treated as half-collisions and the photon-molecule interaction is represented by the dipole operator. It was found that the photoionization cross section is governed by resonant structures identified as the discrete vibrational levels of the H_2 lying above the ionization thresholds. The dissociative excitation and recombination of H_2^+ and HD^+ at low to high energies are completely modeled by computing the K-matrix in the 2^{nd} order and accounting for all the relevant symmetries and all the Rydberg series of dissociative states belonging to each symmetry.

Full quantum time independent close-coupling calculations were done for cross sections and rate constants of molecular collisions. The best available potential energy surfaces were used and a very good agreement has been found with experiments for rate constants of He induced rotational excitation

of CN. In the case of reactive molecular collision between O and OH good agreement has been found for rate constants at low temperature with the extrapolated data, but less good agreement with recent measurements at lower temperatures.

A. Larson: Theoretical studies of electron interactions with molecular ions and mutual neutralization: BeH and HeH

Dr Larson discussed electron collisions e + HeH^+ and e + BeH^+ including processes of dissociative recombination (DR), resonant vibrational excitations (VE) and resonant dissociative excitations (DE) and discussed mutual neutralization (MN) of HeH and BeH systems. The electronic resonant states of HeH are calculated using the full Configuration Interaction (CI) method with a large basis set. Non-adiabatic couplings between the resonant states are computed using a method developed by V. Sidis. Cross sections for VE and DE of HeH^+ in different vibrational states are computed by solving a driven Schrödinger equation and including autoionization using a local model. The cross sections become large when the energy is high enough to capture into the resonant states. The computed cross section for DE with the ion in the ground vibrational state is in very good agreement with measurement. The MN reaction, $He^+ + H^- \rightarrow He^* + H$, will be studied using strictly diabatic states.

Previously, the DR cross-sections of BeH^+ were obtained by including the capture into electronic resonant states and electronic couplings between the neutral states. Using the multi-channel quantum defect theory, the non-adiabatic couplings to the Rydberg states are now also incorporated. The indirect process results in sharp oscillations in the cross section and it influences the low temperature thermal rate coefficient for the reaction. Resonant VE and DE of BeH^+ in different vibrational states are investigated. The cross sections for these reactions are significant also at relative low energies. An *ab initio* quantum description of the MN reaction in collisions between $Be^+ + H^-$ is performed with the full CI of a very large basis set.

H. Takagi: Processes of electron and molecular ion collisions relevant to divertor plasma: hydrogen molecular ion and its isotopes

Dr Takagi presented data on molecular ion and electron collisions of H_2^+, HeH^+/NeH^+, CH^+, H_3^+ and their isotopes D, T. The processes include dissociative recombination (DR), dissociative excitation (DE) and vibrational (V) and rotational (N) transitions. The multichannel quantum defect theory (MQDT) is applied for H_2^+, with potential energy curve crossing and for HeH^+ and H_3^+ without crossing. The electronic parameters as the quantum defect and the CI strength of various excitations are employed from R-matrix calculations.

The cross sections of DR and vibrational and rotational transitions at the energies from 1 meV to 1 eV are compiled on the five isotopes. For the energies from 0.3 eV to 11 eV, the cross sections are compiled on the vibrational transition, DE, and DR, with the principal quantum number of produced excited hydrogen atom specified.

R. Janev: Electron- and ion-impact processes with hydrogen and light plasma impurities

Dr Janev outlined the progress made on the following electron and ion collisions with hydrogen and light impurities. For electron collisions, 1) the process of dissociative electron attachment (DEA) on vibrationally excited $H_2(v)$, proceeding via the $^2\Sigma_g^+$ Rydberg resonant state, has been studied within the local complex potential model of resonant theory for this process. 2) The elastic and electronic excitation processes in e – BH_2 collisions have been studied in the energy range 0 (threshold) – 8eV with the molecular R-matrix method. 3) The electron impact excitation of lowest two excited states, $A(^1\Sigma^+)$ and $B(^1\Pi)$, of $BeH^+(v)$ ion has been studied within the Coulomb-Born approximation.

For ion collisions, 4) the elastic and related transport (momentum transfer and viscosity) cross sections for the H^++Be, C and Be^+, C^++H collisions have been calculated in the CM energy range 0.1meV – 10 keV by the quantum-mechanical MOCC method. The multichannel coupling affects the cross sections only for ECM > 100-200 eV. 5) Using the AOCC method with a large AO basis and appropriate model potentials, the state-selective and total electron capture cross sections have been calculated for the N^{5+}+H and O^{6+}+H collisions in the energy range 0.5 – 100keV/u. 6) The excitation and electron capture processes in H^++$He(2s^1,^3S)$ collisions are currently being studied by using the AOCC method by using a large AO basis on both centers (all states with $n \leq 7$ plus pseudo-states with n = 8-13). The electron – ion core interaction in singlet and triplet cases is described by separate model potentials.

State-selective electron capture and excitation cross sections up to n = 6 have been calculated in the energy range 1 – 200 keV/u.

2.5 Heavy Particle Collisions

B. He: Theoretical progresses on heavy particle collisions

Dr He presented the progress made on the theoretical study of the collisional processes between hydrogen particles (H^+, H, H_2) and the light element atomic and molecular plasma impurities such as Li, Be, B, C, N from about 10^{-5} eV/amu to 10^5 eV/amu. The cross-sections are computed using the Quantal Molecular Orbital Close-Coupling (QMOCC) method and the two-center Atomic Orbital Close-Coupling (AOCC) method. The QMOCC method is based on Born-Oppenheimer approximation and the molecular structure data are obtained by using MRD-CI package. This method is usually suitable for projectile energy below 1 keV/u. The two-center AOCC method assumes that the projectile moves in a straight line and it is suitable for the projectile energy beyond 1 keV/u.

Calculated cross-sections are presented for the following processes: 1) radiative and nonradiative charge transfer in collisions of Be^{2+} and B^{3+} ions with H atoms, 2) charge transfer and dissociation for the collision of $H_2^+(1s\ \sigma_g)$ with $He(1s_2)$, 3) charge transfer of H^+-$Li(2p_{0,\pm1})$. 4) polarization degree difference for the $3p\ ^2P_{3/2} - 3s\ ^2S_{1/2}$ transition of $N^{4+}(3p\ ^2P_{3/2}\ )$ produced in N^{5+}-He and N^{5+}-H_2 collisions. In general, the QMOCC and AOCC methods agree well in the overlapped region and with the available experimental and other theoretical results. Differences with measurements were found for the dissociation cross-sections of $H_2^+(1s\ \sigma_g)$ with $He(1s_2)$, which indicate that the process is very complex and more work is needed.

I. Rabadan: Calculations of charge exchange cross sections for some ion-atom and ion-molecule systems

Dr Rabadan presented the theoretical study of ion-atom and ion-molecule collisions. The group applies a variety of methods, a fully quantum-mechanical treatment calculations, in which both nuclear and electronic degrees of freedom are treated quantum mechanically, a semi-classical formalism to use straight-line nuclear trajectories and quantum-mechanical electrons, and the classical trajectory Monte Carlo (CTMC) method of both nuclear and electron motions to calculate cross sections for elastic scattering, charge exchange (CE) and ionization processes.

A large scale quantal calculation has been applied to obtain elastic and CE cross sections in collisions of B^{5+} with H(1s) at very low collision energies. Ionization and CE in collisions of B^{5+} with H(n=1,2), at higher energies were described with the CTMC and semi-classical methods. The full quantal and semiclassical methods were applied to both collisions of Li^+ with H and H^+ with Li. Progress in the calculation of CE cross section for the systems $H^+ + N_2$ and for mutual neutralization collisions $H_2^+ + H^-$ is presented and compared with available experimental data and other calculations. The $(HN_2)^+$ system is being studied using MOLPRO to obtain multi-reference configuration interaction wave functions. Also, a two center model potential has been developed to run CTMC calculations that include the anisotropy of the target molecule.

D. Schultz: Recent calculations involving light species for fusion

Dr Schultz reported on the recent calculations for heavy-particle elastic collisions and transport processes and for inelastic processes of charge transfer and excitation. Since about 1997 the ORNL group has produced successive works containing very accurate cross sections for elastic and related transport processes needed in fusion plasma edge modeling, beginning with the comprehensive treatment of (H^+, H) colliding with (H, H_2, He) that was published as Volume 8 of the IAEA "Green book" (APID) series. In subsequent publications additions to this initial database have been made which improve or extend it as summarized in a recent paper [P.S. Krstic and D.R. Schultz, Phys. Plasmas 16, 053503 (2009)]. New elastic and transport cross sections in that work include those for neutrals and ions of Li, B and B in a hydrogen plasma. In the presentation Dr Schultz showed comparisons between results obtained from classical trajectory Monte Carlo (CTMC) calculations and fully quantum cross sections.

The most recent work extends these elastic cross section and transport cross section calculations to O and N. The transport cross sections for $H^+ + O$ and $O^+ + H$ via the CTMC method are added to the

database and those for H^+ + N and N^+ + H as well as complementary fully quantum mechanical results for H^+ + O and O^+ + H are planned. It is the goal to complete the dataset for ions lighter than Ne to provide not only explicit new data for impurity species common in fusion devices, but also to facilitate determination of trends of behavior with varying nuclear charge.

The Oak Ridge atomic physics group carries out benchmark experiments using merged beams for inelastic collisions and these motivate new theoretical calculations. Measurements of inelastic collisional data of hydrogen-like C, N, and O ions colliding with atomic hydrogen were compared with calculations using the AOCC method for charge transfer, excitation and ionization processes. The agreement is excellent over the energy range of about 200 eV/u to 10 keV/u, with the experimental data extending down to about 0.01 eV/u and the theoretical data up to 200 keV/u. Future work is planned on cross sections for charge transfer in H^++H and C^{6+}+H collisions including excitation of excited states n>1. These calculations would be done using CTMC and using the lattice time dependent Schrödinger equation (LTDSE) method as a benchmark.

3. Discussion and Work Plan

The meeting participants first discussed light element atomic and molecular data needs in general and then reviewed their individual plans and possible collaborations.

3.1 Work Needed on Electron-atom Collision Data

Cross sections for electron impact on light atoms and ions have been the domain primarily of the Auburn group, here represented by Teck Lee, and data for e^- + (Be, B^+, C^{2+}) are in very good shape. The next isoelectronic sequences are in progress. Validation remains difficult but it should be done.

3.2 Work Needed on Heavy Particle Collision Data

For the case of one-electron systems the atomic orbital close-coupling (AOCC) approach gives benchmark quality results. Data need to be assembled for electronic excited targets and we stress the need for evaluated and recommended data. The JAEA database has data for charge transfer in collisions H + X^{q+} for H^*(2s) and H^*(2p).

Elastic scattering cross sections and related transport cross sections were calculated fully quantum mechanically for singly-charged ion-atom scattering of H on Li, Be and B by Krstić and Schultz and for H on Be and C by Liu, Wang and Janev. The ion-atom elastic scattering cross sections are needed still for H + N and H + O (to be done at ORNL; H + O was done using CTMC but not fully QM).

3.3 Work Needed on Electron-molecule Collision Data

We need to inventorize experimental studies of electron collisions with light hydrides: LiH, BeH, BH, BeH_2, BH_2 and their ions. Work of that nature has been done at the Institute for Ion Physics and Applied Physics at Innsbruck (T. Märk) for hydrocarbons, but apparently not for these molecules. There is recent work on e^- + BH_2^+ that used the ORNL crossed electron ion beams apparatus [M. Fogle et al., Phys. Rev. A **82**, 042720 (2010)]. Anything from CRYRING? Anything else?

There is much work on dissociative recombination of H_2^+ and H_3^+, also for molecular excited states (Takagi, Schneider). DR of HeH^+ at low energy was studied by H. Takagi and DR of BeH^+ by both A. Larson and I. Schneider. The LiH^+ ion is very weakly bound, it is not of practical interest. We don't know theoretical work on electron collisions with BH^+ or BH_2^+; this needs work. For electron collisions with $C_xH_y^+$ see the Janev-Reiter database at Jülich, which is being updated.

3.4 Work Plan

In the area of elastic heavy particle collisions it is planned (D. Schultz) to calculate cross sections and transport moments for collisions H^++N and H+N^+ by classical trajectory Monte Carlo (CTMC) and for collisions H^++O and H+O^+ using MOCC; this will complete the sequence of elastic collision calculations for hydrogen + light element. Beyond this it is hoped to calculate elastic cross sections and transport moments for elastic collisions of H^+ with N_2 and O_2 using CTMC.

To support neutral beam and gas puff studies it is planned (R. Janev and IAPCM group: B. He, L. Liu, J. G. Wang) to calculate charge transfer cross sections for N^{5+} + He and N^{5+} + H_2 and for H^+ +

$Li^*(1s^2,2p_{-1,0,1})$. Benchmark calculations are planned (D. Schultz) for charge transfer (total and state-selective) in $H^+ + H$ and $C^{6+} + H$. For the process $H^+ + He^*(1s,nlm;2s)$ comprehensive calculations including excitation and charge transfer are planned by R. Janev and IAPCM, D. Schultz; also by I. Bray after extension of the CCC approach to such calculations.

Ion-molecule charge transfer processes for $H^+ + H_2$, CO and N_2 are to be studied at UAM (I. Rabadán and L. Méndez). Studies are also planned (B. He et al.) for $H^+ + BeH$, $H^+ + BH$, $Be^{2+} + H_2$ and $B^{3+} + H_2$.

Comprehensive MOCC calculations (total and state-selective and differential) of the mutual neutralization for $He^+ + H^-$ have been started by A. Larson and for $H_2^+ + H^-$ by I. Rabadán and L. Méndez. Semiclassical calculations for mutual neutralization in $Be^+ + H^-$ are planned (A. Larson). Closely related to these studies of mutual neutralization are calculations of dissociative recombination and dissociative excitation, which are planned by A. Larson for $HeH^+(*)$, He_2^+, BeH^+ and BeH_2^+ and by Z. Mesei and I. Schneider for BeH^+ and $BeHe^+$.

Concerning light element spectroscopy the NIST Atomic Spectra Group is planning to complete the first row elements with new compilations for F and Ne.

In the area of electron-atom collisions the Auburn group plans to complete the GCR calculations for B, C and Ne; this requires further cross section calculations still for processes e + C (ground state calculations using RMPS method) and for e + C, C^+ and C^{2+} excited states. Electron impact excitation of C is also to be studied by V. Stancalie.

New experimental studies of electron-molecule collisions are planned (P. Defrance, J. Lecointre) for targets HeH^+, OH_x^+, $C_xH_y^+$ and C_2^+ and at Fudan University (B. Wei) for neutral targets C_xH_y and N_2. The detailed state resolved calculations using MQDT of collisions $e + H_2^+(v,n)$ are to be extended to higher energies (H. Takagi).

Appendix 1

List of Participants

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Appendix 2

Agenda

Monday, 23 May **Meeting Room: A05-31**

09:30 – 09:50 R. Forrest/D. Abriola, B.J. Braams: Opening, adoption of the agenda

Session I. Chair: A. Larson

09:50 – 10:20 V. Stancalie: Atomic data for plasma modeling: research projects at INFLPR
10:20 – 10:50 I. Bray: Benchmark calculations for electron scattering on atomic hydrogen and helium

10:50 – 11:20 *Coffee break*

11:20 – 11:50 T. Lee: Atomic collision data for light atoms and ions
11:50 – 12:20 J. Reader: NIST database work on spectra of light elements and brief update for tungsten

12:20 – 14:00 *Lunch*

Session II. Chair: R. Janev

14:00 – 14:30 All: Data status for atomic processes (electron-atom and radiative)
14:30 – 15:00 P. Defrance and J. Lecointre: Electron impact fragmentation of molecular ions
15:00 – 15:30 B. Wei: Progress of the interaction between e^- and molecules at Fudan University

15:30 – 16:00 *Coffee break*

16:00 – 16:30 J.B. Mitchell: Dissociative recombination: recent results and developments
16:30 – 17:30 All: Discussion on experimental work

19:30 – *Social dinner (outside VIC)*

Tuesday, 24 May **Meeting Room: A05-31**

Session III. Chair: B. Wei

09:00 – 09:30 J.Z. Mezei: Reactive collisions of diatomic systems with electrons, atoms and photons: recombination, excitation, ionization and dissociation
09:30 – 10:00 A. Larson: Theoretical studies of electron interactions with molecular ions and mutual neutralization: BeH and HeH
10:00 – 10:30 H. Takagi: The processes of electron and molecular ion collisions relevant to divertor plasma: hydrogen molecular ion and its isotopes

10:30 – 11:00 *Coffee break*

11:00 – 11:30 R. Janev: Electron- and ion-impact processes with hydrogen and light plasma impurities
11:30 – 12:30 All: Data status and data needs for electron-molecule processes

12:30 – 14:00 *Lunch*

Session IV. Chair: H. Takagi

14:00 – 14:30 B. He: (Tentative) Studies of heavy-particle collision processes in fusion edge plasma
14:30 – 15:00 I. Rabadan: Calculations of charge exchange cross sections for some ion-atom and ion-molecule systems
15:00 – 15:30 D. Schultz: Recent calculations involving light species for fusion

15:30 – 16:00 *Coffee break*

16:00 – 17:00 All: Data status and data needs for heavy particle collision processes

Wednesday, 25 May **Meeting Room: A05-31**

Session V. Chair: P. Defrance

09:00 – 09:30 H.-K. Chung: Database and knowledge base developments at IAEA
09:30 – 12:00 Comprehensive review of data status and data needs

12:00 – 13:30 *Lunch*

Session VI. Chair: B. Braams

13:30 – 16:30 All: Development of Work Plan; Wrap Up

16:30 – *Close of Meeting*

SUMMARIES

Atomic data for plasma modeling - Research projects at INFLPR

Viorica Stancalie
National Institute for Laser, Plasma & Radiation Physics
Magurele, Romania

The objective of our work is to provide accurate atomic data for plasma spectroscopy. Theoretical methods employed are perturbative, non-perturbative, semi-classical and classical. We describe, briefly, the computational studies, including relativistic and non-relativistic calculation of electron-impact cross sections for plasma diagnostics.

A detailed semi-classical analysis of dielectronic recombination of Li-like into Be-like ions (IOP Conf Ser. **140**, 1995) has been done in order to compare the efficiencies of different recombining ways according to the electron temperature in plasma. A new model calculation that retains the essential ingredients of the full R-matrix Floquet theory, namely a bound state coupled non-perturbatively by the field to an autoionizing state and to the continuum, has been developed (Physics of Plasmas **12** (2005) 100705, and Physics of Plasmas **12** (2005) 043301). Results from the calculation, taking full account of the electron collision and radiative processes in a consistent way, show a Z-dependence over the isoelectronic lithium sequence.

A special attention has been paid to the possibility of using the Coulomb Green's function and its Sturmian representation to calculate positions of bound and excited Rydberg states. Results have been compared with those obtained by other theoretical methods and a very good agreement has been observed.

The influence of plasma opacity effects on hydrogen (H-α and Ly-β) and Li-like oxygen emission lines from the RFP EXTRAP T2R plasma (Phys. Scr. 2002), and total radiated power simulation (Phys. Scr. **71**, 2005) has also been performed.

The research plans for the present CRP include detailed study of electron excitation of neutral carbon over an energy range from threshold to 150 eV.

NIST database work on spectra of light elements and brief update for tungsten

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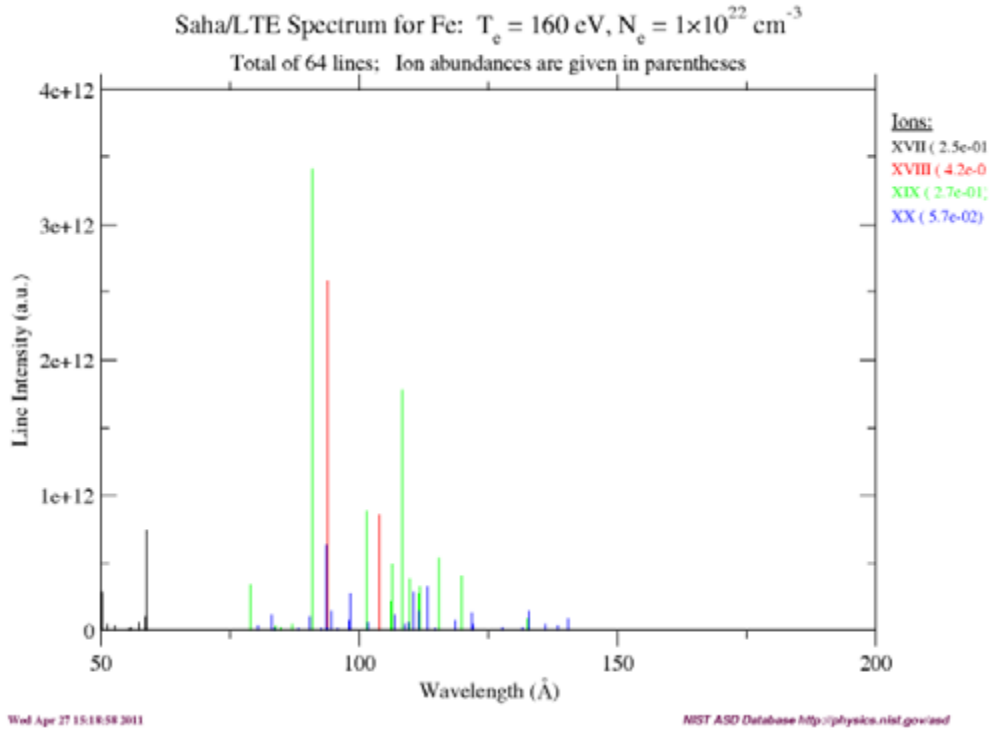
Work at NIST on the spectra of light atoms is concentrated mainly on critical compilations of papers that have appeared in the literature and dissemination of the data through online databases. Examples of our compilations include:

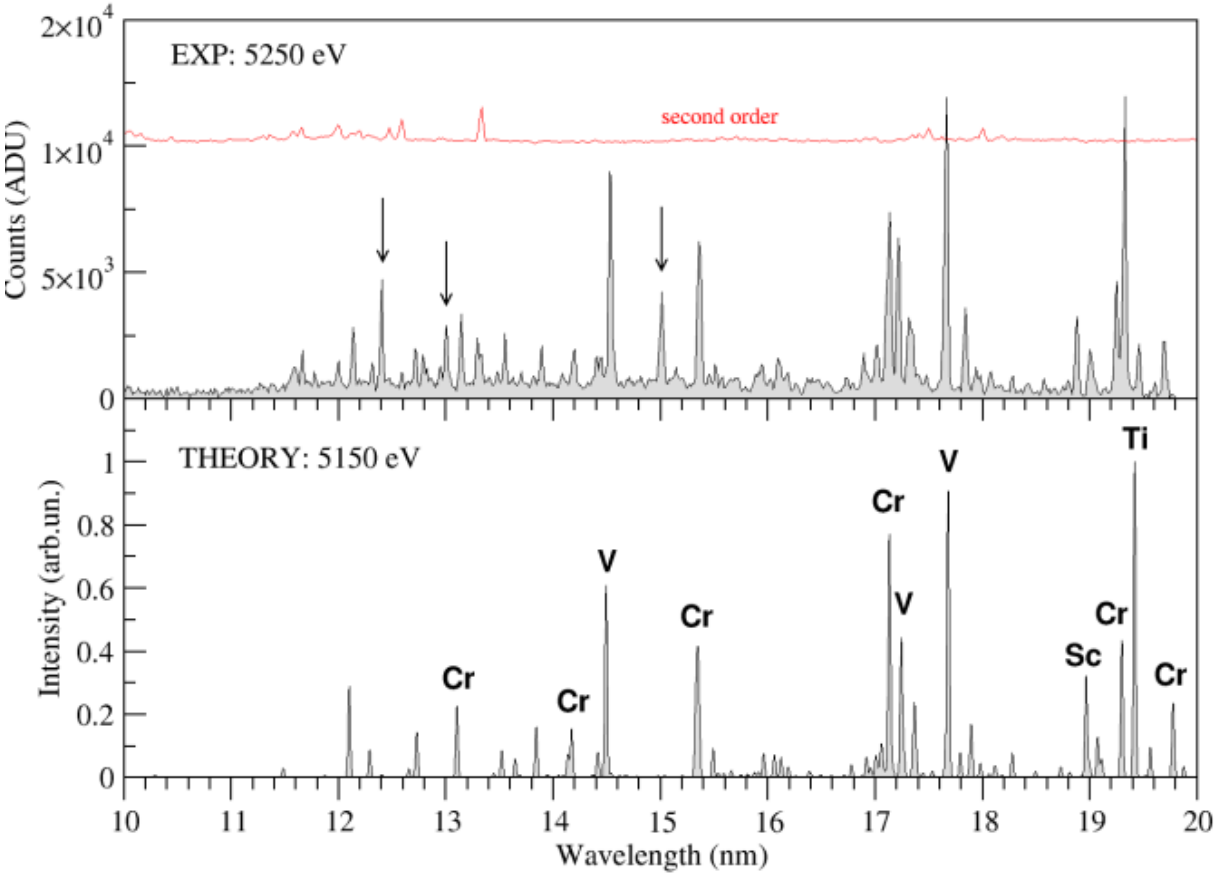
1. "Accurate atomic transition probabilities for H, He, and Li," W. Wiese and J. Fuhr, J. Phys. Chem. Ref. Data **38**, 565 (2009).
2. "A Critical Compilation of Experimental Data on Spectral Lines and Energy Levels of H, D, and T," A. Kramida, At. Data Nucl. Data Tables **96**, 586 (2010).
3. "Tables of Atomic Transition Probabilities for Be and B," J. Fuhr and W. Wiese, J. Phys. Chem. Ref. Data **39**, 013101 (2010).
4. "Energy Levels and Wavelengths for Ar II – Ar XVIII," E. B. Saloman, J. Phys. Chem. Ref. Data **39**, 033101 (2010).

Current work concerns transition probabilities for F and Ne. Because of advances in the theoretical calculations we are able to compile many more lines with accurately calculated values.

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 contains data for 950 spectra and over 180,000 transition wavelengths. Online tools include production of Saha equilibrium plots of spectra (example to lower right for Fe XVII-XX) and Grotrian diagrams. 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 50 recent papers.



New observations [1] for tungsten with the NIST EBIT have produced data for magnetic dipole transitions within the $3d^n$ ground configurations of W^{47+}-W^{55+}. These normally forbidden lines appear at electron beam energies of 4.5-7.0 keV. Since the appearance of these lines is sensitive to the electron density, their intensities serve as indicators of conditions in a tokamak plasma. Similar data have been obtained for isoelectronic ions of Hf, Ta, and Au. Spectra of W at 5250 eV are compared with collisional-radiative modeled spectra (arrows indicate impurities; identifications by isoelectronic sequence). The current status of spectra for tungsten is given in a new report by Kramida [2].



[1] "Spectroscopy of diagnostically important magnetic-dipole lines in highly charged 3dn ions of tungsten," Yu. Ralchenko et al., Phys. Rev. A **83**, 032517 (2011).

[2] "Recent progress in spectroscopy of tungsten," A. Kramida, Can. J. Physics, in press (2011).

Electron Impact Dissociation of Molecular Ions

Pierre Defrance and Julien Lecointre
Catholic University of Louvain, Belgium

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.

Molecular species studied in the frame of this CRP are grouped into the five following categories:

1. Light ions: H_2^+, D_2^+ and D_3^+, D_2H^+

For H_2^+, the particular importance of the internal energy, the vibrational population, has been underlined. Dissociation of H_3^+ isotopologues have recently discussed comprehensively in the two following papers, especially as regards isotope effects in the fragmentation.

"Absolute cross sections and kinetic energy release distributions for electron impact dissociation of D_3^+" J. Lecointre, M.O. Abdellahi El Ghazaly, J.J. Jureta, D.S. Belic, X. Urbain and P. Defrance, *J. Phys. B: At. Mol. Opt. Phys.* 42 (2009) 075201

"Isotope effects in electron impact dissociation of D_2H^+" P. Defrance, J.J. Jureta, J. Lecointre and X. Urbain, *J. Phys. B: At. Mol. Opt. Phys.* 44 (2011) 075202

2. Hydride ions: HeH^+, OH^+, OH_2^+, OH_3^+ and isotopologues *(unpublished)*

For HeH^+, experimental results are available for the production of He^+ and He^{2+}. They will be analysed taking into account the vibrational population measured in a separate charge transfer experiment. The reliable collection of the H^+ fragment was not possible due to the large KER but this experiment will be considered in a soon future.

3. Hydro(deutero)-carbon ions: $C_2D_3^+$, $C_2D_4^+$ and isotopologues $C_2D_3H^+$, $C_2D_2H_2^+$ *(unpublished)*

The hydrocarbon and deuterocarbon families ($C_mH_n^+$ and $C_mD_n^+$) which play a particular role in the plasma studies are systematically investigated in our laboratory. Previous results were published for the methane series (CD_n^+, n= 1–4), for C_2D^+ and $C_2D_2^+$. See number of references in the list here below. Experimental results have been obtained for $C_2D_3^+$ and $C_2D_4^+$. The collected data need to be analyzed in detail in order to determine separately the contributions of dissociative excitation and ionization, as well as the associated energy thresholds and KERDs. The standard procedure will be applied to put these data in a form which is suitable for plasma modelling applications.

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.

5. Nitrogen: NH^+, ND^+ and N_2^+

Dissociation of the nitrogen hydride has recently been made available to the community. In addition, dissociation of N_2^+ was published earlier.

"Electron impact dissociation and ionization of NH^+: formation of N^+ and N^{2+}" J. Lecointre, J.J. Jureta and P. Defrance, *J. Phys. B: At. Mol. Opt. Phys.* 43 (2010) 105202

"Electron impact dissociation of ND^+: formation of D^+" J. Lecointre, D.S. Belic, S. Cherkani-Hassani and P. Defrance, *Eur. Phys. J. D* 61 (2011) in press

"Electron Impact dissociation and ionisation of N_2^+" E.M. Bahati, J.J. Jureta, D.S. Belic, H. Cherkani-Hassani, M.O. Abdellahi and P. Defrance, *J. Phys. B: At. Mol. Opt. Phys.* 34 (2001) 2963

Study of the interaction of e^- and molecules at Fudan University

B. Wei, Z. Chen, X. Wang, R. Hutton, Y. Zou
Fudan University, Shanghai

The interaction between low energy electrons and methane molecules plays a very important role in defining the plasma conditions in the edge region of Tokamaks. The priority for this CRP is to study electron impact ionization and DI (dissociation ionization) for H_2 and CH_4, later also for N_2 and O_2. These measurements will be performed on the Recoil Ion and Electron Momentum Spectrometer (RIMS) at Fudan University. By measuring the momenta (and thus angle and energy) of all particles involved in a collision in coincidence, the excitation, ionization and fragmentation of e.g. a molecule hit by an electron can be studied.

The advantage of the RIMS is that is allows one to measure the time of flight, TOF, and the impact position on the detector of the all fragments produced in the collision. From this information the collision process can be reconstructed. To accurately measure the interaction of a low energy electron with a molecule, the resolution of the TOF and detector has been optimized. A supersonic gas jet target has been employed here to produce the cold molecular beam. The collision system was tested through studies of the interaction of ns laser pulses with methane molecules in 2010. Singly charged ions of CH_3^+, CH_2^+ , CH^+, C^+, H^+ and H_2^+ were observed in the TOF spectra. However, there is no CH_4^+ ion because the dissociation energy is much lower than the ionization energy. The liberation of an H_2 molecule from CH_4 was also observed in our experiment [1].

A low energy electron gun coupled with an ultra-fast pulse generator has been installed and tested at the RIMS. To measure the TOF of the collision products using the RIMS a time-zero point for the interaction is a pre-requisite. In our case, the time-zero point is given by using a pulsed electron beam. In this case the resolution of the TOF strongly depends on the width of the electron beam pulse. An ultra-fast pulse generator has been used to produce the pulsed electron beam. The pulse widths generated are between 0.5 ns and 1 ns and pulse repetition frequency is up to 100 kHz. The energy of the electron beam range covers a range from a few eV to 2 keV. Fig. 1 shows the current of the pulsed electron beam as a function of the beam energy. At lower beam energies, the electron trajectories can easily be bent by stray fields, either electric or magnetic. Since the earth's magnetic is not shielded in the present RIMS set up electron beams with energies lower than around 300 eV are quite weak, and hence are not shown in Fig. 1.

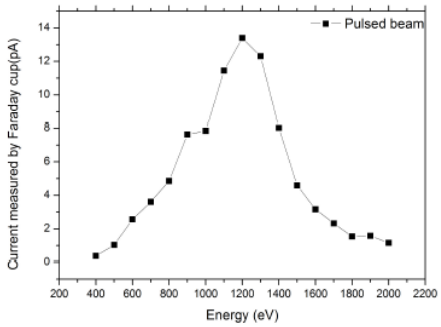


Figure 1, Faraday Cup measurement of the electron current after it passes through a x mm Molybdenum aperture.

Recently, the collision system using a pulsed electron beam was tested through studies on the interaction between low energy electrons with methane and N_2 molecules. Fig. 2 shows the time of flight spectrum of CH_4 measured at incident electron beam energies of 50 and 100 eV. The pressure in the main chamber is 3×10^{-9} mbar. During the experiment, the extraction field in the Time of Flight part of the spectrometer was 2 V/cm for the 50 eV electron beam and 4 V/cm for the 100 eV electron beam. The H_2O^+ ions, see figure 2, originated from residual water in the vacuum chamber. The broadening of the TOF peaks is caused by the initial velocities of the ions. This broadening can be used to estimate the kinetic energy of the ions. For the CH_3^+ ions, the kinetic energy is below 50 meV. This implies that these ions are mainly produced from dissociation. Combining the TOF spectra with position spectra of the ions, a more accurate kinetic energy for the CH_3^+ ions has recently been obtained. Ions produced from either Coulomb explosion or dissociation can be identified from the measured kinetic energies, and in this way, the relative dissociation cross sections can be deduced.

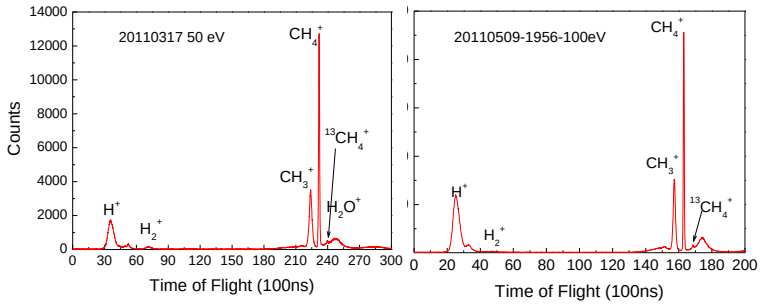


Figure 2, TOF spectra of methane excited by 50 and 100 eV pulsed electron beams.

In conclusion, a low energy pulsed electron beam system has been tested and can be used for experiments on e - molecule interactions. The interaction between the electrons and molecules has recently been measured and the data is being analyzed. To reduce the effects caused by residual/stray magnetic effects, a new Titanium chamber has been designed and is now being manufactured. Sets of Helmholtz coils will be employed to shield the interaction region from the Earth's magnetic in future experiments.

[1] Z Chen, X Wang, B Wei, S Lin, R Hutton and Y Zou, Ionization and dissociation of methane in a nanosecond laser field, *Phys. Scr.* T144 (2011).

Recent Developments in Dissociative Recombination

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There have been a number of recent developments in dissociative recombination research as it relates to ITER, that should be highlighted. These concern primarily experimental and modelling issues and this document will not touch upon the topics of the other scientists involved in DR studies that are present at the meeting.

The topic of branching ratios in general is a topic fundamental to DR especially how it influences the formation of radical and stable neutral molecules that again might play a role in particle formation. It should be remembered that the reactions of neutral radicals to form cyclic compounds are responsible for the formation of soot in combustion, though the role played by ions in flames is at best uncertain. In the near wall plasma environment, ion processes may well be more important since neutral species are rarer. Modelling studies by Pernot and collaborators [1] at the Université de Paris-Sud have shown that if one compares the yields of individual neutral species in ion-chemistry models (in this particular case, the ionosphere of Titan), and if one assumes that DR reactions of hydrocarbon ions primarily decay via the ejection of a hydrogen ion (which is assumed by most Titan ionospheric models) and if one compares these predictions with those coming from a model where actual measured branching ratios are used, differences of up to 5 orders of magnitude are found! This shows very clearly the need for branching ratio studies.

In early merged beam studies of DR performed in Canada in the 1970's, it was noticed that cross sections for polyatomic species typically displayed a sharp fall-off above 0.1 eV. This has since been seen in many storage ring studies and clearly this has important consequences for ITER chemistry where plasma temperatures are likely to be well above ambient. In a recent analysis, Jungen and Pratt [2] have explained this phenomenon on the basis that the recombination is dominated by the indirect process (initial capture into a vibrationally excited, neutral Rydberg state) in which the propensity rule ($+\Delta v=1$) dominates the capture. When the electron energy exceeds that between the v'=0 and v'=1 levels of the ion, where the capture must now involve a $\Delta v=2$ transition, this will be much less effective and so the cross section drops precipitously. This assumes of course that the recombining ion is primarily in the ground v=0 level.

H_3^+ continues to be an active subject of research and a very recent experiment at the TSR ring in Heidelberg has examined the influence of rotational excitation on the rate of the recombination. This is a very beautiful study but an important outcome is that even though a cryogenically cooled storage trap was used to produce the ions, the internal rotational temperature of the ions was never found to be below 150K. This suggests that ion cooling by storage in the ring leads eventually to an equilibrium value for the internal energy of the ions as they are de-excited/re-excited by passage through the electron cooler. As observed in earlier merged beam experiments in Canada, the extraction field in the ion source plays an important role in determining the excitation state of the ions as collisions outside the source can lead to re-heating. Indeed in the TSR experiments using a conventional Penning source and a normal extraction field, the ions were found to have a rotational temperature of several thousands of degrees! This clearly has important significance for earlier measurements taken in storage rings.

Finally, the world will soon have a new storage ring facility for dissociative recombination research and this will be in Langzhou in China. This machine will have a higher magnetic rigidity that previous rings used for DR and so heavier ions and higher mass resolution experiments can be performed there. Experimental operation of this new ring is expected to commence in 2012/2013.

References

[1] S. Plessis et al. J. Chem. Phys. **133**, 134110 (2010)

[2] C. Jungen and S.T. Pratt, J. Chem. Phys. **133**, 214303 (2010)

[3] A. Petrignani et al. Phys. Rev. A **83**, 032711 (2011)

Reactive collisions of diatomic systems with electrons, atoms and photons: recombination, excitation, ionization and dissociation

J. Zs. Mezei[1], F. Lique[1], S. Niyonzima[1], D. Backodissa[1], M. Jorfi[1], K. Chakrabarti[1,2], O. Motapon[1,3], Ch. Jungen[4] and I. F. Schneider[1]

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Reactive radiative and collisional elementary processes involving neutrals - H_2, HD, OH CN, He - and molecular cations - H_2^+, HD^+ - have been studied in Le Havre and Orsay.

1. Photoabsorption [1]

In the present work we have studied the Q(N) (N = 1 − 4) photoabsorption transitions from the $X^1\Sigma^+_g$ ($v'' = 0$) ground and from the vibrationally excited molecular state ($v'' = 1,...,10$) to the $np\pi^1\Pi^-_u$ ($v' = 0$, …; n=2-6) Rydberg states. We have computed the energy levels, the wave functions and the spontaneous emission Einstein coefficients, using a method based on the multichannel quantum defect theory (MQDT), where the radiative transitions are treated as half-collisions and the photon-molecule interaction is represented by the dipole operator. In order to address the photoionization, in addition to the closed channels, we have to account for the ionization channels as well, which are open.

The comparison with the existing experimental results and other theoretical data revealed that the transition lines are globally correct to approx. 1 cm^{-1}, while the intensities are in very good agreement with the experimental findings.

We have found that the photoionization cross section is governed by resonant structures identified as the discrete vibrational levels of the H_2 lying above the ionization thresholds. Moreover we found that the gain in the cross section due to the resonances comparatively to the background is about two orders of magnitude at low energies, while at higher energies this is more than a factor of two. The major contribution to the cross section is coming from resonances of the lowest lying excited electronic states.

2. Dissociative recombination at high energy [2]

Whether at low energy – i.e. below the dissociation threshold of the target molecular ions - the dissociative recombination is dominated by Rydberg resonances, at high energy, they completely disappear. However, new states, built on the vibrational continuum of the molecular ion, play an essential role, and strongly affect the dissociative recombination cross sections. More specifically, the vibrational excitation of the ion, effective at low energy, is extrapolated into the vibrational continuum, resulting in dissociative excitation. In the case of H_2^+/H_2 system (and its isotopomers), two ionic cores are involved in this process, and we took them both into account. Our calculations give very good agreement with recent experiments in storage rings and previous theoretical evaluations. We are about to apply our MQDT tool to BeH^+/BeH system, within collaboration with Åsa Larson (abstract in the same volume).

3. Atom-diatom collisions

Full quantum time independent close-coupling calculations were done in order to calculate reaction cross sections and rate constants. The best available potential energy surfaces were used in the calculation. Very good agreement has been found with experiments for rate constants of He induced rotational excitation of CN [3]. In the case of reactive molecular collision between O and OH good agreement has been found for rate constants at low temperature with the extrapolated data, but less good agreement with resent measurements at lower temperatures [4].

References

[1] J. Zs. Mezei, I., F. Schneider, Ch. Jungen and E. Roueff: in preparation

[2] O. Motapon et al: J. Phys. Conf. Series, in press

[3] F. Lique et al: J. Chem. Phys. **132**, 024303 (2010)

[4] F. Lique et al: J. Chem. Phys. **131**, 221104 (2009)

Theoretical studies of electron interaction with molecular ions and mutual neutralization – HeH and BeH

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Department of Physics, Stockholm University

Reactions driven through electronic resonant states of HeH and BeH are discussed. These reactions are dissociative recombination (DR), resonant vibrational excitations (VE) and resonant dissociative excitations (DE). Another process is mutual neutralization (MN).

HeH

The electronic resonant states of HeH are calculated using the full Configuration Interaction (CI) method with a large basis set. To obtain the autoionization widths electron scattering calculations are carried out using the Complex-Kohn variational method. The target ion is then described with a multi-reference CI wave function. Non-adiabatic couplings between the resonant states are computed using a method developed by V. Sidis [1].

Cross sections for VE and DE of HeH^+ in different vibrational states are computed by solving a driven Schrödinger equation and including autoionization using a local model. The non-adiabatic couplings between the resonant states are neglected. The cross sections become large when the energy is high enough to capture into the resonant states. The computed cross section for DE with the ion in the ground vibrational state is in very good agreement with measurement [2].

The MN reaction, $He^+ + H^- \rightarrow He^* + H$, will be studied using strictly diabatic states. Autoionization will be included using the local model and the cross section will be computed by numerically solving a Matrix-Riccati equation for the radial wave function.

BeH

We have previously [3] studied DR of BeH^+ including the capture into electronic resonant states. Electronic couplings between the neutral states were included using a quasidiabatization procedure. Using the multi-channel quantum defect theory, the non-adiabatic couplings to the Rydberg states are now also incorporated. The indirect process results in sharp oscillations in the cross section and it influences the low temperature thermal rate coefficient for the reaction. Resonant VE and DE of BeH^+ in different vibrational states are investigated. The cross sections for these reactions are significant also at relative low energies. In order to perform an *ab intitio*, quantum description of the MN reaction in collisions between $Be^+ + H^-$ structure calculations of potentials and non-adiabatic interactions are needed using a full CI with a very large basis set. Up to 12 states of $^2\Sigma^+$ symmetry are needed and couplings out to 60 a_0 have to be computed.

Plans

The plan for the next coming period of this CRP is to study high energy DR of HeH^+ for different vibrational states of the target ion. The branching ratios and ion-pair formation will be computed. Mutual neutralization will be studied in collisions between $He^+ + H^-$. Another reaction that will be investigated is the direct DE of HeH^+. We investigate a new theoretical approach to study the direct DE reactions. The direct DE of HeH^+ and He_2^+ will be investigated.

For BeH^+ we plan to include the rotational motion of the system in the MQDT treatment of DR. Mutual neutralization in collisions $Be^+ + H^-$ can be studied using a semiclassical method.

Direct and resonant dissociative excitation of He_2^+ will be computed.

Another interesting reaction is DR of BeH_2^+. To study this reaction quantum mechanically including all degrees of freedom and all relevant states, however, is very demanding and it is not clear how relevant this ion is for the plasma.

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Processes of electron and molecular ion collisions relevant to divertor plasma: hydrogen molecular ion and its isotopes

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We focus on the molecular species of H_2^+, D_2^+, T_2^+, HD^+, and DT^+ in this report. The processes relevant to divertor plasma taken up here are the following; $H_2^+(v,N) + e \rightarrow$

$H(n) + H(1s)$ dissociative recombination (DR)

$H^+ + H(1s) + e$ dissociative excitation (DE)

$H_2^+(v', N') + e$ vibrational(v) and rotational(N) transition

Theoretical calculation is now limited to the collision energies lower than 11 eV because there are complex and many electronic excited states of molecular ions above this energy region. The main mechanism of DR in hydrogen molecular ion is a transition into a dissociative two-electron excited state from single-electron continuum state. This mechanism is induced by the configuration interaction (CI).

The method of calculation is different depending on the collision energies. At lower energies than 1 eV, because the off-the-energy-shell effect (higher order perturbation effect) affects the electron collisions, the CI strength of off-the-energy-shell is also required. In addition, the indirect process with rotational de-excitation contributes to electron collisions. Those subjects could be achieved by the

multichannel quantum defect theory (MQDT) and algebraic solution for the CI scattering with clarifying the energy dependence of the CI. At higher energies than 1 eV, the ion-core exited Rydberg states can dissociate, and even the DE can occur. This problem is overcome by introducing discretized dissociative states to the MQDT, and by using the concept of MQDT not only to the electronic Coulombic functions but also to the dissociative functions. The electronic parameters as the quantum defect and the CI strength of various excitations are employed from the results of R-matrix calculations.

The cross sections of DR and vibrational and rotational transitions at the energies from 1 meV to 1 eV are systematically compiled on the five isotopes. For the energies from 0.3 eV to 11 eV, the cross sections are compiled on the vibrational transition, DE, and DR, where the principal quantum number of produced excited hydrogen atom is indicated. The result will be utilized for a simulation of divertor plasma, which should contribute to the design of a divertor and diagnostics of divertor plasma.

A new method for more complete calculation based on MQDT is now progressing aiming at higher collision energies.

Electron- and ion-impact processes with hydrogen and light plasma impurities

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In the period between the two CRP RCMs the following research has been accomplished within the project:

The process of dissociative electron attachment (DEA) on vibrationally excited $H_2(v)$, proceeding via the $^2\Sigma_g^+$ Rydberg resonant state, has been studied within the local complex potential model of resonant theory for this process. The DEA cross sections and reaction rate coefficients have been calculated for all 14 vibrational states of $H_2(X^1\Sigma_g^+)$ [1].

1. Using the molecular R-matrix method, the elastic and electronic excitation processes in e – BH_2 collisions have been studied in the energy range 0 (threshold) – 8 eV. The target has been described by the CAS CI, with 22 states being used in coupled channel calculations. The cross sections for rotationally elastic and momentum transfer processes, as well as for excitation of lowest two excited electronic states, have been calculated [2].
2. The electron impact excitation of lowest two excited states, $A(^1\Sigma^+)$ and $B(^1\Pi)$, of $BeH^+(v)$ ion has been studied within the Coulomb-Born approximation. The cross sections for v-v' state selective transitions have been calculated from threshold to 1000 eV. v-v' scaling relations have been established for both the cross sections and reaction rate coefficients [3].
3. The elastic and related transport (momentum transfer and viscosity) cross sections for the H^++Be, H^++C, Be^++H and C^++H collisions have been calculated in the CM energy range 0.1 meV – 10 keV by the quantum-mechanical MOCC method. The multichannel coupling affects the cross sections only for E_{CM} > 100-200 eV [4].

Using the AOCC method with a large AO basis and appropriate model potentials, the state-selective and total electron capture cross sections have been calculated for the N^{5+} +H and O^{6+}+H collisions in the energy range 0.5 – 100 keV/u [5].

The excitation and electron capture processes in H^++He($2s^{1,3}S$) collisions are currently being studied by using the AOCC method by using a large AO basis on both centers (all states with $n \leq 7$ plus pseudostates with n = 8-13). The electron – ion core interaction in singlet and triplet cases is described by separate model potentials. State-selective electron capture and excitation cross sections up to n = 6 have been calculated in the energy range 1 – 200 keV/u.

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Calculations of charge exchange cross sections for some ion-atom and ion-molecule systems

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This talk presents the theoretical results obtained by the group in Madrid. We have used a variety of methods, from full quantal calculations, in which both nuclear an electronic degrees of freedom are treated quatum mechanically, to classical mechanics (classical trajectory Monte Carlo) to calculate cross sections for elastic scattering, charge exchange (CE) and ionization processes.

Full quantal methodology has been applied to obtain elastic and CE cross sections in collisions of B^{5+} with H(1s) at very low collision energies. This work is published in [1], and contains data on C^{4+} + H(1s) not included in this presentation. Ionization and CE in collisions of B^{5+} with H(n=1,2), at higher energies, have been published in [2]. Given the wide energy range covered, we employed CTMC and semi-classical methods.

Using the full quantal and semiclassical methodologies, we have studied both collisions of Li^+ with H and H^+ with Li. This work is published in [3].

Progress in the calculation of CE cross section for the systems $H^+ + N_2$ and $H_2^+ + H^-$ is presented and compared with available experimental data and other calculations. $(HN_2)^+$ system is being studied using MOLPRO to obtain multi-reference configuration interaction wave functions. Also, a two center model potential has been developed to run CTMC calculations that include the anisotropy of the target molecule. For H_3 system, 32 full configuration interaction wave functions are calculated in a relatively small basis set of GTOs. In this case, the difficulties arise due to the large number of states involved in the collision. Given the preliminary character of these results, agreement with experiment and other theoretical calculations is encouraging.

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Summary of Presentation

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As part of the ongoing efforts of the Oak Ridge National Laboratory (ORNL) Atomic Physics for Fusion program, which involves integrated work in experimental and theoretical data production and data center activities focused on collection, evaluation, and dissemination of data, D.R. Schultz presented recent accomplishments relevant to the present CRP for heavy-particle elastic and transport processes, charge transfer, and excitation.

Since about 1997, the ORNL group has produced successive works containing very accurate elastic and related transport data needed in fusion plasma edge modeling, beginning with comprehensive treatment of (H^+, H) colliding with (H, H_2, He), including all hydrogen isotopologues, published as Volume 8 of the IAEA "Greenbook" series. In approximately sixteen subsequent publications, additions to this initial database have been made which improve or extend it, including treatment of, for example, protons colliding with Li, Be, B, C, Ne, Ar, Kr, and Xe. References to these works are summarized in a recent paper (P.S. Krstic and D.R. Schultz, Phys. Plasmas 16, 053503 (2009)). During the first year and a half of the present CRP this database has added to by calculations of the transport cross sections for H^+ + O and O^+ + H via the CTMC method. In the final year and a half of the CRP, similar calculations will be completed for H^+ + N and N^+ + H as well as complementary fully quantum mechanical results for H^+ + O and O^+ + H. If time permits the CTMC method will also be used to treat H^+ + O_2 and H^+ + N_2. The goal is to complete the dataset for ions lighter than Ne to provide not only explicit new data for impurity species common in fusion devices, but also to facilitate determination of trends of behavior with varying nuclear charge.

Especially owing to the recent undertaking of novel experimental measurements in the ORNL group regarding hydrogen-like C, N, and O ions colliding with atomic hydrogen, calculations using the AOCC method were made for comparison. Results of the measurements and calculations were presented and showed excellent agreement over the energy range of about 200 eV/u to 10 keV/u, with the experimental data extending down to about 0.01 eV/u and the theoretical data up to 200 keV/u. In addition, benchmarked by these unique measurements at the total cross section level, the theoretical work also provided state-selective charge transfer data needed for emission modeling and diagnostics.

Work was also reported that aimed to create a very large, state-of-the-art AOCC method dataset for excitation of all levels of atomic hydrogen up to $3d_m$ states by proton impact needed for interpretation of diagnostics such as those based on the motional Stark effect. These data are already being used for this purpose by workers at the Forschungszentrum in Jülich. In the final year and a half the work will be extended for C^{6+} + H excitation and charge transfer using the CTMC, AOCC, and LTDSE methods.

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