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

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

18–20 November 2009

Prepared by

B.J. Braams
International Atomic Energy Agency, Vienna, Austria

January 2010

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

The first 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 18–20 November 2009 at IAEA headquarters, bringing together experts representing 14 institutions. Participants summarized their recent and ongoing work pertinent to the research project. The specific objectives of the CRP and a detailed work plan were formulated. The discussions, conclusions and recommendations of the meeting are summarized in this report.

January 2010

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1. Introduction

On the advice of the A+M Data subcommittee of the International Fusion Research Council (IFRC) the Nuclear Data Section has initiated a Coordinated Research Project (CRP) on "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" with the objective to generate data for a number of radiative and collisional processes in ions of atoms and molecules of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen at temperatures and densities typical of the edge and divertor region of fusion reactors. Processes include electron impact excitation and ionization, radiative excitation, ionization, emission and recombination, auto-ionization and dielectronic recombination as well as charge exchange and heavy particle excitation and ionization. Eleven institutions are participating at the inception of the CRP and were represented, together with additional experts, at this first Research Coordination Meeting (RCM). The specific tasks of the RCM are to review ongoing and planned work of the participants in the CRP, to promote interaction between the participants, and to prepare a plan of work for the expected duration of the CRP, 2010–2014.

Participants described their ongoing research pertinent to the CRP and discussed plans for future work. A presentation on specific data needs for ITER was also given. A detailed work plan for the duration of the CRP was then formulated. 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. Section 4 provides conclusions. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2.

2. Summary of Presentations

D.H. Abriola (acting Section Head, Nuclear Data Section) opened the meeting and welcomed the participants. He reviewed the general objectives of the CRP and the specific tasks of this first Research Coordination Meeting (see Section 1). B.J. Braams (Unit Head, Atomic and Molecular Data Unit) reviewed the proposed agenda, which was adopted without change. Participants briefly introduced themselves. The meeting was attended by representatives of all the institutions participating in the CRP and further by Dr Steve Lisgo of ITER, France, Dr John Curry of the Atomic Spectroscopy Group at NIST, USA, and Dr Robert E.H. Clark of UT San Antonio (and past A+M Unit Head, IAEA). For the IAEA also Dr Hyun-Kyung Chung of the A+M Unit participated in the meeting.

The presentations are briefly summarized below. Most contributions are available in full through the A+M Unit web pages for this CRP (http://www-amdis.iaea.org/CRP/LightElement/) and the reader is asked to look at the original presentations for further information, including co-authors, attributions, citations and other pointers to the literature. 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 Data and Electron-atom Collisions

I. Bray, Curtin University of Technology, Australia: The convergent close coupling method for electron-atom scattering

Dr Igor Bray (representing D.V. Fursa) of the Centre for Antimatter–Matter studies at Curtin (http://www.positron.edu.au/) described briefly the Convergent Close Coupling (CCC) method, developed in Australia during the 1990s, and discussed computational studies of electron-atom scattering. The CCC theory is meant to be applicable at all energies for the major excitation and ionisation processes. A recent development is a surface integral approach to scattering theory that is

valid for short and long-range potentials including Coulomb potentials (Kadyrov et al.). The approach involves an expansion in one-electron and two-electron atomic states including continuum states; this limits the application to collisions on atoms having one or two valence electrons only. I. Bray showed convergence studies and comparisons with experiment for several systems. The calculations provided fully differential cross-sections for e^-+(H,Li,Na) including excitation and ionization channels. These studies show almost no substantial discrepancies between CCC and experiment for electron-impact excitation or ionisation of quasi one- and two-electron targets and for photon-impact single and double ionisation of He. Work is underway to extend CCC to positron collisions with quasi one- and two-electron targets, multi-channel proton collisions, and more complicated targets such as inert gases and molecules starting with H_2^+.

T.-G. Lee, Auburn University, USA: Electron impact on light atomic species: collisional data for tokamak edge plasma and divertor regions

Dr Teck Lee (representing M. S. Pindzola) presented recent and ongoing work in the Atomic and Spectroscopic Physics group at Auburn University (http://www.physics.auburn.edu/research/atomic) on light element collision data for fusion and astrophysical plasma. The theoretical methods employed are advanced non-perturbative close-coupling, perturbative distorted-wave, semi-classical and classical. The objective is to obtain accurate fundamental collisional data and also to produce high quality generalized collisional-radiative (GCR) rate coefficients that are of interest to the plasma modeling community.

In recent years GCR coefficients were calculated for the H, He, Li and Be isonuclear sequences; see PPCF 51, 105006 (2009), ADNDT 92, 813 (2006) and ADNDT 94, 257 (2008). Work on GCR data sets for the B and C isonuclear sequences is ongoing. Calculations for the electron impact excitation of neutral B and B^+ were published in JPB 40, 1131 (2007) and JPB 36, 1337 (2003), respectively. The remaining calculations to be carried out are for neutral C and the C^+ ion. The ionization of the ground states of B, B^+, C and C^+ were published in the following papers: PRA 76, 042704 (2007), PRA 78, 012704 (2008), PRA 62, 042705 (2000) and PRA 78, 052708 (2008), respectively. Calculations for electron impact ionization from excited states of the B isonuclear sequence were recently completed and it is next intended to calculate ionization from the excited states of the C isonuclear sequence.

In other work the Auburn group has studied processes involving heavy particle collisions with atoms and ions, including charge exchange, excitation and ionization for p+H, B^{4+}+H, p+He^+, He^{2+}+Li^{2+}, and p+Li. These studies were published in PRA 72, 062703 (2005), JPB 39, 2877 (2006), JPB 40, 3629 (2007) and PRA 68, 013404 (2003), respectively. Also some calculations were done for the single ionization of light diatomic molecules by electron and heavy particle impact that are of fusion interest, namely e+H_2, e+H_2^+, e+Li_2, e+Li_2^+, e+C_2, p+H_2^+, and He^{2+}+H_2^+. The reports can be found in the following papers: PRA 73, 052706 (2006), JPB 38, L285 (2005), PRA 78, 042703 (2008) and PRA 72, 022720 (2005). Final state resolved dielectronic recombination rate coefficients for ground and metastable states of H-like to Mg-like ions were calculated and are archived at http://amdpp.phys.strath.ac.uk/tamoc/DATA/DR/.

The presentation concluded with an assessment of the applicability and quality of the various theoretical methods. For neutral He and H, the excited state ionization cross sections were calculated using the quantal close-coupling methods (e.g., R-matrix with pseudostates and/or convergence close-coupling methods). These data were used to scrutinize the accuracy of both the classical and perturbative methods. It is found that the non-perturbative methods must be used for the lowest n-shells of H, He and He^+. For the excited states, semi-classical methods for H and He come into agreement with the non-perturbative close-coupling calculations for the highest n-shell that can be calculated (i.e., n=4). For He^+, excited state ionization perturbative DW methods are in good agreement with the non-perturbative results up to n=4, but are worsening as n increases further. Thus, including comparison with other light species, the following tentative general conclusions are made: (1) The semi-classical results become progressively worse with increasing ion charge q. (2) For low-charged (q=+1 and +2) ions, the non-perturbative methods should be employed for low n-shell ionization; scaled top-up is required for higher n-shell for which semi classical (e.g., ECIP) results

should be valid. (3) For moderate- to high-charged (q>+2) ions, in general the perturbative DW method becomes more accurate with increasing ion-charge for low n-shell ionization, and the contribution to the total ionization for the excited states is less important. Studies for such trend (DW vs. RMPS vs. ECIP) for boron and carbon are underway. It would be desirable to find a scaling law for the high n-shell ionization cross section for elements with Z>3 and low q.

R. E. H. Clark, University of Texas, San Antonio, USA: Atomic data for kinetics modeling of light element plasmas

Dr Bob Clark discussed data needs for fully kinetic modelling of plasma based on evolution equations for the population densities of individual excited states. Many excitation states must be followed in general, if one is not in the very low-density (coronal) or high-density (LTE) regime. Rate coefficients are needed for upward and downward transitions, but they are related via detailed balance. Comparisons were shown between the Plane-Wave Born approximation (PWB) and first-order many-body perturbation theory (FOMBT), showing good agreement in some cases but very large differences for forbidden transitions in electron impact excitation of C^+. Resonances are not treated correctly by either PWB or FOMBT and require the use of R-matrix methods or of Convergent Close Coupling, but these methods are much more expensive. The resonance states must then be included in the collisional-radiative model. This leads to very large models, for example in work by James Colgan et al. at Los Alamos on the order of 10^4 levels are used for boron and carbon. A database must have a comprehensive set of energy levels, including resonances, and cross sections consistent with those energy levels for all transitions. Bundling must be considered, but it requires a complete data set at the start. Bob Clark recommends that the LANL group be represented in the CRP.

J. Curry, National Institute of Standards and Technology, USA: Spectroscopic research projects at NIST on light elements

Dr John Curry described the spectroscopic databases and allied research in the Atomic Spectroscopy Group at NIST (http://physics.nist.gov/Divisions/Div842/Gp1/). The Atomic Spectra Database (ASD), version 3.15, contains now numerical data for 950 spectra, 144,000 transition wavelengths and 77,000 energy levels. Auxiliary tools provide Grotrian diagrams, Saha-equilibrium radiation plots, line ID plots, and spectral modelling by the FLYCHK code. ASD receives around 50,000 queries per month. Bibliographical databases are available for energy levels and wavelengths, atomic transition probabilities, and line shapes and shifts. Recent comprehensive compilations for ASD were done for all the lightest elements: H (D, T), He, Li, Be, and B; they are underway for other first- and second-row elements. There are also studies of charge-exchange recombination spectroscopy, in particular for Ar. Data for tungsten are being re-evaluated and extended. Future plans include new compilations for H, D, T (energy levels and wavelengths), F and Ne (transition probabilities), and Ar and Cl (energy levels and wavelengths). Spectral measurements are being carried out for Mg.

2.2 Heavy Particle Collision Processes

D.R. Schultz, Oak Ridge National Laboratory, USA: Recent calculations involving light species for fusion

Dr Dave Schultz provided an overview of the atomic and molecular physics work at Oak Ridge and then presented his research plans for the present CRP. Oak Ridge has three centres concerned with A+M data: the Controlled Fusion Atomic Data Center (databases; http://www-cfadc.phy.ornl.gov/), the Multicharged Ion Research Facility (experiment; http://www.phy.ornl.gov/atomic/MIRF/Mainmenu.htm) and the Atomic, Molecular, and Optical Theory group (http://www.phy.ornl.gov/theory-amo/). Answering specific requests for data from the plasma science community is the highest priority for the Data Center, and this is accomplished through rapid feedback to requests using existing data sources or quick calculations, and through longer term data production projects. A major ongoing project is connected with the revision of the database for collisions of H and H^+ (all isotopes) on (H, H_2, He); also on Li, Be, B and selected reactions involving heavier atoms and ions. Fully quantal calculations

are carried out for differential cross-sections and for particle, momentum, and energy transport moments.

For the present CRP the planned work is calculations of state selective charge exchange with use of the Lattice Time-Dependent Schrödinger Equation (LTDSE) method. The method involves discretization of the (effective) one-electron Schrödinger equation on a multidimensional grid. Examples were presented for the reactions of Be^{4+}+H, He^{2+}+H and H^{+}+H.

L. Méndez, Universidad Autónoma de Madrid, Spain: Calculation of charge exchange cross sections at low collision energies

Dr Luis Méndez, of the Atomic and Molecular Collisions Centre at UAM, Madrid (http://tcam.qui.uam.es/) described computational studies of charge exchange at low collision energies — low enough that it is not possible to employ an approximation of unperturbed heavy particle trajectories, but electronic excited states can nevertheless be important. Processes already studied include $N^{2+}+H \rightarrow N^{+}+H^{+}$ (at various spin states), $Li^{+}+H \rightarrow Li+H^{+}$, $Be^{+}+H \rightarrow Be+H^{+}$, and $H^{+}+Be \rightarrow H+Be^{+}$. The vibrational close coupling (VCC) method was employed to study the collision process $H^{+}+H_2$ while allowing for vibrational excitation, dissociation, nuclear exchange, electron capture, dissociative capture, and capture with nuclear exchange. Preliminary work was described concerning the reaction $H^{+}+CH \rightarrow H+CH^{+}$. Planned and possible future work concerns:

1. Elastic, charge transfer and excitation cross sections for collisions between ions and atoms; in particular, reactions between Be ions and H (D, T) atoms. Similar systems can be considered if required.

2. Collisions of ions with small molecules at energies between 1 and 100 eV/amu. The group at UAM is developing methods to incorporate nuclear exchange processes and to improve the quantum chemistry techniques to evaluate the molecular wavefunctions and potential energy surfaces. This project will be carried out in collaboration with Prof. B. Pons (Bordeaux, France), and Profs. Halász and Vibók (Debrecen, Hungary).

J. B. A. Mitchell, Université de Rennes I, France: Ion-molecule reactions of light elements: missing information

Dr Brian Mitchell of the Institute for Physics at Rennes (http://www.ipr.univ-rennes1.fr/wiki/index.php/FR/home) discussed the status of experimental work for bimolecular cation-molecule reaction kinetics. There is an important compilation of data by V. G. Anicich (JPL report 03-19: http://hdl.handle.net/2014/7981). Singly charged ions are of interest in gas phase kinetics and in astrochemistry in addition to fusion and data are available for many ion-molecule reactions involving H^{+}, H_2^{+}, H_3^{+}, He^{+}, He^{2+}, He_2^{+}, HeH^{+}, Li^{+} and Be^{+}. However, there are fewer data for multiply charged ions colliding with molecules, and then mainly for the H_2 molecule. The formation of other molecules in plasma is poorly understood. Photon-stimulated reactions may play an important role. The FALP-MS afterglow and the CRESU supersonic flow experiments at Rennes can be used to study formation of molecular cations.

J. G. Wang, Institute of Applied Physics and Computational Mathematics, Beijing, China: Theoretical studies on heavy particle collisions

Dr Jianguo Wang of the IAPCM (http://www.iapcm.ac.cn/) described charge transfer calculations including electronic excitation and ionization. The computational approach is based on molecular orbital close-coupling (MOCC) theory or on the two-center atomic orbital close-coupling (TC-AOCC) theory. Starting point is a multi-reference with single and double excitations (MRDCI) molecular electronic structure calculation for the reaction complex; this is followed by a scattering calculation using a close-coupling approach. Calculations were shown for single and double charge transfer including excitation in the reaction $O^{3+}+He \rightarrow (O^{2+}+He^{+}, O^{+}+He^{2+})$ and for charge transfer plus excitation in the reaction $He^{+}+Ne \rightarrow He+Ne^{+}$. The effect of Debye shielding in non-ideal plasma

(modifying the electronic structure) was considered in calculations of charge exchange, excitation and ionization for collisions of He^{2+} on H. Calculations of the characteristic charge exchange spectrum were shown for $O^{8+}+H \rightarrow O^{7+}+H^+$, of interest for neutral beam diagnostics.

Work is in progress on charge transfer with excitation in reactions of ions of Be and B (all charge states) with H. Future plans include charge transfer calculations involving molecules: H^++(BeH,BeH_2,BH,N_2) and ($Be^{4+},B^{5+},C^{6+},N^{7+}$)+$H_2$.

R. K. Janev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia: Data status and needs for heavy-particle collision processes in fusion edge/divertor plasma

Dr Ratko Janev reviewed the status of light element atom-atom and atom-molecule (including ions) collision data for fusion and presented ongoing and planned work in connection with the present CRP. For the collision of protons on He there are good excitation data for targets He(1s) and He(2s) singlet and good ionization and charge exchange data for target He(1s); data for more highly excited target states are needed. Probably direct calculation must be done for the n=2,3,4 initial states; then scaling for higher n. Likewise for impact by He^+ and He^{2+} on H, H_2 or He there are good data for excitation, ionization and charge exchange for ground state targets, some excitation data for excited targets, but not enough on ionization and CX for excited targets, and there are gaps for low impact energies. For proton impact on Li targets there are AOCC calculations for ground and excited state targets (excitation, ionization and charge transfer), but experimental data for ionization and CX exist only for target Li(2s). The presentation continued with a review of data for Li^{q+}+(H,H_2), p+(Be,B), (Be^{q+},B^{q+})+(H,H_2,He) and further remarks on collisions involving C, N, and O; please see the transparencies for this and please see Section 4 for the planned work.

2.3 Electron-molecule Collision Processes

P. Defrance, Université Catholique de Louvain, Belgium: Electron impact ionization and dissociation of molecular ions

Dr Pierre Defrance described experimental work carried out in the Atomic, Molecular and Optical Physics group at UCL employing the animated crossed electron-ion beam method (Lecointre et al., J. Phys. B 39 (2006) 3275). The molecular ion beam of well-defined energy (a few keV) interacts at right angles with an electron beam whose energy is tuned from a few electron volts up to 2.5 keV. Product ions are separated from the primary ion beam by using a double focusing 90° magnetic analyzer. Product ions are further deflected by a 90° electrostatic spherical deflector and directed onto the channeltron detector. Three-dimensional imaging of the dissociative charge transfer events is realized in a separate set-up. The molecular ion beam intersects a collimated Potassium jet, on which a two-colour excitation can be applied to produce Rydberg states. Position sensitive detectors consisting of microchannel plates and a resistive anode are located 2 m downstream and operate in coincidence, enabling the reconstruction of the velocity vectors of the fragments. (More advanced detectors will be available for multiple fragment detection).

Absolute cross-sections and kinetic-energy-release distributions (KERD) have been published for CD_n^+ (n=1–4), H_2^+, D_3^+ and NeD^+, for example. The work in the group is concerned with fusion plasma as well as plasma processing and atmospheric ions. For fusion plasma, especially the hydrocarbon and deuterocarbon families ($C_mH_n^+$ and $C_mD_n^+$, m=1-3) are of interest and are systematically investigated at UCL.

Dissociative charge transfer with ground state or laser excited target has been demonstrated to provide direct access to the internal excitation of the molecular ions. When long-lived neutral states are populated, that decay via predissociation, the coincident detection of the neutral fragments allows the reconstruction of the KERD, which is a signature of the internal energy of the parent molecular ion. Such a technique was successfully used for H_2^+, HD^+, D_2^+, HeH^+, HeD^+, O_2^+, and H_3^+. Its general applicability must however be tested on larger systems, e.g. hydrocarbon ions. This method will be coupled to the afore-mentioned electron-impact studies.

B. Wei, Fudan University, Shanghai, China: Studies of the interactions between electrons and molecules based on a reaction-microscope

Dr Baoren Wei of the Fudan Institute of Modern Physics (http://imp.fudan.edu.cn/) described proposed research based on the recoil ion momentum spectrometer (RIMS) that is currently being tested at the Shanghai EBIT laboratory. The unique feature of RIMS, and the reason such instruments are important to the proposed measurements, is the ability to reconstruct the dynamics of a collision from position and momentum data for the collision products. For fairly complex collisions this requires multi-hit features and the Shanghai RIMS has this through the fast timing of the electronics and data acquisition systems. Experiments can be done at low collision energies (at Shanghai from 1 eV up to several keV) and provide energy resolution in the range of a few eV or less under favourable circumstances. The Fudan group proposes to measure cross-sections for ionization and fragmentation of cold molecules by low energy electron collisions. These measurements require the development of a super-sonic gas jet target to ensure good energy properties of the molecular beam. A second development, which will be made specifically for this project, is a low energy electron beam. After combining the electron beam with the RIMS, the experimental set up will be tested through studies of sub keV electron beams colliding with methane (CH_4). Subsequently cross-sections for ionization and dissociation of other hydrocarbon molecules will be measured. The measured data will be published and shared with the IAEA through its atomic and molecular databases. Future measurements will aim at cross-sections for the excitation and dissociation of molecules by electron impact. This research is supported by the IAEA through the present CRP and further by the Chinese National Fusion Project for ITER. In conclusion Dr Wei drew attention to the International Conference on the Physics of Highly Charged Ions, HCI2010, which will be held at Fudan University, 30th August – 3rd September 2010.

H. Takagi, Kitasato University, Japan: Theoretical calculation on electron and molecular ion collisions relevant to divertor plasma

Dr Hidekazu Takagi described theoretical and computational work on dissociative recombination and molecule-assisted recombination in low-temperature divertor plasma (from below 1 eV up to 30 eV). Rovibrational molecular excitation and dissociation is included in these calculations and one is interested in state-specific electron-impact cross sections. The principal computational bottleneck is the need to include many electronic states to cover the wide range of collision energy. The computational approach to overcome this bottleneck is based on multichannel quantum defect theory (MQDT) and a discretization of the dissociative states, followed by an R-matrix scattering calculation. Molecular targets of interest include H_2, H_2^+, H_3^+, HeH^+, CH, CH^+, and NeH^+.

M. Larsson, Stockholm University, Sweden: Experimental studies of electron scattering on molecular ions

Dr Mats Larsson, of the Molecular Physics Division at Stockholm (http://mol.physto.se/index2.htm), described experiments on dissociative recombination. Early experiments were based on stationary afterglow (following termination of a microwave discharge) and then afterglow in a flowing gas. At present ion storage ring experiments are favoured as they provide better control of the collision parameters in a steady-state environment. The Stockholm CRYRING "first generation" ion storage ring is to be shut down after a final set of experiments in December 2009. (It will be moved to Germany.) A first generation storage ring is operating in Heidelberg and second generation (electrostatic) storage rings in Aarhus, Denmark (ELISA), Tsukuba, Japan (KEK) and Tokyo, Japan (TMU); however, these are not much used for fusion-related atomic physics studies. New second generation storage rings are in Lanzhou, China (heavy ion research), Stockholm University (DESIREE; commissioning in 2010), Heidelberg, Germany (a cryogenic ring scheduled for 2012), and there is proposal for a facility at ORNL, USA. The DESIREE facility at Stockholm will be used, as complementary to earlier CRYRING studies, for bound electron scattering and recombination studies (positive ion - negative ion collisions) relevant to plasma physics and fusion.

A. Larson, Stockholm University, Sweden: Theoretical studies of electron scattering on molecular ions

Dr Åsa Larson, also of the molecular physics division (http://mol.physto.se/index2.htm), presented theory and computation for electron impact processes on molecular ions, including scattering and dissociative recombination. Starting point is the solution of the multi-state electronic structure problem and an electron scattering calculations of resonant states. This is followed by diabatization of all the states, determination of diabatic coupling coefficients and autoionization widths, and then wavepacket calculations of nuclear dynamics. It can be carried out in practice for a 2-atom or 3-atom molecular system. An example process of much interest in fusion is the radiative and dissociative recombination of BeH^+, with excited BeH as an intermediate state. (Experimental studies are scarce or nonexistent because of the toxicity of Be.) The electronic structure calculations must use multi-reference configuration interaction (MRCI), and for the scattering calculations the Complex Kohn variational method is used. The calculations can be carried out for excited initial states as well as for ground states, at greater cost due to the (typically) much larger number of accessed excited intermediate states. Sample calculations were shown for $e^-+BeH^+ \rightarrow Be^*+H$. New work is focussing on dissociative recombination in the collision processes $e^-+BeH_2^+$ and $e^-+CH_2^+$. For this three-atom system the electronic structure part and the electron scattering calculations are similar to the two-atom case, but for the nuclear dynamics the Multi-Configuration Time-Dependent Hartree (MCTDH) method is employed.

2.4 ITER Data Needs

S. Lisgo, ITER, France: ITER overview and requirements for light element atomic data

Dr Steve Lisgo described the ITER status and its current time schedule (tokamak core and first plasma in 2018, start of H/He experiments in 2021) and its main needs for atomic and molecular data. ITER plans to operate initially with a mixed surface: C divertor, W baffle, Be first wall. The main atomic species of interest are therefore the proper plasma constituents H, D, T and He; Be and C as unavoidable impurities; Li due to its use in a diagnostic beam; N and Ne because N_2 or Ne gas injection may be used for power control and mitigation of ELMs and disruptions; O because of H_2O wall contamination; and then heavier elements W from the surface, possibly Ar for power control (but N_2 and Ne are presently favoured for this purpose), and finally Fe and Cu from abnormal events. Among the light elements only B is absent; ITER is not planning to boronize the wall.

In the divertor a cool (below 1 eV) high-density "detached" plasma is foreseen and molecules will be present; the molecular species of primary interest are H_2, H_2^+, H_3^+ (and their isotopes as goes without saying), also vibrationally excited, and hydrocarbons and LiH and BeH and their ions. Due to the planned He campaign there is also much recent interest in molecular ions containing He. N_2 may be injected and is therefore of interest. There will be a dedicated neutral beam for impurity diagnostics. Atomic and molecular data are required for plasma temperatures down to below 1 eV, but also for collisions with H at up to 150 keV for the diagnostic neutral beam and up to 1 MeV for the main heating neutral beams. Photoionization can be an important process in parts of the divertor region where plasma is not otherwise expected. The atomic and molecular data are used in a variety of fluid and kinetic modelling codes and the principal source of atomic data is ADAS [see PPCF **48** (2006) 263–293]; also important are AMJUEL [D. Reiter], a general repository including the Janev-Reiter hydrocarbon data; HYDHEL [Janev-Langer], a database for H and He and their molecules; and H2VIBR [Sawada, Fujimoto, Goto, Reiter], a collisional-radiative model for $H_2(v)$. There is an Integrated Tokamak Modelling (ITM) activity in Europe (also in the US) that seeks standardized interfaces to the atomic, molecular, nuclear and surface data used for modelling; this is important to ITER. In conclusion, among all data needs those for vibrationally excited H_2 (all isotopes) appear most important, and the need for He data (including molecules and metastable states) has received new emphasis.

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

Methods and codes exist for a wide range of electron-impact excitation and ionization processes; however, it is important to exercise these codes for situations required in plasma modelling. In particular, more attention must be given to excited initial states, as metastables may be very long-lived in the light elements (different from the case of high-Z elements) and their presence has a significant impact on power loss. It is proposed that collision data for e^-+He(n=2,3,4) should be revisited, especially near threshold. The same applies to other light targets: H, He, Li and Be and their ions and at least the n=2 initial state for B and C and their ions. (But check what has been done for this to-date in ADAS.) Benchmark calculations at the highest level of theory should be done at least for He. These calculations are expensive as excitation from excited states can access many states of high angular momentum already at very low plasma temperature. Scaling rules and simplified methods for computation of processes beginning with excited states should be investigated as well, e.g., based on the distorted-wave (DW), plane-wave (PW), classical trajectory Monte Carlo (CTMC), or Exchange Classical Impact Parameter (ECIP) methods. However, calculations on the two-electron e^-+H process already serve as a warning against the DW and PW methods at n=4 or n=5.

3.2 Work Needed on Heavy Particle Collision Data

For the primary plasma components, H and He, negative ion data need attention. Cross-sections for mutual neutralization, H_2^++H^- and H_3^++H^-, need to be validated up to 1 keV. Vibrationally resolved data involving H_2 and H_2^+ should be extended to higher energies. ITER is planning a major He-plasma campaign and processes involving metastable and excited He have not all been covered; data are needed for H^++He(n=2,3,4), for (He^+,He^{2+})+H_2 and for collisions involving HeH^+ and He_2^+.

Secondary light elements are Li, Be, B, C, N and O. Charge transfer and ionization data for H^++Li are important for Li neutral beam studies and need to be checked. Charge transfer cross sections also need to be checked for all Li ions colliding with H and with H_2. In general, for all secondary species, charge transfer with H(n=2,3,4) and with electronic or vibrationally excited H_2 and H_2^+ needs to be checked. Finally, for the charge transfer collisions H^++(Be,B,C,N,O) the elastic channel needs more attention.

3.3 Work Needed on Electron-molecule Collision Data

For the simplest processes, e^-+(H_2,H_2^+), it would be very nice to have experimental data, vibrationally resolved, for dissociative excitation and recombination (case of H_2^+), but probably theory will be all that can be done. Theory is also required for the collision process e^-+HeH^+ (dissociative excitation, recombination, and ionization), vibrationally resolved. (Experimental DR data exist for v=0.) For He-plasma studies data are needed for the formation of He_2^+ (e.g., via three-body processes) and for its destruction by electron impact (DE, DI and DR). The formation of hydrides XH and XH^+ (X=Li,Be,B,C,N,O) is not adequately understood; here also surface processes must be important. Vibrationally resolved data are needed for all channels of e^-+XH^+ (X=Li,Be,B,C,N,O) and for e^-+(C_2,N_2,O_2) and their ions. Finally the most important three-atom molecules for which electron-impact data are required are H_3^+, BeH_2^+, CH_2^+, and NH_2^+.

3.4 Work Plan

I. Bray, D.V. Fursa – The group at Curtin plans to carry out Convergent Close Coupling (CCC) calculations to obtain benchmark cross-sections for e + H, He, Li, Be, especially near thresholds and involving initially excited states. They plan to develop codes based on similar theoretical methods for proton impact (hoping for collaboration within the CRP), and to develop codes for light molecules and apply those to obtain benchmark results for e + H_2^+ and e + H_2.

T.-G. Lee, M.S. Pindzola – The main plan of the Auburn group for this CRP is to produce high-quality generalized collisional-radiative (GCR) rate coefficients for the light element isonuclear series. Work has been completed for H, He, Li, and Be, while work is in progress for B and C. It is further planned to compute single and double charge transfer cross-sections for He^{2+}+He collisions.

J. Curry – The principal ongoing projects at NIST on light element spectroscopy concern compilation of transition probabilities for F and Ne, and compilation of wavelengths and energy levels for Be, B, F, Ne. A new compilation of wavelengths and energies for hydrogen isotopes is also in progress.

R.E.H. Clark – Bob Clark recommends that the group of James Colgan at LANL be involved in the CRP for computations on B and C: energy levels, transition probabilities, photoionization, autoionization, and electron-impact excitation and ionization. An open-access interface to this data is being constructed.

D.R. Schultz – The work at ORNL for this CRP is based on the Lattice Time-Dependent Schrödinger Equation Method (LTDSE). It is planned to calculate elastic and transport cross sections for proton impact on O, N, O_2 and N_2, cross-sections for H excitation due to collisions with H^+ and C^{6+} for beam emission spectroscopy, and benchmark results for ionization in H^++H across a broad range of energies.

L. Mendez – The work of the Madrid group will focus on the calculation of total cross sections for heavy particle collisions. Specific atomic collisions to be studied are B^{5+}+H charge transfer (with H(n=2)), H^++Li all channels, and low-energy elastic cross sections for H^++Be, Be^++H and Li^++H. Other similar systems can be considered if required. Molecular collisions to be studied are H^++H_2, H^++CH and H^++N_2 at energies between 1 and 100 eV/amu, mutual recombination in H_2^++H^-, and the processes (He^{2+},Li^{3+},Be^{4+})+H_2. The group is developing methods to incorporate nuclear exchange processes and to improve the quantum chemistry techniques to evaluate the molecular wavefunctions and potential energy surfaces. The molecular collision studies will be carried out in collaboration with Prof. B. Pons (Bordeaux, France) and Profs. Halász and Vibók (Debrecen, Hungary).

J.B.A. Mitchell – It is planned to study two- and three-body reactions forming HeH^+, He_2^+ and $HeNe^+$ and Ne_2^+ ions in edge and divertor plasma. This study will include literature surveys and data evaluation, and experiments using CRESU for the three-body association leading to HeH^+ and He_2^+. Also experiments are planned on dissociative excitation of HeH^+, He_2^+, $HeNe^+$ and Ne_2^+ (collaboration with Pierre Defrance, UCL), and on mutual neutralization in H^-+(H_2^+,H_3^+) if a collaboration is available. Experimental and theoretical data on dissociative recombination for light elements will be collated.

J. Wang – Charge transfer and excitation in the reactions Be^{q+}+H, B^{q+}+H, H^++He*, and H^++Li*; also charge transfer in the reactions H^++(B,Be,C).

R.K. Janev – It is planned to study dissociate excitation (DE) in the Coulomb-Born approximation for electron impact on LiH^+, BeH^+ and BH^+ (collaboration with R. Celiberto, Bari); charge transfer and excitation using the AOCC approximation for the collision of $(Li,Be,B,C,N)^{q+}$+H (collaboration with J. G. Wang, IAPCM, Beijing); and to evaluate published data for heavy particle impact collisions involving He, N, and N_2.

P. Defrance – The work plan at UCL for this CRP is the study of dissociative excitation and ionization of $C_2H_n^+$, n=3-6, HeH^+, NH^+, OH^+ and BeH^+ (and H→D variants) by electron impact in the energy range from threshold to 2.5 keV. Coordination with ORNL/Auburn experiments will be useful. The collected data will be analyzed in order to determine separately the contributions of dissociative excitation and ionization, as well as the associated energy thresholds and KERDs. In cases where it is possible, vibrationally excited states populations will be evaluated for each target molecule.

B. Wei – The priority at the Fudan EBIT for this CRP is to study electron impact ionization and DI (detecting ion products) for H_2 and C_nH_m; later also for N_2 and O_2. These measurements require the development of a super-sonic gas jet target to ensure good energy properties of the molecular beam. A

second development, specifically for this project, is a low energy electron beam. Combining the electron beam with the RIMS, the experimental set up will first be tested through studies of sub-keV electron beams with methane.

H. Takagi – At Kitasato, collaborating with IMS and ISAS, it is planned to compute more reliable cross sections for electron impact DR, DE, and vibrational and rotational transitions in HeH^+, HeD^+, HeT^+, and H_2^+; also in CH^+, H_3^+, and in NeH^+ and other noble gas hydrides in collaboration with Dr Florsecu-Mitchell. Fully state-specific cross sections will be provided at low energies (below 1eV).

M. Larsson – The principal experimental effort at Stockholm will be devoted to mutual neutralization and dissociation by collision of H^- with H^+, H_2^+, $H+3^+$, H_5^+ and HeH^+.

Å. Larson – It is planned to compute cross-sections for electron-impact DE and DR of HeH^+, for mutual neutralization $He^+ + H^-$, for electron-impact dissociative excitation of H_2, and for dissociative recombination of H_2O^+, CH_2^+, BeH_2^+, and BH^+.

4. Conclusions

The presentations and discussions at this first Research Coordination Meeting of the CRP on "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" resulted in the identification of data needs for further modelling of tokamak plasma and light element impurities in the near-wall region. Broadly speaking, effort is most needed to obtain fully resolved cross-sections for collision processes involving electronically excited atomic targets and electronically and vibrationally excited molecular targets. Another recent area of interest is processes involving HeX^+ molecular ions (X=H,He,Li,Be,B,C). More specific data needs were enumerated and a detailed work plan was drawn up for the participants and their co-workers. The progress in meeting the objectives of the CRP will be evaluated at the second RCM, which is to be held in approximately 18 months.

Appendix 1

IAEA first Research Coordination Meeting on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

18–20 November 2009, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA first Research Coordination Meeting on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions

18–20 November 2009, IAEA Headquarters, Vienna, Austria

Agenda

Wednesday, 18 November **Meeting Room: A23-11**

09:30 – 10:00 D. Abriola, B. Braams: Opening introductions, adoption of the agenda

Session I. Chair: M. Larsson

10:00 – 10:40 I. Bray: The convergent close-coupling method for electron-atom scattering

10:40 – 11:10 *Coffee break*

11:10 – 11:50 T. Lee: Electron impact on light atomic species: collisional data for tokamak edge plasma and divertor regions

11:50 – 12:30 R. Clark: Atomic data for kinetics modeling of light element plasmas

12:30 – 14:00 *Lunch*

Session II. Chair: R. Clark

14:00 – 14:40. J. Curry: Spectroscopic research projects at NIST on the light elements

14:40 – 15:20 S. Lisgo: ITER overview and requirements for light element atomic data

15:20 – 15:50 *Coffee break*

15:50 – 16:20 Discussion on atomic data issues

16:20 – 17:00 D. Schultz: Recent calculations involving light atoms and ions

19:30 – *Social dinner (outside VIC)*

Thursday, 19 November

Session III. Chair: D. Schultz

09:00 – 09:40 L. Mendez: Calculation of charge exchange cross sections at low collision energies

09:40 – 10:20 B. Mitchell: Ion-molecule reactions of light elements: missing information

10:20 – 10:50 *Coffee break*

10:50 – 11:30 J. Wang: Theoretical studies on heavy particle collisions

11:30 – 12:10 R. Janev: Data status and needs for heavy-particle collision processes

12:10 – 13:40 *Lunch*

Session IV. Chair: R. Janev

13:40 – 14:10 Discussion on heavy particle collision issues

14:10 – 14:50 P. Defrance: Electron impact ionization and dissociation of molecular ions

14:50 – 15:20 *Coffee break*

15:20 – 16:00 B. Wei: Studies of the interactions between electrons and molecules based on reaction-microscopes

16:00 – 16:40 H. Takagi: Theoretical calculation on electron and molecular ion collisions relevant to divertor plasma

19:30 – *Social dinner (outside VIC)*

Friday, 20 November

Session V. Chair: P. Defrance

09:00 – 09:50 M. Larsson / A. Larson: Experimental and theoretical studies of electron scattering on molecular ions

09:50 – 10:20 Discussion on electron – molecule (or mol. ion) collision issues

10:20 – 10:50 *Coffee break*

Session VI. Chair: B. Braams

10:50 – 12:30 All: Development of Work Plan

12:30 – 14:00 *Lunch*

14:00 – 16:00 All: Development of Work Plan; Wrap Up

16:00 – *Close of Meeting*

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