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Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma

Summary Report of the First Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

10–12 August 2011

Report prepared by

B. J. Braams

IAEA Nuclear Data Section

December 2013

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Abstract

The First Research Coordination Meeting of the IAEA Coordinated Research Project (CRP) on "Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma" was held 10-12 August 2011 at IAEA Headquarters in Vienna. Participants reviewed the status of the database on molecular processes of H and He, identified data needs and made plans for development of new data in connection with the CRP. The proceedings of the meeting are summarized here. Participants' summaries and work plans are also provided.

December 2013

Contents

1. Introduction 7

2. Presentations 8

D. Abriola, B. J. Braams: Opening 8

D. Reiter: Collisional-radiative and transport modeling for ITER 8

P. Krstic: Vibrationally resolved ion-molecule collisions 9

K. Sawada: Revision of collisional-radiative models and neutral transport code for hydrogen and helium species 9

J.-S. Yoon: Evaluation of cross section for electron impact with hydrogen and their combination molecules in fusion plasma 9

U. Fantz: Application and evaluation of state-resolved atomic and molecular data in population models for hydrogen, deuterium and helium 9

R. Celiberto: From elementary processes to modeling of molecular plasmas in thermonuclear fusion 10

H.-K. Chung: Databases in the atomic and molecular data unit 10

X. Urbain: Electronic and atomic collisions with hydrogen and helium ions: State-specific study of associative, dissociative and reactive processes 10

X. Ma: State-resolved cross section measurements in low and intermediate energy Ion-He/H2 Collisions 10

A. E. Orel: Theoretical studies of electron driven resonant processes in H_2^+ and HeH^+: Dissociative recombination, vibrational excitation and dissociative excitation 10

O. Motapon: Low energy reactive collisions of electrons with H_2^+ and isotopomers: Computations and comparison with measurements 11

Ch. Jungen: Dissociative recombination of molecular hydrogen and diatomic hydride ions: direct and indirect processes 11

V. Kokoouline: Inelastic processes in collisions between the H_3^+ ion and an electron: Rotationally and vibrationally resolved cross-sections for dissociative recombination and (de)excitation of H_3^+ 11

3. Discussion on data status and data needs 11

General remarks 11

Note on CR models for H and He 11

Electrons and protons, e^- and H^+ 12

Atomic and molecular hydrogen, H and H_2 12

Electronic excited H 12

Vibrationally excited H_2 12

Rotationally excited H_2 12

Electronic excited H_2 13

Molecular cation H_2^+ 13

Excited H_2^+ 13

Negative ion H^- 13

Electronic excited H^- 14

Negative molecular ion H_2^- 14

Protonated molecular hydrogen H_3^+ 14

Electronic excited H_3^+ 14

Helium and its ions and molecular ions 14

Presentation of data 15

Opportunities for benchmark experiments 16

4. Workplan 16
D. Reiter 16
P. Krstic 16
K. Sawada 16
J.-S. Yoon 16
U. Fantz 17
R. Celiberto 17
X. Urbain 17
X.-W. Ma 18
A. Orel 18
O. Motapon 18
C. Jungen 18
V. Kokoouline 19

Recommendations and Conclusions 19

Appendix 1: List of Participants 20

Appendix 2: Agenda 21
Wednesday, 10 August Meeting Room: A07-42 21
Thursday, 11 August Meeting Room: A07-42 21
Friday, 12 August Meeting Room: A07-42 22

Appendix 3: Summaries by Participants 23
Collisional-radiative and transport modeling of hydrogen and helium for ITER 23
Vibrationally resolved ion-molecule collisions 24
Revision of collisional-radiative models and neutral-transport code for hydrogen and helium species 26
Evaluation of Cross Section for Electron Impact with Hydrogen and Helium and Their Combination Molecules in Fusion Plasma 27
Application and Evaluation of State-Resolved Atomic and Molecular Data in Population Models for Hydrogen, Deuterium and Helium 28
Recent advances on state-to-state approach in non-equilibrium hydrogen plasma modelling: focus on electron-H_2 resonant collisions 30
Electronic and Atomic Collisions with Hydrogen and Helium Ions: State-Specific Study of Associative, Dissociative and Reactive Processes 31
State-Resolved Cross Section Measurements in Low and Intermediate Energy Ion-He/H_2 Collisions 33
Theoretical studies of electron driven resonant processes in H+2 and HeH+: Dissociative Recombination, Vibrational Excitation and Dissociative Excitation 34
Low Energy Reactive Collisions of Electrons with H_2^+ and isotopomers: Computations and comparison with measurements 35
Molecular Rydberg states: between spectroscopy and dynamics 36
Rotationally and vibrationally resolved cross-sections for dissociative recombination and (de-) excitation of H_3^+ by electron impact 38

1. Introduction

The divertor of a magnetic confinement fusion experiment is the region where plasma that flows along magnetic field lines interacts with a material boundary. The divertor has two primary roles: power handling and particle control. Both issues require a high density, low temperature plasma regime and this is achieved by friction between plasma and neutral gas together with radiative cooling.

Neutral particles are pumped out from the divertor region in order to remove impurities and (in a reactor) helium ash. In much of the divertor region the plasma is relatively cold and dense with typical temperature in the range 1 eV – 5 eV and electron density in the range $2\times10^{14}/m^3$ – $1\times10^{15}/m^3$. Hydrogen molecules are formed on the walls and under some conditions also by volume recombination, and in parts of the divertor region the plasma transitions to a neutral gas. These conditions of detached or semi-detached divertor plasma are desirable in order to spread the heat load on the wall area, but they are difficult to create and control. The principal objective of divertor physics for nuclear fusion is to develop strategies for stable plasma operation with low peak heat load on material boundaries and with good pumping efficiency for particle control.

Molecular processes and interaction of the plasma electrons and ions with molecules and molecular ions are critical features of the divertor plasma and the correct treatment of these atomic and molecular processes together with that of the plasma-wall interaction is the preeminent concern of edge and divertor plasma modelling. In the area of atomic and molecular (A+M) physics the principal difficulty in modelling the mixture of neutral and ionized species in the plasma boundary region is the need to take into account reactions involving electronically and rovibrationally excited states. The ability to calculate accurately the population balance of excited states is also essential for interpreting spectroscopic diagnostics of the edge plasma.

Simulation of near-wall plasma in fusion devices therefore requires cross-sections for collisional, photon-induced and radiative processes that are resolved with respect to excited state of the incoming and outgoing particles. The existing databases have gaps and quite large uncertainties in this area. Even for such a relatively simple process as dissociative recombination of hydrogen: $e^- + H_2^+ \rightarrow H + H$ there are difficulties; the incoming H_2^+ and the outgoing H + H may be in some excited state, and the cross-section for the collision depends strongly on the vibrational state of the H_2^+. The database is especially sparse for processes involving the molecular ions HeH^+ and He_2^+, which are of much recent interest due to the plans for an extensive helium campaign on ITER before its nuclear phase.

The presence of large regions of dense, low temperature plasma in the ITER divertor places much greater demands on atomic and molecular data than do existing experiments. In ITER neutral-neutral collisions will be important, giving rise to viscous effects in the neutral gas. For accurate simulation of the molecular reaction kinetics also ion-molecule collisions must be considered. Opacity and radiation transport must be explicitly included in the modelling as the mean free path for Lyman series radiation can be less than 1 cm.

The IAEA Atomic and Molecular Data Unit, part of the Nuclear Data Section, aims to support research into nuclear fusion through the provision of internationally recommended atomic, molecular, plasma-material interaction and material properties databases. The main mechanism available to the Unit to encourage the development of new data is that of the IAEA Coordinated Research Project (CRP). A CRP brings together research groups from around the world to work on a shared goal, such as the development of data for a well-defined class of atomic, molecular or plasma-material interaction processes.

Following advice from the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council at their meetings in April 2008 and April 2010 the IAEA initiated a CRP on "Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma". The purpose of this CRP is to evaluate existing data for atomic and molecular processes of hydrogen and helium that are relevant to fusion, generate new fundamental atomic and molecular data where this is needed, and assemble the information into a knowledge base and numerical

databases for use by the fusion community. The primary focus of the CRP is on processes under conditions prevalent in the near-wall plasma, but the improved database will also be of interest for the simulation of H and He neutral beam injection systems and of the interaction of the beam with the core plasma.

The CRP is expected to have three Research Coordination Meetings (RCM) over the course of about 4 years. The First RCM was held 10-12 August 2011 at IAEA Headquarters in Vienna. This report contains the proceedings of that meeting together with the assessment of research needs and a description of the workplan for the duration of the CRP. Participant summaries are also provided. Appendix 1 contains the list of participants and Appendix 2 contains the Meeting Agenda.

2. Presentations

D. Abriola, B. J. Braams: Opening

The meeting was opened by Dr D. Abriola on behalf of Dr R. A. Forrest, Head of the Nuclear Data Section. Dr Abriola noted the mission of the Nuclear Data Section to provide internationally recognized and validated databases in support of nuclear energy and applications including fusion energy. IAEA Coordinated Research Projects offer a unique opportunity for cooperative work to develop such databases. Dr Abriola stressed the importance of plasma-wall interaction for the viability of fusion energy production and the role of molecular processes in determining plasma behaviour near material boundaries. Atomic and molecular data have a key role in modelling and simulation of the near-wall plasma. Dr Abriola welcomed the participants to Vienna and wished for a productive meeting.

Participants then briefly introduced themselves. The agenda for the meeting was reviewed and adopted.

For the following talks presentation materials are available through the CRP web pages of the A+M Data Unit, http://www-amdis.iaea.org/CRP/. Participants' summaries are included later in this in this report. Therefore the talks are only briefly summarized here.

D. Reiter: Collisional-radiative and transport modelling for ITER

Dr Reiter of Forschungszentrum Jülich spoke about collisional-radiative and transport modelling for ITER. (Joint work with R. K. Janev and B. Kueppers.) The centre-piece of these activities at Jülich is the EIRENE code, which solves the Boltzmann transport equation in three-dimensional (3d) geometry by a Monte Carlo approach. EIRENE includes a collisional-radiative (CR) model for hydrogen, helium and hydrocarbons and it includes models for particle-surface interaction processes of sputtering, reflection, adsorption and desorption. The modelling for ITER includes treatment of vibrationally excited hydrogen and of radiative transport through the Lyman series. The principal source of the hydrogen and helium data for ITER modelling remains the 1986 book of R. K. Janev et al. [R. K. Janev, W. D. Langer, K. Evans, Jr. and D. E. Post, "Elementary Processes in Hydrogen - Helium Plasmas: Cross Sections and Reaction Rate Coefficients", Springer Verlag, 1986]. For other modelling with use of EIRENE databases are maintained and are accessible through the EIRENE home page [http://www.eirene.de/]. In particular the HydHel database concerns processes for hydrogen and helium and the AMJUEL database contains additional atomic and molecular data. There are also databases for the methane, ethane and propane families (including breakdown to atomization) and the silane family.

To support the A+M databases for EIRENE there is an online tool HydKin [http://www.hydkin.de]. HydKin can be used to construct a CR model condensation, perform spectral (timescale) and sensitivity analysis, perform fragmentation pathway analysis and evaluate reduced models. The model condensation that is done in HydKin leads to a system of differential-algebraic equations: instead of coupled Boltzmann equations for, say, N species one arrives at Boltzmann evolution equations for N-M

species coupled to an algebraic system of order M. This reduction is obtained without an a priori bundling of states.

P. Krstic: Vibrationally resolved ion-molecule collisions

Dr Krstic, Physics Division, Oak Ridge National Laboratory, spoke on vibrationally resolved ion-molecule collisions. In the divertor region of fusion devices at temperature down to 1 eV and density up to $1\times10^{15}/cm^3$ the dominant species are neutral H and H_2; other species include He and impurities. Atoms can be electronically excited and molecules may be ro-vibrationally as well as electronically excited. This greatly affects cross sections; for example the charge transfer cross section for H colliding with H^+ increases as n^4 with principal quantum number n. The processes of molecule-assisted recombination (MAR) and molecule-assisted dissociation (MAD) depends strongly on the population of vibrationally excited molecules. Some tests of the sensitivity of divertor plasma simulations to atomic data were presented in [D. P. Coster et al., AIP Conf. Proc. 1125 (2009) 112] and for the case of hydrocarbon data in [D. Reiter et al., Phys. Scr. T138 (2009) 014014]. The necessary data with consideration of electronic and ro-vibrational excitation, as well as isotope dependence, are difficult and in many cases impossible to obtain by experiment and high-quality theoretical data are sparse. This is true even for such a simple ion-molecule collision process as $H^+ + H_2$ that involves only 2 electrons and 3 nuclei; e.g., see [D. W. Savin et al., ApJ 607 (2004) L147].

K. Sawada: Revision of collisional-radiative models and neutral transport code for hydrogen and helium species

Dr Sawada described the ongoing development of collisional radiative (CR) models for hydrogen and helium in fusion plasma. This is joint work between K. Sawada at Shinshu University and M. Goto at National Institute for Fusion Studies (NIFS) and it has its roots in work by T. Fujimoto at Kyoto University. The models are applied to RF plasma as well as divertor plasma. Special issues addressed in the presentation are radiation trapping and inclusion of rotational excited states.

J.-S. Yoon: Evaluation of cross section for electron impact with hydrogen and their combination molecules in fusion plasma

Dr Yoon described the work in the Data Centre for Plasma Properties (DCPP) in the National Fusion Research Institute (NFRI) to produce evaluated and recommended data for industrial and fusion applications. The data evaluation is done in the context of and following procedures set by the National Standard Reference Data (SRD) project and the result may be Qualified or Validated or Certified (in order of increasing stature) Standard Reference Data. Terminology and methods of ISO-GUM (Guide to Uncertainty in Measurement) are carefully followed.

In this framework cross section data for electron collisions with hydrogen molecules are evaluated and recommended values are provided as far as possible. The HD and D2 molecules are considered along with H_2.

U. Fantz: Application and evaluation of state-resolved atomic and molecular data in population models for hydrogen, deuterium and helium

Density and temperature in the scrape-off layer and divertor plasma vary between approximately $10^{18}/m^3$ to $10^{21}/m^3$ and from below 1 eV to about 50 eV. The atomic and molecular data must be condensed into a collision radiative model including molecular species to support modelling and interpretation of diagnostics. The flexible code Yacora [D. Wünderlich et al.] is used to construct CR models for H and He including molecules.

In her presentation Dr Fantz provided a detailed description of the capabilities of the Yacora code and its application to hydrogen and helium in ionizing and recombining divertor plasma and in negative ion sources.

R. Celiberto: From elementary processes to modelling of molecular plasmas in thermonuclear fusion

In cold and partially molecular plasma one may have to deal with a non-Boltzmann vibrational distribution function of ground state molecules, a non-Boltzmann electronic state distribution function for atoms and molecules and possibly also a non-Maxwell electron energy distribution function. It means that one needs a Master equation approach to vibrational kinetics, electronic state kinetics and ionization and recombination processes, possibly coupled to a Boltzmann equation for the electron energy distribution function. This may all be incorporated into a particle-in-cell direct simulation Monte Carlo (PIC-DSMC) approach.

Dr Celiberto described the work at Bari to acquire the large set of cross section data required for PIC-DSMC modelling of low-temperature hydrogen plasma, with special attention to resonant electron-molecule collisions.

H.-K. Chung: Databases in the atomic and molecular data unit

Dr Chung provided an overview of the databases maintained by the IAEA atomic and molecular data unit and of the CRP mechanism by which data are developed. ALADDIN is the principal numerical database, covering atomic and molecular (A+M) and also particle-surface or plasma-material interaction processes. AMBDAS is a bibliographical database and since 2010 the Unit also is developing a broader wiki-style knowledge base. Coordinated Research Projects (CRP) are normally focussed on development and evaluation of data for a well-defined class of processes. Activities of the Data Centre Network (DCN) and the Code Centre Network (CCN) were briefly described as well.

X. Urbain: Electronic and atomic collisions with hydrogen and helium ions: State-specific study of associative, dissociative and reactive processes

Dr Urbain described the merged and crossed beam set-ups at UCL (Louvain) and their application for studies of ion-ion, ion-atom and electron-molecular ion collisions. It is possible to measure absolute cross sections for dissociative excitation and dissociative ionization, measure energy thresholds and kinetic energy release distributions and in some cases diagnose electronic and vibrational states contributing in the collisions. Collisions that have been studied or for which work is in progress include $HeH^+ + e^-$ (dissociative excitation and ionization) and $H^+ + H^-$, $H_2^+ + H^-$, $He^+ + H^-$ (mutual neutralization). In work at FLASH in Hamburg the XUV photo dissociation of HeH^+ was studied. Work is underway on state-to-state collision studies for $H^+ + H_2$ and isotopic variants. These and other studies provide fundamental data for collisional processes involving H, H^+, H^-, He, He^+, He^{2+}, He^-, H_2, H_2^+, H_3^+, HeH^+, He_2^+ and isotopic variants. Cross sections may be obtained for collisions with electrons and collisions among themselves and for photon-induced processes.

X. Ma: State-resolved cross section measurements in low and intermediate energy Ion-He/H2 Collisions

Dr Ma described research done using the Cooler Storage Ring (CSR) and the ReMiLa Reaction Microscope at the Heavy Ion Research Facility in Lanzhou. The systems to be studied are (1) $H^+ + He$ (E_p = 15 - 300 keV/u); (2) $He^{q+} + He$ (q=1, 2; E_p = 5.0 - 150 keV/u); (3) $C^{q+} + He/H_2$ (q=2, 3, 4, 5; E_p = 2 - 125 keV/u); (4) $Ar^{q+} + H_2$ (q=2, 3, 4, 5, 6; E_p = 0.7 - 45 keV/u). The experimental set-up and opportunities were described with special attention for collisions of He_2^+ on He and on H_2.

A. E. Orel: Theoretical studies of electron driven resonant processes in H_2^+ and HeH^+: Dissociative recombination, vibrational excitation and dissociative excitation

Dr Orel described calculations of electron-molecule collisions based on the Complex Kohn Variational Method for reactions leading to dissociative recombination, vibrational excitation and dissociative

excitation. Different approaches for the direct processes and for resonant (via electronic excited state) were presented. Sample calculations were shown for electron collisions with HeH^+, He_2^+ and H_3^+. Dr Orel also described calculations for mutual neutralization in collisions $H^+ + H^-$.

O. Motapon: Low energy reactive collisions of electrons with H_2^+ and isotopomers: Computations and comparison with measurements

Dr Motapon described the Multichannel Quantum Defect Theory and its application to calculations of cross sections for state-to-state transitions and dissociative recombination of H_2^+ and isotopic variants. Theory and calculations were presented for rotationally resolved transitions including resonance effects at low collision energy (below about 0.2 eV). These processes are relevant for ro-vibrational relaxation of the population of H_2^+ molecular ions.

Ch. Jungen: Dissociative recombination of molecular hydrogen and diatomic hydride ions: direct and indirect processes

Dr Jungen described Multichannel Quantum Defect Theory and its application to calculations of spectroscopy and dynamics of highly excited (Rydberg) and super-excited H_2 including the competition between dissociation, ionization and fluorescence. Experiments have been done using the Bessy II synchrotron radiation source in Berlin. For small or moderate internuclear distance all electronic excited states in H_2 are effectively Rydberg states; they are important as resonances in dynamical processes and can be described using scattering theory.

V. Kokoouline: Inelastic processes in collisions between the H_3^+ ion and an electron: Rotationally and vibrationally resolved cross-sections for dissociative recombination and (de)excitation of H_3^+

Dr Kokoouline described comprehensive cross section calculations for electron collisions with H_3^+ including vibrational, rotational, electronic and nuclear spin degrees of freedom and Jahn-Teller coupling. Hyperspherical coordinates are used and the scattering matrix is obtained using quantum defect theory. State-to-state and state averaged cross-sections for dissociative recombination, rotational, and vibrational excitation have been determined.

3. Discussion on data status and data needs

General remarks

This section of the meeting report is intended to provide an overview of hydrogen-helium species and processes that are of interest in fusion experiments and to provide pointers to available data. The description is informal and it is missing authoritative citations; more detailed information should be assembled in a subsequent report.

In this section "H" or "hydrogen" means H, D, T unless it is made clear that it means specifically the ^1H isotope. He normally means ^4He; the isotope ^3He is only of peripheral interest in fusion research. (It is formed in the $D + D \rightarrow {}^3He + n$ fusion reaction and one may want to diagnose its presence.)

Note on CR models for H and He

Existing CR data sets need to be upgraded to provide isotopically correct and consistent data for H, D, T, and that is a task within this CRP. Note the big difference between HD on one hand and HH or DD on the other (or DT vs DD/TT) in the rate of radiative decay to the ground state. For the case of electron-molecule collisions where data are available only for ^1H molecules one may extrapolate to other isotopes by matching vibrational energy (and not vibrational quantum number).

The existing CR databases are separate for H and for He. It would be a major effort and a major step to integrate the two and provide "off-diagonal blocks" in the matrix.

In order to construct the transition matrix that underlies the CR model one wants to rely on detailed balance. What if the underlying states are themselves condensed states? There are cases in the EIRENE database where detailed balance is violated. Example: non-resolved rotational excitations.

Electrons and protons, e^- and H^+

These are the primary plasma constituents; always important and normally present in similar number density. However, for atomic (ionic) excitation and ionization in hot plasma collisions with e^- are much more important than collisions with H^+ due to the higher collision frequency.

Atomic and molecular hydrogen, H and H_2

In present experiments H and H_2 are formed on walls; H_2 quickly dissociates but H is important throughout the divertor and edge plasma. In ITER one expects a large region of recombining plasma with transition to neutral gas, so H_2 is very important for divertor plasma behavior there. (Alcator C-Mod would come closest among existing experiments.)

Electronic excited H

H(n) is the first constituent in any collision radiative model of hydrogen excitation and ionization in divertor plasma. Key processes are formation of H(n) by dissociation of H_2 and H_2^+; collisions of H(n) with e^-, H^+ and with any other charged plasma constituents (H_2^+, H_3^+, He^+, He^{2+}, impurities).

In most cases only the principal quantum number, n, is of interest, but the orbital and magnetic quantum numbers are of interest for processes of the diagnostic neutral beam, and even for accurate calculation of absorption of the heating beam. (O. Marchuk, Yu. Ralchenko, …)

Vibrationally excited H_2

$H_2(v)$ is of interest whenever H_2 is of interest; if H_2 is present then it is likely to be vibrationally excited. Key processes to determine the population: excitation and de-excitation by collisions with H^+, with e^-, and with other H_2; dissociation of H_3^+ (as a reaction intermediary). Collisions with He^+, He^{2+} are also of interest and the importance of vibrational excitation of H_2^+ in those collisions needs to be checked. For collisions with H^+ there is the important resonant process $H_2(v=3,4) + H^+ \rightarrow H_2^+ + H$.

Data status: Full 15*15 matrix is included in Sawada model and it is agreed that it is important to consider about that many vibrational levels explicitly. Calculated data only for v=0, v=1, v=2, then scaling. We should upgrade to proper consistent calculated data for all v→v' transitions; these calculations are feasible (Orel for e-impact? Krstic for H^+ impact?). Many data are already available; they need to be incorporated into the CR models. Issue of re-assembly of the database that underlies the CR model.

We need to inventorize data for the (e,2e) process, $e^- + H_2 \rightarrow H_2^+ + 2e^-$, including resolution of the vibrational excitation of the H_2^+; and also $e^- + H_2 \rightarrow H + H^+ + 2e^-$. We also need to inventorize data for excitation into the triplet state of H_2, vibrationally resolved.

Rotationally excited H_2

On the one hand, should be important; if H_2 is present then it is likely to be rotationally excited. On the other hand, one usually tries to capture the effects of rotation in some relatively simple approximations. The most important processes that determine the population are collisions with H^+, with e^-, and with other H_2 and dissociation of H_3^+.

Why do we tend to ignore effects of rotation, or capture the effect in some simple way? A pragmatic reason to neglect the effect in the database is that it is a huge effort to include it in; in practice one just assumes some rotational temperature and one copies the cross sections from j=0.

A justification for ignoring it would be that it exists in a relatively narrow band (thermal, not high temperature). But if the rotational temperature is high then it is should not be ignored. For some processes rotation can in practice be ignored; just use a frozen sudden impact approximation (e.g., electron impact). On the other hand, particle exchange greatly influences rotation. Rotational excitation is important for H^- production.

Electronic excited H_2

Primarily important for diagnostic purposes. Emission from decay of electronic excited state is the only way to measure H_2; therefore one needs a quantitative model. Note that the electronic excited state is expected to be vibrationally (and rotationally) excited. Ground state is S_0; excited states S_1 and T_0, but we really need the singlet and triplet systems up to n=3 including vibration.

Most important processes that determine the population: Collisions of H_2(vib) with H^+ and with e^-. Dissociation of H_3^+? All this data needs to be benchmarked; we have multiple datasets and really need to establish recommendations.

Coupling singlet-triplet is said to be not important. We need to check on the coupling of electronic excited H_2 to H(n); they would be connected via dissociation.

Molecular cation H_2^+

This species is short-lived; if the plasma is hot enough to form H_2^+ from H_2 then it is hot enough that the H_2^+ will quickly dissociate. So, H_2^+ is primarily important as an intermediary for complete breakup and ionization of H_2. Key processes are formation by H_2 + (e^-,H^+); collisions with (e^-, H^+, H, H_2).

Excited H_2^+

Vibrational and rotational excitations are relevant in the same situation as for H_2; and in practice one seeks to ignore issues of rotational excitation. The electronic excited state is not of fusion interest.

We need to clarify the connection between vibrationally excited H_2^+ and electronic excited H (both formation and dissociation of H_2^+). This is a key issue for MAR and is important in linear plasma devices. Resonance effects are very important here; therefore isotope effects will be important.

Negative ion H^-

Neutral beams are employed to heat the plasma. In order to create a high-energy (200 keV – 1 MeV) neutral beam one must start with negative ions, H^-, because the positive ions cannot be neutralized efficiently enough. Therefore, processes involving H^- at MeV collision energy are relevant for fusion development. Note that the heating beam on ITER will be D, not T.

Besides the neutral beam interest, H^- is diagnosed on linear plasma devices and so data are of interest to support diagnostics. We don't know very well what role H^- has in tokamak divertor plasma.

The process $H^- + H \rightarrow H_2(v)+e^-$ or $H+H+e^-$ needs much attention; it is an important process to remove H^-. There are measurements by D. Savin with X. Urbain. These measurements serve as benchmark for calculations of Cizek on $H + H^-$ and on $e^- + H_2$ (including vibrationally excited H_2).

The key production processes in edge plasma are electron attachment to vibrationally (and rotationally) excited H_2. Surface processes are important, but they are not part of this CRP. Destruction takes place by mutual neutralization with H^+, H_2^+, H_3^+, He^+, He^{2+}.

There is also interest in $H^- + H_2$ at very high energy (1 MeV), all reaction channels, as a process in the negative ion-based neutral beam injector.

Electronic excited H^-

Not of interest.

Negative molecular ion H_2^-

Of interest as a reaction intermediary. H_2^- lives for μs, D_2^- lives for ms, T_2^- close to 1s. These are very minor species.

Protonated molecular hydrogen H_3^+

The trihydrogen cation H_3^+ (protonated H_2) is very important in interstellar medium, but in fusion edge plasma it is mainly of interest as a reaction intermediary. It needs to be formed from H_2^+, which is itself rare in fusion plasma, and it quickly dissociates at temperatures where H_2^+ might exist. It can be measured on linear machines through the absorption spectrum. Therefore its chemistry is of interest to us for interpretation of laboratory experiments. In low temperature plasma H_3^+ is of special interest because H_2 can be destroyed through H_3^+ at lower energies than via electron impact.

Key processes to determine the population of H_3^+: Formation by $H_2 + H_2^+$ or (as an unstable intermediary) $H + H_2^+$, $H^+ + H_2$. The H_3^+ will normally be created vibrationally and rotationally excited and the molecular state influences all further cross sections. Collisions with e^- and H^+ are the most important processes that affect the excited state population.

Important collision processes: $e^-+H_3^+$, $H^++H_3^+$, $H+H_3^+$, $H^-+H_3^+$; maybe also collisions with He, H_2 and with H_2^+. Collision with H^- is of interest for negative ion beam production. Data are available for these processes with H_3^+ in the ground state. One needs data for electronic and molecular excited states and then data resolved for excitation of the reaction products; e.g. collisions $e^- + H_3^+$ producing vibrationally and rotationally excited H_2. Also the present calculated data do not describe higher energy channels leading to $H_2 + H^+$ or to $H_2^+ + H$, and more attention is needed for the exit channel $H_2 + H^*$.

The present data are not isotopically resolved and this is important for fusion applications.

General question: how to describe the vibrational and rotational state for database purposes? Use vibrational energy, rotational energy?

Electronic excited H_3^+

Important for the breakup process. Need to consider S_0, S_1, T_0; states may be asymptotic to $H_2 + H^+$ or to $H_2^+ + H$. Higher electronic excited states for formation of H(n), etc.

Helium and its ions and molecular ions

Helium is produced in fusion reactions and the expected concentration n_{He}/n_e is about 0.05 in ITER D-T plasma. However, operation of ITER will commence with a non-nuclear phase of two years or longer during which the primary plasma constituents will be ^1H (protonium) and He in any mixture ratio including that of pure He. The objective of this phase is to study full-power operation of the edge and divertor plasma without activating the vacuum vessel. On present experiments helium may be injected as a minority species for divertor pumping studies or for other studies and it is also sometimes used as the main plasma constituent. In addition helium may be used in a diagnostic neutral

beam. These various situations explain the interest of helium in fusion plasma. Atomic and molecular data are needed for processes that involve helium in the low-temperature divertor plasma, processes that involve an energetic helium neutral beam interacting with plasma, processes in the source or neutralization region of a helium neutral beam, and processes that involve a hydrogen neutral beam interacting with helium in the plasma.

For modelling helium in divertor plasma it is always necessary to consider excited and metastable He and excited He^+. (Metastable helium normally means the ground state triplet configuration, 1s2s $^3S_1$, also denoted He(2^3S_1) or He^*, which has a lifetime of ~8000 s. However, the 1s2s $^1S_0$ configuration, He(2^1S_0), is also long-lived, with a lifetime of ~20 ms.) Collision processes involving these species are the core of a CR model. For the case of a hydrogen-helium plasma with neglect of molecules the key processes to determine the population and develop the CR model are collisions involving e, H, H^+, He, He^+ and He^{2+} including excited states, radiative decay of excited states and, in some regimes and for a limited set of states, also photon-induced processes.

The principal database for electron impact processes involving ground state and excited He is due to Ralchenko, Janev, Kato, Fursa, Bray and de Heer [ADNDT 94 (2008) 603–622]. The collision process $e+H^*$ would be a good candidate for benchmark calculations.

Helium may also be used in a diagnostic neutral beam, especially for study of fast alpha particles produced in fusion (initial energy 3.5 MeV). For that application the neutralization (charge transfer) process $He^+ + He \rightarrow He + He^+$ and the double charge transfer $He^{2+} + He \rightarrow He + He^{2+}$ at MeV collision energy are important. One needs to know absolute cross sections including the branching between the ground state and the metastable states He(2^3S_1) and He(2^1S_0) in the outgoing He^0 channel.

Processes involving the helium anion He^- are important for producing a high energy (100 keV – 1 MeV) helium neutral beam for plasma diagnostics. The anion may be produced by collisions He^* + (Li,Na,K,Rb,Cs). It autoneutralizes, but also charge transfer collisions $He^- + He \rightarrow He + He^-$ are of interest. (Probably also $He^- + He \rightarrow He + He + e^-$.) Several states of the anion can be relevant and the branching between ground state and long-lived excited states in the He^0 neutralization product is also important. (For beam penetration one wants to maximize the production of ground state He^0.)

Molecules HeH^+ and He_2^+ may be formed in the divertor region and comprehensive data for processes of these molecules are required in preparation for the initial non-nuclear phase of ITER. The most important processes for formation of HeH^+ are collisions involving vibrationally excited H_2^+ or metastable He: collisions $H_2^+(v>3)$ + He and H_2 + He(2^3S_1). A somewhat exotic process to form HeH^+ is in the collision $He^+ + H^-$. (It may serve as a benchmark.) He_2^+ may be formed in collisions He + He(n>3) (measurements in Saclay) or $He^* + He^*$. In a hydrogen-helium plasma He_2^+ can also be formed via collisions $He + HeH^+$.

Measurements of $e + HeH^+ \rightarrow (e^- + He + H^+$ and $e^- + He^+ + H)$ are being carried out (P. Defrance, unpublished); calculations were done by A. Larson and A. Orel and are being revisited. The dissociative neutralization channel $e^- + HeH^+ \rightarrow H + He$ has been measured by A. Wolf et al. Excited states of the product are produced preferentially. We need to assemble information about the process $e^- + He_2^+$.

In order to produce a high-energy helium neutral beam the favoured process appears to use the negative ion, He^-. However, it is also conceivable to use a beam of HeH^+ (or even He_2^+). What are the processes by which such a beam might be neutralized in an injector box? See [Sakakita et al., JPFR-S 8 (2009)].

Presentation of data

There are some things on which all are in agreement and yet they need to be emphasized. The basic data are cross sections, not rate coefficients. Modellers can average over a Maxwellian if needed; they cannot invert the averaging process. If fit functions are used then they must be of a form that scales

correctly to the extremes of the energy range. (The choice between fit functions and tabular representation is not clear-cut in general.)

Opportunities for benchmark experiments

Following the discussion on data needs participants considered what may serve as benchmark experiments. In the case of molecular data these would probably involve molecular ions, because it is so difficult to prepare a neutral molecule in a well-defined ro-vibrational state. Collisions $e^- + H_2^+$ at very low energy (A. Wolff, unpublished?) could be a good benchmark. Perhaps also $H^- + H_2^+$ if it is possible to characterize the final state of the H or H_2. Even more elementary, the collision process $H^- + He^+$.

4. Workplan

D. Reiter

CR model development for H / H_2 / H_2^+ system and for He system; especially work towards isotopically correct model and investigate the need to combine the H and He CR models into one. The coupling would be through processes involving HeH^+; maybe other couplings too.

Integration of the CR model into HydKin for public exposure. Once CR submatrices are complete (including forward-reverse process, detailed balancing..), carry out sensitivity analysis.

P. Krstic

It is planned to include all isotopic combinations (H, D, T) in an expanded range of energies (also energies below 0.5 eV or above 10 eV), using the fully quantum-mechanical treatment for reactions (1-8, below), with explicit inclusion of the nuclear exchange. This will be achieved by taking into account a large basis of rotational transitions.

1) $H^+ + H_2(v_i) \leftrightarrow H^+ + H_2(v_f)$, $v_{i,f}$ = 0-14

2) $H^+ + H_2(v_i) \leftrightarrow H(1s) + H_2^+(v_f)$, v_i = 0-14, v_f = 0-19

3) $H^+ + H_2(v_i) \leftrightarrow H^+ + H + H$, v_i = 0-14

4) $H + H_2^+(v_i) \leftrightarrow H + H_2^+(v_f)$, $v_{i,f}$ = 0-19

5) $H + H_2^+(v_i) \leftrightarrow H^+ + H_2(v_f)$, v_i = 0-19, v_f = 0-14

6) $H + H_2^+(v_i) \leftrightarrow H + H^+ + H$, v_i = 0-19

7) $H^+ + H + H \leftrightarrow H^+ + H_2(v_f)$, v_f = 0-14

8) $H^+ + H + H \leftrightarrow H + H_2^+(v_f)$, v_f = 0-19

K. Sawada

CR model development for H / H_2 / H_2^+ system and for He system with Dr. Fantz.

J.-S. Yoon

Evaluation and compilation of cross section data from literature, leading finally to full data sets for CR model in collaboration with U. Fantz and with K. Sawada.

Evaluation of experimental data in collaboration with the Asia-Pacific Atomic data Network (A-PAN) members Y. Itikawa, T. Kato, H. Tanaka, S. J. Buckman, M. J. Brunger, H. Choi, V. P. Shevelko and others. For evaluation of theoretical data we will need more help from theoreticians inside the CRP.

Finally we will categorize data as Recommended data, Compiled (or Collected) data and Unknown data. Transfer data to U. Fantz (or others) in order to check with experiment.

U. Fantz

Identification of relevant processes in recombining and ionizing divertor plasmas.

Continuation of CR model activities on H_2, H and He. Comparison with experiments.

Comparison with Sawada's model → identify differences and gaps in the data.

Try to make a model with D_2 → Celiberto data???

R. Celiberto

Cross sections for electron collisions with H_2.

Calculate cross sections (needed by plasma modelers) for state-resolved transitions involving excited electronic states. The following are already available.

Optically allowed triplet-triplet e-H_2 electronic transitions, vibrationally resolved, are available for these processes (impact-parameter method):

$a\ ^3\Sigma_g^+ \rightarrow d\ ^3\Pi_u$

$c\ ^3\Pi_u \rightarrow h\ ^3\Sigma_g^+$

$c\ ^3\Pi_u \rightarrow g\ ^3\Sigma_g^+$

[A. Laricchiuta, R. Celiberto and R. K. Janev, Phys Rev. A 69, 022706 (2004)].

Optically forbidden singlet-triplet e-H_2 electronic transitions are available for these processes (Born-Rudge approximation):

$X\ ^1\Sigma_g^+ \rightarrow d\ ^3\Pi_u$ (for vi = 0, 1, 2, 3)

$X\ ^1\Sigma_g^+ \rightarrow a\ ^3\Sigma_g^+$ (to be checked)

[Capitelli et al, J. Phys. B: At. Mol. Opt. Phys. 43, 144025 (2010)].

Possible collaborative work on electron collisions with He_2^+ (see also Ann Orel's work plan).

X. Urbain

1) Mutual neutralization $H^+ + H^-$, total and partial cross section, isotope effect (H+D, D+D).

2) Mutual neutralization $He^+ + H^-$, idem.

3) Proton impact ionization of H_2(v=0) between 10 eV and 1000 eV: total cross section, H_2^+(v) distribution, isotope effect.

4) Dissociative excitation and ionization $HeH^+ + e^-$: branching $He + H^+$, $He^+ + H$, KER distributions, isotope effect.

5) Electron impact ionization of H_2(v=0): H_2^+ vibrational distribution from threshold, isotope effect.

X.-W. Ma

1) Measure the state-distribution of H neutralization at keV energies.

2) Measure the branching and partial cross sections in H and H2/He collisions at keV energies.

3) Measure the total and differential charge exchange cross sections between heavy ions and H_2/He at keV energies.

A. Orel

1) Resonant vibrational and dissociative excitation in HeH+. Study effects of target vibrational excitation, study effects of isotopic substitution, calculate final state distributions (including ion-pair).

2) Resonant dissociative recombination in HeH+. Study effects of target vibrational excitation, study effects of isotopic substitution, calculate final state distributions (including ion-pair).

3) Direct dissociative excitation; same issues as above.

4) Resonant dissociative recombination, vibrational and dissociative excitation in H_2^+ (at energies above 0.2 eV); same issues as above.

5) Mutual Neutralization in $He^+ + H^-$ collisions.

6) Possible collaborative work on He_2^+.

O. Motapon

Planned work:

1. Improvement of the input data relevant for high energy DR/DE computations of H_2^+, using the computations of Jungen, Telmini, Argoubi on resonant states and their autoionization widths.

2. Perform systematic DR/DE and vibrational excitations computations of cross sections for H_2^+ and isotopomers in the energy range that is relevant for fusion modelling needs.

3. Perform rate coefficients computations. Check scaling rules.

4. Collaborative work with A. E. Orel on the low energy DR of He_2^+.

C. Jungen

Planning benchmark calculations on electronically excited H_2, combining spectroscopy with decay processes and considering all symmetries (singlet/triplet and gerade/ungerade) and all degrees of freedom (electronic, vibrational and rotational). This will involve two-electron R-matrix calculations combined with Multichannel Quantum Defect theory. This effort should lead to results concerning some of the processes discussed in this meeting:

1. $H + H(nl) \rightarrow H + H(nl') \ (n>1)$
2. $H + H(nl) \rightarrow H_2^+(v) + e^-$
3. $H^+ + H^- \rightarrow H(n) + H$
4. $H^+ + H^- \rightarrow H_2^+(v) + e^-$
5. $H_2^+(v) + e^- \rightarrow H + H(n)$
6. $H_2^+(v) + e^- \rightarrow H^+ + H^-$

It is hoped, in particular, that the theoretical treatment of last two processes(5 and 6, DR), will lead to benchmark results of a new level of quality, to be compared, hopefully, with DR experiments in which the initial distribution of vibration/rotation levels is better characterized than now. The issue here is the appearance and assignment of resonances in the cross section which has not been explained quite satisfactorily in the DR cross sections of any molecular ion. The exception is DR of H_2^+ where the best results today are those of Motapon, Schneider et al. in comparison with the Heidelberg TSR results (Wolf and collaborators), but where again further improvement is desirable. Process 4 relates to the interesting subject of `heavy' Rydberg states.

V. Kokoouline

Collect and/or produce data on processes for electron interactions with H_3^+:

- Cross sections and rate coefficients for the dissociative recombination of H_3^+ being in the ground or in an excited vibrational state.
- Branching ratios for the final products in dissociative recombination of H_3^+
- Cross-sections for vibrational (de-)excitation of H_3^+ by an electron impact

Collect and evaluate data (experiment and theory) on the formation of H_3^+ at energies relevant to the divertor region: Reactions: $H_2^+ + H_2 \rightarrow H_3^+ + H$.

Calculate rate coefficients for the three-body recombination of hydrogen: $H+H+H \rightarrow H_2+H$.

Recommendations and Conclusions

Participants reaffirm the objective of this CRP to obtain isotopically complete and state-resolved recommended data for relevant processes of hydrogen and helium in fusion edge plasma. Specific data needs were discussed and are summarized. Broadly one may highlight the need for consideration of simultaneous electronic and vibrational excitation, consideration of isotope effects for molecular processes at low energy especially where resonances are involved, treatment of rotational degrees of freedom in molecules and treatment of non-adiabatic behaviour of excited states.

Appendix 1: List of Participants

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Appendix 2: Agenda

Wednesday, 10 August — Meeting Room: A07-42

09:20 – 09:50 D. Abriola, B. Braams: Opening, introductions, adoption of the agenda

Session I. Chair: U. Fantz

09:50 – 10:25 D. Reiter: Hydrogen and helium collisional radiative modeling with ITER divertor code B2-EIRENE, assessment and possible revision of database

10:25 – 11:00 P. Krstic: Overview of the H-He collisional processes and data. Vibrationally resolved ion-molecule collisions

11:00 – 11:20 *Coffee break*

11:20 – 11:55 K. Sawada: Revision of collisional-radiative models and neutral-transport code for hydrogen and helium species

11:55 – 12:30 J.-S. Yoon: Evaluation of cross section for electron impact with hydrogen and their combination molecules in fusion plasma

12:30 – 14:00 *Lunch*

Session II. Chair: P. Krstic

14:00 – 14:35 U. Fantz: Application and evaluation of state-resolved atomic and molecular data in population models for hydrogen, deuterium and helium

14:35 – 15:10 R. Celiberto: From elementary processes to modeling of molecular plasmas in thermonuclear fusion

15:10 – 15:30 *Coffee break*

15:30 – 15:50 H.-K. Chung: Databases in the Atomic and Molecular Data Unit

15:50 – 17:20 All: Review and discussion of database status and needs

19:30 – *Social dinner (outside VIC)*

Thursday, 11 August — Meeting Room: A07-42

Session III. Chair: V. Kokoouline

09:00 – 09:35 X. Urbain: Electronic and atomic collisions with hydrogen and helium Ions: state-specific study of associative, dissociative and reactive processes

09:35 – 10:10 X. Ma: State-resolved cross section measurements in low and intermediate energy ion-He/H_2 collisions

10:10 – 10:40 All: Review and discussion of experiments

10:40 – 11:00 *Coffee break*

11:00 – 11:35 A. Orel: Theoretical studies of electron driven resonant processes in H^{2+} and HeH^{+}: Dissociative Recombination, Vibrational Excitation and Dissociative Excitation

11:35 – 12:10 O. Motapon: Low energy reactive collisions of electrons with H^{2+} and isotopomers: computations and comparison with measurements

12:10 – 13:40 *Lunch*

Session IV. Chair: X. Urbain

13:40 – 14:15 C. Jungen: Dissociative recombination of molecular hydrogen and diatomic hydride ions: direct and indirect processes

14:15 – 14:50 V. Kokoouline: Inelastic processes in collisions between the H_3^+ ion and an electron: Rotationally and vibrationally resolved cross-sections for dissociative recombination and (de)excitation of H_3^+

14:50 – 15:10 *Coffee break*

15:10 – 17:00 All: Review and discussion of needs from theory and computation

Friday, 12 August Meeting Room: A07-42

Session V. Chair: D. Reiter

09:00 – 10:30 Breakout into 3 groups: Prepare overviews of status and needs for database, experiment and theory

10:30 – 12:00 All: Review status and needs

12:00 – 13:30 *Lunch*

Session VI. Chair: B. Braams

13:30 – 15:00 All: Development of Work Plan

15:00 – 16:00 All: Sketch of Meeting Report; Wrap Up

16:00 – *Close of Meeting*

Appendix 3: Summaries by Participants

Collisional-radiative and transport modelling of hydrogen and helium for ITER

D. Reiter, R. K. Janev, B. Küppers

Forschungszentrum Jülich, IEK-4, Germany

The current ITER computational engineering activities for edge plasma and plasma surface interaction (divertor) issues are carried out with the B2-EIRENE code, version SOLPS 4.3. Atomic and molecular data are brought into this integrated edge plasma tool mostly via the kinetic (Monte Carlo) Boltzmann solver EIRENE. The relevance of precise and comprehensive hydrogenic A&M processes within this computational model is obvious, as only those processes and their associated friction, plasma cooling effects etc. provide access to the favourable "detached divertor" regime, on which the planned ITER operation is based. This regime is characterized by a (hydrogen-) chemical complexity not otherwise encountered in fusion plasmas. Helium is the ash of the fusion process and without control of its concentration the fusion flame in ITER would be choked by its own ash within 100 seconds, well short of the planned 600 – 1000 seconds of plasma operation per discharge.

Edge and divertor plasma modelling for ITER falls already into the category of "computational engineering", whereas all other applications of edge transport modelling codes today, e.g. to the ASDEX-Upgrade and JET tokamaks (2D) or the LHD and W7X stellarators (3D), etc. are largely "computational science" activities still. This necessarily leads to particular consequences also for atomic and molecular databases within the B2-EIRENE code package. Computational parameter scans in the multi-dimensional parameter space of the ITER divertor are extremely slow and expensive, both with respect to human and to computational resources. One single data point (i.e. one single run with B2-EIRENE on a particular set of ITER input parameters) takes about 3 months on current computers. (This figure is a constant since about 15 years: the increasing complexity of the physical model compensates rapid speedup and availability of CPUs.)

Exchanges of code modules or of A&M databases are only carried out if either missing physics has been clearly identified or if significant improvement of the data quality is to be expected. The A&M databases of the EIRENE code are upgraded continuously and these updates are activated in many applications in Europe, mainly JET, TEXTOR, ASDEX-Upgrade, Tore Supra, etc., but they are activated in the ITER engineering activities only if the additional benefits over the old model are obvious, for reasons of above mentioned ITER code database management and necessity of backward compatibility in the computational design process. The B2 part (and atomic data in it) is about 15 years old, despite more recent heavy development (e.g., B2 to B2.5, fully developed ADAS interfaces for impurity flow, etc.); the EIRENE part, and related A&M databases used by ITER, are more recent.

Hydrogen databases, as activated in typical ITER (and DEMO) applications are based on the work of Sawada and Fujimoto [1], with a few refinements and extensions in particular with respect to vibrational resolution and MAR and MAD processes (status: 2004).

The **collisional radiative model of helium** used in ITER applications is that of Ref. [2], supplemented with electron cooling rates and with all effective rate coefficients fitted to the same format as in [3], see www.eirene.de, A&M data, AMJUEL.

More recent upgrades of A&M data aspects in ITER modelling were driven by clearly identified gaps in the model (e.g. elastic collisions between Be or C neutrals and protons, an upgrade carried out 2010 by incorporating the related ORNL data), or Lyman opacity data (Einstein coefficients and line shapes for absorption and emission processes, added in 2007).

There are many more recent "minor" upgrades of hydrogen (H, H_2, …) CR databases, such as those compiled by Janev and Reiter (FZJ), Wünderlich and Fantz (IPP Garching) or Sawada (Shinshu University), or of He CR databases (e.g. M. Goto, NIFS). These would quite likely only lead to a revision of the current ITER edge computational tools if significant modifications and improvements of predictive quality of results (in terms of significant changes in the cumulated effects within the H/H_2 or He model through the resulting effective condensed rate coefficients) would be proven. This is despite

the fact that those upgrades are directly useful for most fusion applications to existing experiments which employ the EIRENE code.

Consequences for the current CRP, planned work at FZJ

Some of the inertia to bring new A&M CR data into current edge modelling codes is the inconvenience to update CR data. Exchanging a single process cross section by a better one in a code is trivial. But in an integrated edge code the entire large set of all affected CR model effective "condensed" data, such as multiple (in case of metastables) reaction rates, cooling rates, momentum transfer rates, all change simultaneously with the change of the single cross section (one out of possibly thousands to be improved gradually). This situation is distinct for data for individual processes, which can be implemented or upgraded on a more continuous basis. FZJ plans to use its HYDKIN (www.hydkin.de) online database analysis tool (sensitivity analysis and condensation) and the existing automated EIRENE interface to it, which is currently in place for the hydrocarbon catabolism database, now also for H/H_2 and He CR models. This will avoid the issue with multidimensional fits (in case of effective CR data for H/H_2, which depend on at least 5 independent parameters. It will also allow systematic (algebraic, rather than trial and error) direct sensitivity analysis. (See [4], and note that a CR system with N reactions and M species has N*M sensitivity parameters and, e.g., N = 10000 and M = 100 for the $H/H_2/H_2^+$ system.)

Significant incremental steps of H and He CR models, which might potentially lead to rapid direct impact on ITER and DEMO computational design work and result in visibility of the IAEA data unit activity, might be a proper (physically more sound) treatment of **isotope effects in $H/H_2/H_2^+$ CR models**, or the revision of He CR models to allow coupling to the H/H_2 system (e.g. via HeH^+ processes) or to **helium resonance line opacity effects**.

References

[1] K. Sawada, T. Fujimoto, J. Appl. Phys. 78 (5), 1 September 1995.
[2] T. Fujimoto, Quant. Spectosc. Radiat. Transfer Vol. 21, pp. 433-455 (1997).
[3] R. K. Janev et al., "Elementary Processes in Hydrogen and Helium Plasmas", Springer 1987.
[4] D. Reiter et al., Phys. Scripta T138 (2009) 014014.

Vibrationally resolved ion-molecule collisions

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Typical for the divertor region is formation of the molecules, particularly vibrationally-rotationally excited H_2 and H_2^+. Huge increase of the cross sections (as n^4 for charge transfer) necessitates consideration of electronically excited atomic and molecular states. Vibrationally resolved collisions are crucial for volume plasma recombination schemes MAR and MAD with hydrogen and hydrocarbons, but also for infrared emission plasma diagnostic and for collisional-radiative (CR) models of $H_2/D_2/T_2$ plasma. High rotational temperatures of hydrogen molecules are indicated in divertor plasma, leading to the need to include all vibrational (and possibly rotational) states of the hydrogen molecule and molecular ion. The needs for cross sections in divertor plasma modelling are further analyzed in ref. [1].

Two main issues arise in the plasma modelling of the divertor plasma. These are (1) the sensitivity of the plasma modelling to the particular atomic and molecular processes and (2) need for self-consistent database of the blocs of processes (and the whole database matrix) in the integral CR modelling. Needless to say, high importance of the self-consistent processes derived at the "same footing" arises also from the unitarity requirements of the mutually competing processes. Investing large effort to satisfy these requirements we have derived full unitary database of the reacting $H^+ + H_2(v)$ and $H + H_2^+(v)$ systems, leading to the set of cross sections resolved with respect to initial and final vibrational state for collisionally induced excitation, charge transfer, dissociation and association processes on the two lowest adiabatic electronic surfaces of the H_3^+ quasimolecular system [2-6]. This unitary set of data was obtained by state-of-the-art fully quantum-mechanical technique, in the huge set of vibrational states (including dissociative continuum, which was here discretized in a large box).

The only approximation used was the Infinite Order Sudden Approximation for rotation, effectively freezing diatomic rotations during the collisional reactions, leading to the calculation for various diatomic angles and performing the angle ensemble average at the level of the cross sections. IOSA limits the range of center-of-mass collision energies to about 0.5 eV from below, while requirement of accuracy and proximity of the excited electronic states of H_3^+, with chosen density of the dissociative continuum, limits the applicability of the obtained set from above to about 10 eV.

A narrower set of reactions, was also considered by Ichihara et al. [7] using classical approach to nuclear motion of both projectile and the diatomic target, which was restricted to $H_2(v)$ (no hydrogen molecular ion). Comparison shows that this set has satisfactory accuracy only for higher initial vibrational states, in agreement with Bohr's principle of correspondence.

The considered reactions are

1) $H^+ + H_2(v_i) \leftrightarrow H^+ + H_2(v_f)$, $v_{i,f}$ = 0-14

2) $H^+ + H_2(v_i) \leftrightarrow H(1s) + H_2^+(v_f)$, v_i = 0-14, v_f = 0-19

3) $H^+ + H_2(v_i) \leftrightarrow H^+ + H + H$, v_i = 0-14

4) $H + H_2^+(v_i) \leftrightarrow H + H_2^+(v_f)$, $v_{i,f}$ = 0-19

5) $H + H_2^+(v_i) \leftrightarrow H^+ + H_2(v_f)$, v_i = 0-19, v_f = 0-14

6) $H + H_2^+(v_i) \leftrightarrow H + H^+ + H$, v_i = 0-19

7) $H^+ + H + H \leftrightarrow H^+ + H_2(v_f)$, v_f = 0-14

8) $H^+ + H + H \leftrightarrow H + H_2^+(v_f)$, v_f = 0-19

Note that reactions 1) and 4) also contain vibrationally elastic cross sections, when $v_i = v_f$ [4]. Reactions 1-3 are on the $H_2(v)$ target, 4-6 are with $H_2^+(v)$ target and 7-8 are associative 3 body reactions leading to creation of the diatomic molecules and molecular ions. Modification of this approach (with classical motion of the impact particle) was used to expand the upper limit of applicability of the set to about 100 eV [8]. All these data are available at ORNL-CFADC web site (www-cfadc.phy.ornl.gov) as well as in ALADDIN, in both row-tabular and graphical forms.

Although nuclear exchange is included in our calculations it is not separated from charge transfer processes. In the following period we will include all isotopic combinations (H, D, T), in expanded range of energies (below 0.5 eV, above 10 eV), using the fully quantum-mechanical treatment for reactions (1-8), with explicit inclusion of the nuclear exchange. This will be achieved by taking into account explicitly a large basis of rotational transitions.

References

[1] R. K. Janev, D. Reiter and U. Samm, "Collision Processes in Low-temperature Hydrogen Plasmas" (http://www.eirene.de/reports/report_4105.pdf or http://hdl.handle.net/2128/249) (2003).
[2] P. S. Krstic, "Inelastic Processes from Vibrationally Excited States in Slow $H^+ + H_2$ and $H + H_2^+$ Collisions: Excitations and Charge Transfer," Phys. Rev. A 66, 042717 (2002).
[3] P. S. Krstic and R. K. Janev, "Inelastic Processes from Vibrationally Excited States in Slow $H^+ + H_2$ and $H + H_2^+$ Collisions. II. Dissociation," Phys. Rev. A 67, 022708 (2003).
[4] P. S. Krstic, R. K. Janev and D. R. Schultz, "Three-body, diatomic association in cold hydrogen plasmas", J. Phys. B 36 (16), L249-L255 (2003).
[5] P. S. Krstic and D. R. Schultz, "Elastic Processes Involving Vibrationally Excited Molecules in Cold Hydrogen Plasmas," J. Phys. B 36, 385-398 (2003).
[6] D. W. Savin, P. S. Krstić, Z. Haiman and P. C. Stancil, "Rate coefficient for $H^+ + H_2(X\ ^1\Sigma_g^+, v=0, J=0) \rightarrow H(1s) + H_2^+$ charge transfer and some cosmological implications," Astrophys. J. 606, L167 (2004).
[7] A. Ichihara, O. Iwamoto and R. K. Janev, "Cross Sections for the Reaction $H^+ + H_2(v=0\text{-}14) \rightarrow H + H_2^+$ at Low Collision Energies," J. Phys. B. 33, 4747-4758 (2000).
[8] P. S. Krstić, "Vibrationally resolved collisions in cold hydrogen plasma," Nucl. Instrum. Methods Phys. Res. B 241, 58 (2005).

Revision of collisional-radiative models and neutral-transport code for hydrogen and helium species

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We have been developing collisional-radiative models and a neutral-transport code for hydrogen and helium species, which are used to investigate fusion plasmas. Collisional-radiative models of atomic hydrogen and helium have been applied to a helium-hydrogen RF plasma at Shinshu University, Japan, to test whether these models reproduce the observed emission intensities. The electron temperature and density are determined from visible emission line intensities of helium atom considering photoexcitation from the ground state to singlet P states, which is accompanied by radiation trapping [1,2]. From the observed hydrogen Balmer γ line intensity, which is hardly affected by photoexcitation, the atomic hydrogen density is determined using a hydrogen collisional-radiative model that ignores photoexcitation. The atomic hydrogen temperature, which reproduces Balmer α and β line intensities, is determined using an iterative hydrogen atom collisional-radiative model [3] that calculates photoexcitation rates. R-Matrix cross sections for $n \leq 5$ in Ref. [4] are used in the model. The hope is hoped that precise cross sections for higher-lying levels will be produced to determine the atomic density in fusion plasmas.

As a revision of the molecular hydrogen collisional-radiative model, which includes electronic and vibrational states [5, 6], we are developing a model that also includes rotational states. This model will provide more precise effective reaction rate coecients of the molecule. Emission line intensities of hydrogen molecules in plasmas are calculated as a function of n_{H2}, n_e, T_e, and T_v, T_{rot} in the ground electronic state. From observed spectra, these parameters can be determined. In the revised model, assuming Hund's (b) case, the levels are labeled by the principal quantum number of the united atom n, and by Λ, N and J. The number of 2131 levels for $n \leq 4$, listed in Ref. [7], is included in the model. Spontaneous transition probabilities e→a, d→a, i→c, j→c, I→C and J→C in Ref. [8] are included in the model. The values for other transitions are calculated according to Ref. [9]. Transition probabilities to continuum states are also calculated. The vibrationally resolved excitation cross section from the electronic ground state to B, B', B", C, D, D' in Ref. [10] are included in the model; for the excitation to other states, data in Ref. [11, 12] are included. Currently, there is not enough information to derive vibrationally and rotationally resolved cross sections. Tentatively, for an optically allowed transition, we assume that the rate coecients are proportional to Franck-Condon and Hönl-London factors. For an optically forbidden transition, we use the Franck-Condon factor to obtain vibrationally resolved data and divide them evenly for rotational states. Excitation cross sections between excited states are estimated from united atom helium cross sections. Reaction rate coefficients which are essential to determine the vibrational and rotational population of the ground electronic state are included in the model.

References

[1] M. Goto, JQSRT 76, 331 (2003).
[2] K. Sawada et al., Plasma and Fusion Res. 5, 001 (2010).
[3] K. Sawada, J. Plasma Phys. 72, 1025 (2006).
[4] H. Anderson et al., J. Phys. B 33, 1255 (2000), J. Phys. B 35, 1613 (2002).
[5] K. Sawada and T. Fujimoto, J. Appl. Phys. 78, 2913 (1995).
[6] K. Sawada and T. Fujimoto, Contrib. Plasma Phys. 42, 603 (2002).
[7] H. M. Crosswhite, The Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke, John Wiley & Sons Inc (1972).
[8] S. A. Astashkevich et al., J. Quant. Spectrosc. Radiat. Transfer 56, 725 (1996).
[9] James K. G. Watson, Journal of Molecular Spectroscopy 252 5 (2008).
[10] R. Celiberto, R. K. Janev et al., Atomic Data and Nuclear Data Tables 77, 161 (2001).
[11] R. Janev, D. Reiter and U. Samm, Report Forschungszentrum Jülich JUEL 4105, (2003).
[12] W. T. Miles, R. Thompson and A. E. S. Green, J. Appl. Phys. 43, 678 (1972).

Evaluation of Cross Section for Electron Impact with Hydrogen and Helium and Their Combination Molecules in Fusion Plasma

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Hydrogen and Helium are simple atoms and their properties are studied by many researchers since a long time. Several persons have made evaluation data about some collision processes long time ago. So we are interested to evaluate cross sections including various processes such as ionization, excitation, recombination, and attachment for electron impact with hydrogen and helium atoms. The research objective is to provide a more complete data set for electron collisions with hydrogen and helium atoms than those published before.

In order to evaluate the cross section data, we established a data evaluation process and guidelines for the establishment and distribution of Standard Reference Data (SRD). Here SRD is reference data issued by a recognized authority and reference data is data related to a property of a phenomenon, body, or substance, or to a system of components of known composition or structure, obtained from identified source, critically evaluated and verified for accuracy.

In the SRD framework we evaluate the cross sections for electron collisions with hydrogen molecules [1]. In this paper, we complete update of the previous data compilation on the $e+H_2$ collision [2]. After reviewing available cross section data we have determined a set of recommended values of cross section, as far as possible. The general criteria for the selection of preferred data are as follows: In principle, experimental data are preferred to theoretical ones and the reliability of the experimental methods employed is critically assessed. Agreement between independent measurements of the same cross section is generally taken as an endorsement of the accuracy of the measured data. A strong emphasis is placed on the consistency of the results determined by different techniques, and in cases where only a single set of data is available for a given cross section those data are simply shown in this paper, unless there is a strong reason to reject them. In this way, cross section data have been compiled for electron collisions with hydrogen molecules based on 71 references. Cross sections are collected and reviewed for total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational, and electronic states, dissociation, ionization, emission of radiation and dissociative attachment.

Almost all of the cross sections have been revised. However, further studies are still needed to make the cross section data more comprehensive and more accurate. In particular, the following problems should be addressed: The rotational cross section has a large value at the energies up to a few tens of eV. However, no experimental data available at the energies of about 1 eV and higher. Only one old set of measured values is available for the elastic cross sections at the energies of 100 - 1,000 eV. They are not completely consistent with the recommended cross sections in the energy region below 100 eV. Although several sets of experimental cross sections are available for the excitation of electronic states, more detailed measurement should be done for the excitation of triplet states. The total dissociation cross sections are available with fair certainty. Further information is necessary for the details of the dissociation process. Finally, cross section data for the target molecules in their excited states are of practical importance. Any experiment of the electron collision with excited hydrogen molecules would be very valuable.

Also, we evaluate the electron impact cross sections for deuterated hydrogen and deuterium molecules [3]. This work reviews the electron-scattering cross sections for elastic and inelastic processes at different electron energies for both these molecules. The elastic momentum transfer cross sections and inelastic cross sections for electron-impact rotational, vibrational and electronic excitation, emission, dissociation, ionization and dissociative electron attachment have been evaluated. As a result, the electron-impact cross sections for some of the different processes for these molecules could not be reviewed in this paper. This has left us with a partially incomplete picture of the subject. To obtain a real comprehensive picture, the following few problems have to be addressed in the near future: Total electron-impact scattering cross sections (elastic + inelastic) have not been measured so far for both HD and D_2 molecules. The rotational and vibrational excitation cross sections for D_2 reported in the literature are the old sets of measured values. Also, such cross sections are not available for HD molecules at all. No measurements for the appearance energies of HD^+, H^+ from HD and D^+ from HD are

available. Also, total electron impact ionization cross sections for HD molecules have not been reported in the literature.

Our future data evaluation work will include cross section data on total scattering, elastic scattering, momentum transfer, ionization, electron attachment, and excitation of rotational, vibrational, and electronic states. The work plan is to collect data through journal, report, web database and to review available cross section data and comparison and critical evaluation of existing data (experimental and theoretical). Through this processes, we have determined a set of recommended values of cross section, as far as possible.

References

[1] J.-S. Yoon et al., Journal of Physical and Chemical Reference Data, 37 (2), 913 (2008).
[2] H. Tawara et al., Journal of Physical and Chemical Reference Data, 19, 617 (1990)
[3] J.-S. Yoon et al., Report on Progress in Physics, 73, 116401 (2010).

Application and Evaluation of State-Resolved Atomic and Molecular Data in Population Models for Hydrogen, Deuterium and Helium

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Within the scope of the CRP on "Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma" population models for atoms and molecules provide an insight in the relevance of individual processes for a wide range of plasma parameters. Of particular interest are reactions in the cold plasma edge of fusion devices in the temperature range from some (ten) eV to below one eV, which means plasmas in the ionizing and in the recombining regime. These regimes are accessible in low pressure, low temperature plasmas generated in laboratory experiments. Such laboratory plasmas are well suited to benchmark population densities calculated with collisional radiative models.

Since modelling low temperature plasmas requires accurate cross section data around the threshold energy of the processes, a critical evaluation of the used data is required. Another crucial point is the resolution of the electronic states in the atom and molecules, i.e. to what extend the main quantum number is state resolved and, in case of molecules, the resolution in vibrational and rotational levels. For the latter, isotope shifts are to be taken into account.

Therefore, the following research proposal has been suggested: Collisional radiative models for H, H_2 and He will be used as tool to systematically investigate and evaluate the input data. If needed the data basis will be extended by applying simplified codes. Focus will be laid on: reactions connecting H^+, H_2^+ and H_3^+ with atomic and molecular hydrogen, ro-vibrational excitation of hydrogen molecules and its ions, and on production of negative hydrogen ions. Regarding the isotope effect deuterium will be investigated as well, which will allow for some extrapolations to tritium molecules. Calculated population densities are benchmarked by experimental data from several low temperature plasmas to cover a wide range of plasma parameters. Special emphasis will be given to processes in negative ion sources and beams. Besides pure hydrogen, deuterium or helium plasmas, mixtures are investigated as well.

The presentation at the first meeting of the CRP summarizes the status of the activities within the proposed research. The flexible solver Yacora [1] is been introduced and used to construct collisional radiative models for atomic and molecular hydrogen as well as for helium based on the most recent data. The laboratory experiments used for the benchmark of the codes and their diagnostic capabilities are introduced.

For molecular hydrogen the model by Sawada [2] is been used as a starting point with extensions carried out continuously during the last years. At present, the Yacora model for H_2 takes into account the vibrational resolution in the ground state, in all electronic states in the principal quantum number n=2 and in selected states of n=3, neglecting the rotational resolution. The n=4, 5,... levels are only resolved in their multiplet system. Whenever possible the latest data compilation for hydrogen [3] has

been implemented with the option to switch back to data by Sawada and Miles [2,4]. If not available in literature, vibrationally resolved data has been produced by using either the Gryzinski method [5,6] or the impact parameter method IPProg [7] together with Franck-Condon factors or transition probabilities respectively. Franck Condon factors and transition probabilities are calculated with TraDiMo [8, 9]. Cross checks of the cross sections calculated using the Gryzinski method and IPProg with data available in literature showed an agreement within a factor of 2. At present 214 levels and 21645 reactions in total are taken into account. Good agreement of calculated population densities with experimental results [10] is observed for the singlet system. In the triplet system however, usage of the latest data [3] leads to very unsatisfying results, i.e. the calculation is a factor of 5 higher than the measurement. This might indicate that reaction channels are missing such as the effective mixing of electronic levels in the principal quantum number which will be investigated next. As a further step, calculations of non-dissociative and dissociative ionisation cross sections (Gryzinski method) have been started.

The Yacora model for atomic hydrogen implements a collisional radiative model for the excited states of the atom coupled to the atom and the ion. In addition, opacity of emission lines can be treated self-consistently. Coupling to molecular hydrogen offers the possibility to take dissociative excitation into account. The relevance of both effects has been benchmarked by experiments [11]. A critical evaluation of data for electronic excitation from the ground state into excited states revealed discontinuities around the quantum number n=5 [1] caused by the switch from one set of raw data to another. The application of a smoothing procedure results in population densities which are in much better agreement with experimental data, in particular for the Balmer line H_γ. Besides the coupling to molecular hydrogen coupling to the molecular hydrogen ions (H_2^+ and H_3^+) is provided, being of relevance for recombining plasmas. A survey of the data base for dissociative recombination has been carried out.

Implementing an energy dependency of the branching ratios, i.e. break-up into the individual excited states depending on the vibrational excitation of the molecular hydrogen ion [3] resulted in a better agreement with experimental data from recombining plasmas. More precise scaling would be desirable, and particularly data for molecular deuterium ions. The need of branching ratio data for H_3^+ (D_3^+) recombination is been pointed out. Last but not least the model is coupled to the negative hydrogen ion via the mutual neutralization process being of high importance for data interpretation in negative ion sources. Examples of applications of the coupled Yacora model for hydrogen are shown for a variety of experiments (divertor plasmas, linear plasma devices and laboratory experiments) which are either in the ionising or in the recombining regime or in the intermediate regime.

For helium the data compilation by Ralchenko [12] has been implemented in Yacora. The electronic states are resolved up to quantum number n=4 in both multiplet systems resulting in 19 levels and 338 reactions in total. The helium model is been benchmarked against the ADAS package [13] and a very good agreement is been observed. The Yacora model, however, is more flexible, allowing for implementing opacity and diffusion which are of importance for resonance lines and metastable levels respectively. Calculated and experimental data has been compared in a Boltzmann plot and a good agreement for n=2 and n=3 levels is observed only by taking into account these two effects. The next step will concern the benchmark with n=4 data. In addition mixtures of hydrogen and helium will be investigated and measurements of the HeH^+ (HeD^+) density are planned.

References

[1] D. Wünderlich et al., JQSRT 110 (2009) 62.
[2] K. Sawada and T. Fujimoto, J. Appl. Phys. 78 (1995) 291.
[3] R. Janev, D. Reiter, U. Samm, Juel-Report 4105 (2003).
[4] W. Miles, R. Thompson, A. Green, J. Appl. Phys. 43 (1972) 678.
[5] M. Gryzinski, Phys. Rev. 138 (1965) A336.
[6] E. Bauer, C.D. Bartky, J. Chem. Phys. 43(1965) 2466.
[7] A. Burgess, H. P. Summers, Mon. Not. R. Astr. Soc. 174 (1976) 345.
[8] U. Fantz and D. Wünderlich, ADNDT 92 (2006) 853.
[9] D. Wünderlich and U. Fantz, ADNDT 97 (2011) 152.
[10] U. Fantz and D. Wünderlich, APID Series 16 (2011) 76 (in press).
[11] K. Behringer, U. Fantz, New Journal of Physics 2 (2000) 23.
[12] Yu. V. Ralchenko et al., NIFS-DATA-59 (2000)
[13] H.P. Summers, The ADAS User Manual, version 2.6, http://adas.phys.strath.ac.uk.

Recent advances on state-to-state approach in non-equilibrium hydrogen plasma modelling: focus on electron-H_2 resonant collisions

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The theoretical description of a diatomic molecular plasma, out of thermodynamical equilibrium, requires in general the determination of the ground-state vibrational distribution function, the distribution of the excited electronic states and the electron-energy distribution function for free electrons. These quantities, due to the system's non-equilibrium conditions, are expected to show more or less strong deviations from the Boltzmann's or Maxwell's distributions [1].

The determination of the distribution functions can start with the formulation of a set of differential *master equations* describing the time-variation of volume density of atomic and molecular ionic species and neutrals, caused by the collision processes occurring in the system among all the possible species present in the plasma, including walls, and by the absorption and emission of radiation interacting with particles.

An important aspect of this kinetic model, is represented by the fact that every excited species in a given quantum state (vibrational or electronic), acts in the plasma as an independent chemical component, so that a time-evolution equation must be written for the density of each quantum state. This circumstance defines the so-called *state-to-state kinetics* [2].

The final step of the plasma kinetic modelling is the simultaneous solution of the master equation set, coupled with the Boltzmann's equation for the electron energy distribution function and, for those systems where required, with the *fluid dynamics equations* [3], from which the ionic and neutral densities and electron distribution function, resolved in time, are finally obtained.

One of the most powerful tool in the solution of the master equation set is represented by the so-called ab-initio particle method. In Particle-in-Cell/ Direct Simulation Monte Carlo (PIC-DSMC) methodology [4, 5], every macroparticle represents a cloud of real particles carrying all the information necessary to solve the kinetic effects (positions, velocity coordinates and inner degree of freedom, such as electronic and/or vibrational states). They are tracked along their flight in the phase space. For plasma charged particle, the dynamics is coupled self-consistently with the solution of field Maxwell's equations. Moreover, this simulation technique allows a direct implementation of boundary conditions (plasma-wall and gas-wall interactions) reducing any kind of approximation.

The solution of the obtained mathematical system of coupled equations, requires, as external requisite, the knowledge of the impact data, represented by the collision cross sections, for all the processes involving the particle quantum states. The determination of reliable collision cross sections, either through accurate experimental measurements or theoretical calculations, is a non-trivial task which requires a specific experience in atomic and molecular physics [6].

Among all the elementary processes that occur in the plasma, electron-molecule resonant collisions play a fundamental role and represent one of the most interesting subjects in electron-molecule collision studies.

A resonant process in a hydrogen plasma, occurs through the trapping of a free electron in a H_2 molecule, with a formation of a transient species H_2^-. This molecular ion is unstable and can detach the captured electron leaving the H_2 molecule in an excited vibrational state (resonant vibrational excitation or e-V process). Alternatively, if the auto-detachment is not a rapid process, the molecule can suffer dissociation, with a subsequent formation of a stable negative ion, $H^-(1s^2)$, and a neutral hydrogen atom in a given quantum state H(n). This process, known as dissociative electron attachment (DEA), along with the resonant vibrational excitation, plays a paramount role in affecting the vibrational kinetic of the H_2 plasmas [6].

The theoretical calculation of the cross sections for both DEA and e-V processes requires a quantum mechanical description of the resonant collision, which leads, in a first step, to the determination of the bond-length dependent electronic eigenvalues and lifetimes of the H_2^- resonant state [7]. These

quantities, in a second step, enter as complex potential functions in the Schrödinger's equation for the nuclear motion. The solution of this last equation furnishes the resonant nuclear wave function from which, ultimately, the DEA and e-V cross sections can be obtained [8-11].

References

[1] M. Capitelli, R. Celiberto, G. Colonna, G D'Ammando, O De Pascale, P. Diomede, F. Esposito, C. Gorse, A. Laricchiuta, S. Longo and L. D. Pietanza, J. Phys. B: At. Mol. Opt. Phys. 43, 144025 (2010).
[2] M. Capitelli, I. Armenise, D. Bruno, M. Cacciatore, R. Celiberto, G. Colonna, O. De Pascale, P. Diomede, F. Esposito, C. Gorse, K. Hassouni, A. Laricchiuta, S. Longo, D. Pagano, D. Pietanza and M. Rutigliano, Plasma Sources Sci. Technol. 16, S30–S44 (2007).
[3] G. Colonna. L. D. Pietanza and G. D'Ammado, Chemical Physics 398, 37–45 (2012).
[4] C. K. Birdsall and A. B. Langdon, Plasma Physics via Computer Simulation, McGraw-Hill, New York, 1985.
[5] F. Taccogna, P. Minelli, D. Bruno, S. Longo and R. Schneider. Chemical Physics 398, 27-32 (2012).
[6] M. Capitelli, R. Celiberto, F. Esposito and L. Laricchiuta, Plasma Processes and Polymers, 6, 279 (2009).
[7] D. T. Stibbe and J. Tennyson, J. Phys. B 31, 815 (1998).
[8] R. Celiberto, R. K. Janev, J. M. Wadehra and A. Laricchiuta, Phys Rev A 77, 012714 (2008).
[9] R. Celiberto, R. K. Janev, J. M. Wadehra and A. Laricchiuta, Phys Rev A 80, 012712 (2009).
[10] R. Celiberto, R. K. Janev, J. M. Wadehra and J. Tennyson, Chemical Physics 398, 206-213 (2012).
[11] R. Celiberto, R. K. Janev, J. M. Wadehra and A. Laricchiuta, Phys Rev. A 84, 012707 (2011).

Electronic and Atomic Collisions with Hydrogen and Helium Ions: State-Specific Study of Associative, Dissociative and Reactive Processes

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Atomic and molecular collisional processes are experimentally studied in Louvain-la-Neuve (UCL) since many years now. The reactions that are generally investigated in our laboratory cover the energy range from well below 1eV up to several keV. They are of two kinds: (i) between atoms and ions, atomic and molecular, and (ii) between electrons and atomic and molecular species. Experimental data allow the determination of absolute cross sections, energy thresholds, vibrational populations, energy and angular distributions.

Total cross-sections are measured, for the associative ionization and mutual neutralization, and other reactive processes like proton transfer, by means of a merged-beam set-up operating with keV beams [1]. In this apparatus, two ionic beams are merged over a short interaction path. The cationic beam is extracted from an electron cyclotron resonance (ECR) source and the anionic beam is obtained either from a duoplasmatron ion source, or a cesium sputter source. An observation voltage is applied to the merging section. As a result, the cations formed in this region experience an increase of their kinetic energy and become distinguishable from other molecular cations produced along the beam path. A magnetic analyzer allows the intensities of the primary beams to be recorded and the reaction products to be detected by a channel electron multiplier. In mutual neutralization studies, neutral particles leave the observation cell unaffected, and must be detected in coincidence further downstream. Special detectors are used to acquire total and differential cross sections, together with state-specific information.

The relative population of the vibrational levels and, more generally, the degree of ro-vibrational excitation of a given molecular ion, may be inferred from the dissociative charge transfer it undergoes with an appropriate gas target. The three-dimensional imaging of the dissociative charge transfer events is realized in a dedicated set-up, as described in [2]. The molecular ions of interest are accelerated to several keV and collimated before passing through an effusive gas jet. A pair of position sensitive detectors operating in coincidence enables the reconstruction of the velocity vectors of the fragments. The electron capture from alkalis populates a narrow band of excited states of the neutral mol-

ecule subject to rapid predissociation, producing sharp peaks in the kinetic energy release distribution. Alternately, rare gas targets may be used to directly populate the lowest dissociative state, mapping the vibrational wavefunction to kinetic energy release. Developments are under way to extend the technique to multiple fragmentation of triatomic species like H_3^+ and its isotopomers, by means of delay-line and camera based detectors.

Electron-impact ionization and dissociation are studied by means of the animated crossed electron-ion beam method. The apparatus and the experimental method have been described in detail in [3]. A molecular ion beam generated in an ECR source and accelerated to a 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. Due to the transfer of internal potential energy, dissociation fragments exhibit both a broad velocity and a broad angular distribution in the laboratory frame. Product ions are separated from the primary ion beam by using a double focusing 90° magnetic analyzer, and are dispersed according to their velocity in the laboratory frame. They are further deflected by a 90° spherical deflector and directed onto the channel electron multiplier. The magnetic field distribution of the signal is converted into a centre-of-mass distribution of kinetic energies. The high end of this distribution reflects the repulsive character of the dissociative ionization channel, allowing its separation from the dissociative excitation channel.

The above described methods may be combined to unravel the chemistry of hydrogen helium mixtures. Among them, the ion-ion collisions, i.e. reactions $X + H^-$ ($X = H^+$, H_2^+, H_3^+, He^+ or He^{++}), will be studied in merged-beams experiments. Cross sections for $H^+ + H^-$ mutual neutralization were recently measured between 10 meV and 250 eV. The position-sensitive coincident detection of H products has allowed the precise determination of their electronic excitation. The branching ratio among the different principal quantum numbers of the products could also be measured. After this proof-of-principle measurement, we may start looking into the details of less understood mutual neutralization reactions, namely $He^+ + H^-$, $H_2^+ + H^-$, and $H_3^+ + H^-$, the latter two opening the possibility for three-body breakup and ro-vibrational excitation of the products to occur. Isotope effects will also be investigated.

The ion-atom and ion-molecule reactions are ubiquitous in plasmas, and are enhanced by the induced dipole attractive potential. $He^+ + H^*$ and $He^* + H^+$ charge exchange reactions were investigated theoretically by N. Vaeck's group at ULB (Brussels). We want to perform at least one such measurement to benchmark theory. The production of state-selected atomic beams beyond their electronic ground state is clearly challenging. We want to explore a scheme for metastable helium production based on the photodetachment of He^-. Such a beam is also highly needed for electron impact studies (I. Bray et al.) The other route is to neutralize H^+ or He^+ beams on a cesium target, producing a large but unknown amount of metastable atoms, which can be further excited by lasers. The dominant contribution of a minute fraction of Rydberg states is foreseen and must be evaluated. Low energy electron detachment (H^-) and dissociation (H_2^+, H_3^+) in collisions with ground state H and He atoms may also be considered at a later stage.

The dissociative charge transfer provides a reliable diagnostic of the ro-vibrational excitation of H_2^+ ions produced by quite different mechanisms (ECR source [3], REMPI [4]). We have recently achieved similar precision with HeH^+, and could follow the decay of its excitation with trapping time. We believe we can analyze the excitation of reaction products issued from the associative ionization of He^+ with H^-, and of $He(2\,^3S)$ with H, the total cross section being known for both processes [5].

Finally, we mention here the continuation of our electron-impact studies with the help of our animated cross-beams experiment. The $HeH^+ + e^-$ and $He_2^+ + e^-$ collisions may lead to both their dissociative excitation and dissociative ionization. The aforementioned diagnostic tool will be applied to both ion beams to fully characterize the reactants. Measuring the energy thresholds and kinetic energy release distributions for the considered reactions besides their absolute cross sections will certainly help in benchmarking the theoretical work in progress.

References

[1] Nzeyimana T, Naji EA, Urbain X and Le Padellec A, Eur. Phys. J. D 19 (2002) 315.
[2] Urbain X, Fabre B, Staicu-Casagrande E M, de Ruette N, Andrianarijaona V M, Jureta J, Posthumus J H, Saenz A, Baldit E, Cornaggia C, Phys. Rev. Lett. 92 (2004) 163004.
[3] Lecointre J, Belic D S, Cherkani-Hassani H, Jureta J J and Defrance P, J. Phys. B: At. Mol. Opt. Phys. 39 (2006) 3275.

[4] E.M. Staicu-Casagrande, T. Nzeyimana, E.A. Naji, N. de Ruette, B. Fabre, A. Le Padellec and X. Urbain, Eur. Phys. J. D 31 (2004) 469–475.
[5] A Naji, K Olamba, J P Chenu, S Szücs, M Chibisov and F Brouillard, J. Phys. B: At. Mol. Opt. Phys. 31 (1998) 2961.
[6] J.H. Posthumus, B. Fabre, C. Cornaggia, N. de Ruette, X. Urbain, Phys. Rev. Lett. 101 (2008) 233004.

State-Resolved Cross Section Measurements in Low and Intermediate Energy Ion-He/H_2 Collisions

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Charge exchange between ions and atoms/molecules including electron capture, ionization, transfer ionization, and their accompanying simultaneous excitation occurs in various plasmas. These processes are important for understanding the properties of plasmas and the diagnostic of plasma. In the zone of the divertor of a magnetic confinement fusion reactor, the plasma is relatively cold and dense, atomic/molecular processes and the interaction of the plasma electrons and ions with atoms/molecules and molecular ions become important. The cross section data of these processes are essential for divertor plasma modeling. We are going to measure the cross sections of these processes at accelerator facilities. Here, the experimental approach for measuring the cross sections of related charge exchange processes will be given in detail.

Crossed beam technique will be applied in the experiment. A cold target recoil ion momentum spectrometer (COLTRIMS) has been established in the Institute of Modern Physics, Lanzhou and has been employed to study the state-selective electron captures. The setup is installed at a dedicated beam line for atomic physics studies equipped at the 320 kV platform for research with highly charged ions. The ions which are produced in an ion source are directed to the atomic/molecular target in the spectrometer center. It can determine the initial momentum of each charged particles gained in the collision by measuring the flight time and its position on the detector. From the value of longitudinal momentum of a recoil ion, the state selective information related to electron capture can be deduced. Further, the angular differential cross sections can also be obtained because the transverse momentum of the recoil ion is ready to be calculated from the measured momentum.

We plan to study the following processes experimentally for various projectile energies. The collision systems are (1) H^+ + He (E_p = 15 - 300 keV/u); (2) He^{q+} + He (q=1, 2; E_p = 5.0 - 150 keV/u); (3) C^{q+} + He/H_2 (q=2, 3, 4, 5; E_p = 2 - 125 keV/u); (4) Ar^{q+} + H_2 (q=2, 3, 4, 5, 6; E_p = 0.7 - 45 keV/u). In the Coordinated Research Project meeting, the cross sections in the collisions of He_2^+ on atomic helium and molecular hydrogen will be presented. The energy dependence of the state-selective electron capture cross sections will be discussed and compared to the other measured data and theoretical results from different models. The mechanism of the dominating processes will also be analyzed. Finally, the plan of the experimental project will be reviewed.

References

[1] S. I. Krasheninnikov, A. Yu. Pigarov and D. J. Sigmar, Phys. Lett. A 214, 285 (1996).
[2] A. Yu. Pigarov and S. I. Krasheninnikov, ibid. 222, 251 (1996).
[3] R. K. Janev, T. Kato and J. G. Wang, Phys. Plasmas 7, 4364 (2000).
[4] X. Ma, H. P. Liu, L. T. Sun, M. T. Song, X. L. Zhu, et. al. J. Phys.: Conf. Ser. 163 (2009) 012104.
[5] X. Ma, X. L. Zhu, H. P. Liu, et. al. Science in China, Series G 51(2008) 755.
[6] X. L. Zhu, X. Ma, B. Li, S. F. Zhang, et. al. J. Phys.: Conf. Ser. 163 (2009) 012064.
[7] S. Yan, X. Ma, P. Zhang, S. Xu, S. F. Zhang, et. al. Phys. Rev. A 82(2010)052702
[8] J. Anton, B. Fricke, X. Ma, X. L. Zhu, et. al. Physics Letter A 369(2007) 85-89
[9] Zhu Xiao-long, Ma Xin-wen, Li Bin, et. al. Chin. Phys. Lett. 23（2006）587
[10] R. Dörner, V. Mergel, O. Jagutzki, et al. Phys. Rep. 330 (2000) 95.
[11] X. Ma, R. T. Zhang, S. F. Zhang, X. L. Zhu, et al. Phys. Rev. A 83, (2011) 052707.
[12] J. Ullrich, R. Moshammer, A. Dorn, R. Dorner, et al, Rep. Prog. Phys. 66, (2003)1463.
[13] M. Alessi, et al. Phys. Rev. A83 (2011) 014701.

Theoretical studies of electron driven resonant processes in H+2 and HeH+: Dissociative Recombination, Vibrational Excitation and Dissociative Excitation

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We have carried out a number of preliminary studies of the dynamics of H_2^+ and HeH^+ and their isotopes following low-energy electron collisions [1-9]. We are continuing these studies, increasing the accuracy of the calculations and studying reactions leading to dissociative recombination, vibrational excitation and dissociative excitation and possibly ion-pair formation. These calculations will be carried out for a wider range of electron energies than previously explored, and in addition will look at the effect of vibrational excitation of the initial target. Previous work had assumed the target molecule was in its ground vibrational state. For the fusion plasma environment, both the energy of the electron collision and the degree of vibrational excitation is higher than what has been studied before. In addition, final branching ratios will be calculated. We use the complex Kohn variational method to study the electron collisions and a combination of time-dependent and time-independent solutions to the Schrödinger equation to study the dynamics following the collision.

Another important reaction for modeling of the fusion plasmas is mutual neutralization in collisions between H^- and H^+ or He^+. We have previously studied the first of these reactions [10] and we intend to study the second reaction. These reactions are driven by non-adiabatic couplings between the ion-pair state and the covalent states especially at large internuclear distances and the cross section for the reaction will be computed by solving a coupled Schrödinger equation for the nuclear motion where the effect of autoionization will be included.

References

[1] Dissociative excitation of HeH^+ by electron impact, A. E. Orel, T. N. Rescigno and B. H. Lengsfield III, Phys. Rev. A 44 4328 (1991).
[2] The effects of open inelastic channels in the resonant dissociative recombination of HeH^+, A. E. Orel, K. C. Kulander and T. N. Rescigno, Phys. Rev. Lett. 74 4807 (1995).
[3] Resonant enhanced dissociation of a molecular ion below its electronic excitation threshold, K. C. Kulander and A. E. Orel, Phys. Rev. A 54 4992 (1996).
[4] Dissociative recombination of He_2^+ molecular ions, L. Carata, A. E. Orel and A. Suzor-Weiner, Phys. Rev. A 59 2804 (1999).
[5] Dissociative recombination of HeH^+: product distributions and ion pair formation, Å. Larson and A. E. Orel, Phys. Rev. A. 59 3601 (1999).
[6] Ion-pair formation and product branching ratios in dissociative recombination of HD+ Å. Larson and A. E. Orel, Phys. Rev. A. 64 062701 (2001).
[7] Dissociative recombination of He_2^+, J. Royal and A. E. Orel Phys. Rev. A. 72 022719 (2005).
[8] Wave packet study of the products formed in dissociative recombination of HeH^+, Å. Larson and A. E. Orel, Phys. Rev. A. 72 32701 (2005).
[9] Resonant dissociative excitation and vibrational excitation of He_2^+, J. Royal and A. E. Orel, Phys. Rev. A. 75 052706 (2007).
[10] Mutual neutralization in low-energy $H^+ + H^-$ collisions: A quantum ab initio study, M. Stenrup, Å Larson and N. Elander, Phys. Rev. A. 79 012713 (2009).

Low Energy Reactive Collisions of Electrons with H_2^+ and isotopomers: Computations and comparison with measurements

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The Multichannel Quantum Defect Theory is a powerful time-independent method that can be used to study the following reactions between a molecular ion and an electron:

$AB^+(N_i^+, v_i^+) + e^- \rightarrow A + B$ (Dissociative Recombination) (1)

$AB^+(N_i^+, v_i^+) + e^-(\epsilon) \rightarrow AB^+(N_f^+, v_f^+) + e^-(\epsilon')$, with $\epsilon' > \epsilon$ (Ro-vibrational Excitation, RVE) (2)

$AB^+(N_i^+, v_i^+) + e^-(\epsilon) \rightarrow AB^+(N_f^+, v_f^+) + e^-(\epsilon')$, with $\epsilon > \epsilon'$ (Ro-vibrational De-excitation, RVD) (3)

$AB^+(N_i^+, v_i^+) + e^-(\epsilon) \rightarrow AB^+(N_i^+, v_i^+) + e^-(\epsilon')$, with $\epsilon = \epsilon'$ (Elastic Collisions, EC) (4)

and, for high enough collision energies,

$AB^+(N_i^+, v_i^+) + e^-(\epsilon) \rightarrow A + B^+ + e^-(\epsilon')$ (Dissociative Excitation, DE) (5)

where AB^+ stands for a diatomic molecular ion. This method treats all the processes simultaneously and combines the direct and the indirect mechanisms.

Important improvements have recently been brought to our MQDT code through the full description of the rotational couplings at low collision energy and the consideration of two ionic thresholds in DE computations.

At very low collision energies, the rotational effects play a key role on the DR and RVD/RVE of light molecular species with a large rotational constant, such as H_2^+ and isotopomers, in which the indirect process is important [1]. This has been recently put in evidence in the comparison of H_2^+ computations with experiments. Whereas an overall better agreement was found for the DR of $v_i^+ = 0$ with the full consideration of rotations, they have been found to enhance the vibrational superelastic collisions [2]. As well, for HD^+, the assignment of the manifold of resonances appearing on all the partial contributions to the total cross sections has been used to interpret all the structures appearing in the cross section, and then to clearly establish a correspondence between the features observed in the experimental and theoretical cross sections in the energy range 0 to 350 meV. This comparison shows a good agreement between both theory and the experiments performed at the test storage ring (TSR) of Heidelberg [3].

Still at very low energy, we have performed some preliminary computations on state-to-state rotational transitions in HD^+ and H_2^+, inspired by the recent observations of rotational cooling by superelastic collisions at TSR, by merging a beam of rotationally hot HD^+ ions with an electron beam at zero relative energy [4,5]. The SEC anisotropic rate coefficients obtained for the transitions $J \rightarrow J-2$ seem to agree reasonably with the observed ones. As well the cross sections and the thermal rate coefficients are compatible with those of Faure and Tennyson [6] for and Faure [4] for HD^+.

For collision energies exceeding the dissociation threshold, DE enters in competition. The computations have been performed for HD^+ in the range 0 to 12 eV. The results obtained for DR agrees quite well with the other theoretical computations and experiment [7, 8].

References

[1] Vâlcu et al (1998), Europ. Phys. J. D 1 71.
[2] O. Motapon et al (2008), Phys. Rev. A77, 052711.
[3] F. O. Waffeu Tamo et al (2011), Phys. Rev. A, In press.

[4] Shafir et al (2009), Phys. Rev. Lett. 102 223.
[5] D. Schwalm et al (2011), J. Phys. Conf. Ser. 300, 012006.
[6] A. Faure and J. Tennyson (2011), Mon. Not. R. Astr. Soc. 325 443.
[7] O. Motapon et al (2011), J. Phys. Conf. Ser. 300, 012018.
[8] K. Chakrabarti et al (2011), In preparation.

Molecular Rydberg states: between spectroscopy and dynamics

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Multichannel quantum defect theory is a generalization of the Rydberg equation to multiple series or "channels" in atoms and molecules applicable below and above the series limits, i.e. both in the bound and the continuum ranges. In its modern form quantum defect theory owes much to the work of Ham [1], Seaton [2] and Fano [3] and many others, who developed it into a versatile theoretical tool applicable to a variety of problems in molecular spectroscopy and dynamics. A particular strength of quantum defect theory for Rydberg states in molecules is that the theory accounts for non-adiabatic effects by means of the method of frame transformations [3] and is not limited to the Born-Oppenheimer approximation. As such it constitutes an alternative to the standard coupled-equations approach.

In the first part of the presentation I shall discuss the absolute cross sections for the competing decay channels fluorescence, dissociation, and ionization of photoexcited long-lived superexcited H_2 molecular levels. These have recently been measured from the ionization threshold of H_2 up to the H(1s) + H(n=3) dissociation limit [4, 5] and the total and partial natural widths of these levels have been determined. Good agreement is found with first principles calculations carried out by multichannel quantum defect theory for excited levels of $^1\Pi_u^-$ symmetry. The calculations reproduce the balance between the competing decay processes autoionization, predissociation and spontaneous photon emission, as well as its substantial evolution from level to level. These results underline the importance of long-lived resonances in the collision dynamics of superexcited molecular hydrogen.

The second topic to be mentioned here involves far less numerical work; it is actually a two-channel application of multichannel quantum defect theory and it has an analytical solution. The dissociative recombination (DR) of H_3^+ corresponds to the process

$$H_3^+ + e^- \rightarrow H + H_2 \text{ or } H + H + H \qquad (1)$$

To describe this process in a simple fashion [6] we proceed as follows. The ion H_3^+ is stable - it corresponds in essence to a protonated stable closed-shell H_2 molecule. The H_3 molecule on the other hand is unstable towards dissociation; its ground state is purely repulsive, and many of its excited states are strongly predissociated. Our analysis therefore proceeds on the assumption that once an incoming electron is captured, dissociation will be immediate. In other words, the comparatively slow capture process is the rate-determining step, and it is the only one that needs to be considered explicitly. This is why dissociative recombination is approximated here by a two-channel process.

The first channel is the continuum channel corresponding to a free electron impinging on the vibrationless $v_2^+ = 0$ H_3^+ ion. The vibrational quantum number v_2^+ here denotes the non-totally symmetric degenerate bending vibrational mode of the ion (see below). The second channel corresponds to a bound $\ell = 1$ Rydberg series converging to the higher-lying $v_2^+ = 1$ vibrationally excited ion threshold. The two channels are coupled, which means that the bound Rydberg levels are broadened. Their "capture widths" describe the probability for the electron to be stabilized in the electronically bound Rydberg levels n.

From the work of Kokoouline and Greene [7] we know that the strongest vibronic coupling occurring in the H_3 Rydberg manifold involves the two degenerate in-plane pπ orbital components which are Jahn-Teller active via the degenerate v_2 bending vibration. In the framework of the two-channel model just outlined the vibronic capture/autoionization width becomes [6], based on Fermi's Golden rule:

$$\Gamma_a = \Gamma(v_2^+=1 \leftrightarrow v_2^+=0), = 2\pi \frac{2Ry}{(n^*)^3} 2\bar{D}\,\omega^2 . \quad (2)$$

Here *Ry* is the Rydberg constant and $2Ry/(n^*)^3$ is the Rydberg interval, i.e. the inverse of the Rydberg level density. $\bar{D}$ is the Rydberg-scaled Jahn-Teller parameter arising from the linear distortion term which splits the two Jahn-Teller components, while ω is the vibrational frequency corresponding to the degenerate deformation mode. The expression (2) gives the widths of successive members of a regular Rydberg series as decreasing inversely proportional to the cube of the principal quantum number, $(n^*)^3$. From this expression the average DR cross section can be obtained and good agreement with experiment is obtained [6]. This example again underlines the importance of resonant processes in the dynamics of small molecules [8].

References

[1] F. S. Ham, Solid State Phys. 1, 127 (1955).
[2] M. J. Seaton, Rep. Prog. Phys. 46, 108 (1983).
[3] U. Fano, Phys. Rev. A 2, 353 (1970).
[4] M. Glass-Maujean et al., Phys. Rev. Lett. 104, 183002 (2010).
[5] M. Glass-Maujean et al., Phys. Rev. A 82, 062511 (2010).
[6] Ch. Jungen and S. T. Pratt, Phys. Rev. Lett. 102, 023201 (2009).
[7] S.F. dos Santos et al., J. Chem. Phys. 127, 124309 (2005).
[8] Ch. Jungen and S. T. Pratt, J. Chem. Phys. 133, 214303 (2010).

Rotationally and vibrationally resolved cross-sections for dissociative recombination and (de-)excitation of H_3^+ by electron impact

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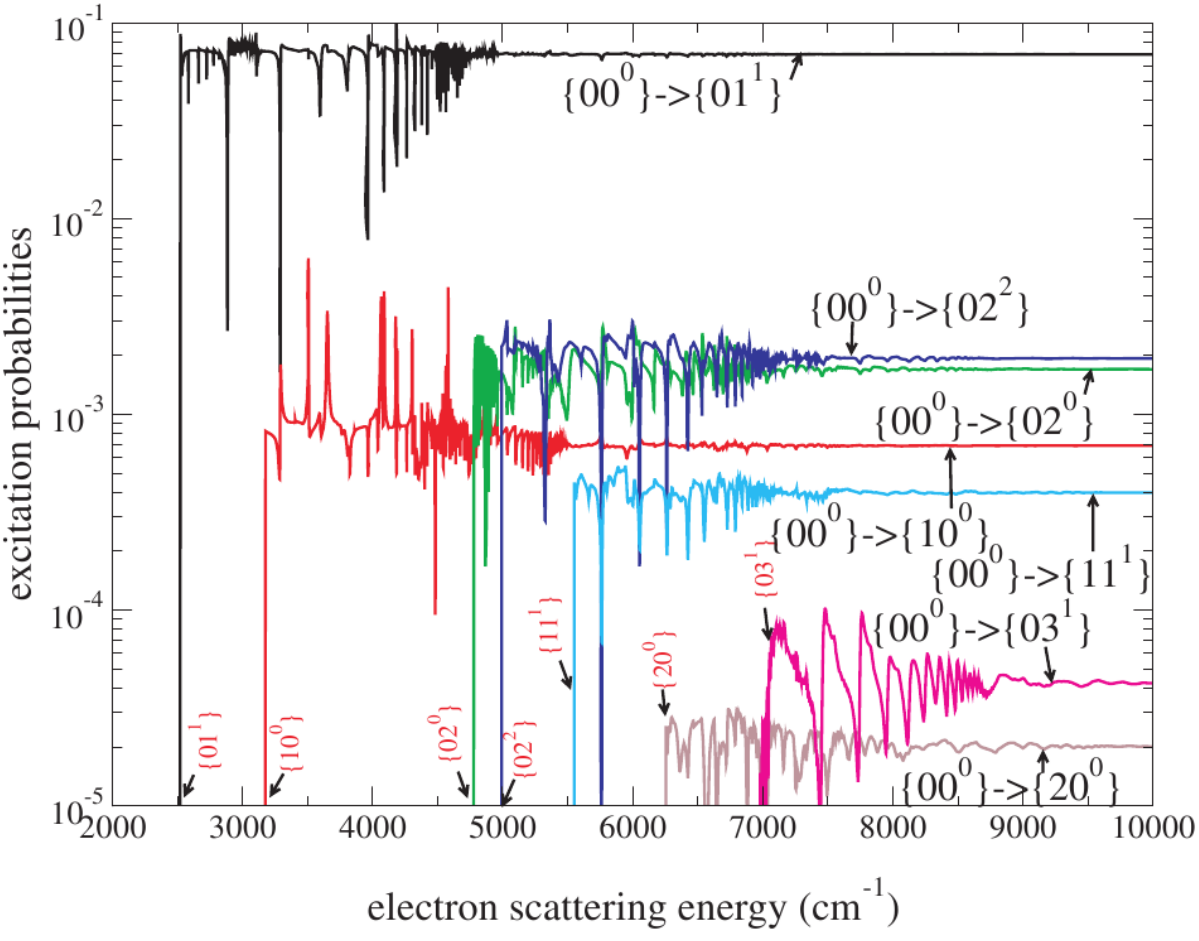
In this talk, I present results of our previous theoretical calculations of cross-sections and rate coefficients for inelastic processes in collisions between the H_3^+ ion and an electron at energies 0-2 eV. I discuss briefly the theoretical approach used to model inelastic electron-H_3^+ collisions [1-4]. In the second part of my talk, I present obtained cross-sections and rate coefficients for the dissociative recombination of H_3^+ with electrons.

The dissociative recombination cross-sections and rate coefficients are available for the ground [1-5] and excited vibrational levels [5,6] of H_3^+, for different initial rotational states [5], and as well as averaged over rotational states [5,6]. Similar calculations have been made for isotopologues of H_3^+: H_2D^+, D_2H^+, and D_3^+ [5,6]. At the end, I will present results on rotational excitation and de-excitation of H_3^+ by an electron impact [7-9]. In these calculations, the same theoretical approach was employed. Similarly to the study of the dissociative recombination, we have considered different initial rotational and vibrational states of H_3^+ [7-9].



The figure gives an example of results obtained in our study of inelastic collisions between H_3^+ and an electron. The shown curves are the probabilities of vibrational excitation from the ground vibrational level {000} of H_3^+ to several excited vibrational levels. Energies of vibrational thresholds are labelled with arrows and the corresponding vibrational quantum numbers.

References

[1] V. Kokoouline, C. H. Greene and B. D. Esry, Mechanism for the destruction of H_3^+ ions by electron collision. Nature 412, 891 (2001).
[2] V. Kokoouline and C. H. Greene, Unified theoretical treatment of dissociative recombination of D_{3h} triatomic ions: application to H_3^+ and D_3^+. Phys. Rev. A 68, 012703 (2003).
[3] V. Kokoouline and C. H. Greene, Theoretical study of the H_3^+ ion dissociative recombination process. J. Phys. Conf. Ser. 4, 74 (2005).
[4] V. Kokoouline and C. H. Greene, Photofragmentation of the H_3 molecule, including Jahn-Teller coupling effects. Phys. Rev. A 69, 032711 (2004).
[5] S. Fonseca dos Santos, C. H. Greene and V. Kokoouline, Dissociative recombination of H_3^+ in the ground and excited vibrational states. J. Chem. Phys. 127, 124309 [8pp] (2007).
[6] L. Pagani, C. Vastel, E. Hugo, V. Kokoouline, C. H. Greene, E. Bayet, A. Bacmann, S. Schlemmer, C. Ceccarelli, Chemical modelling of L183 (=L134N): an estimate of the ortho/para H_2 ratio. Astronomy & Astrophysics 494, 623 [22pp] (2009).
[7] A. Faure, V. Kokoouline, C. H. Greene and J. Tennyson, Near threshold rotational excitation of molecular ions by electron impact, J. Phys. B: At. Mol. Opt. Phys. 39, 4261 (2006).
[8] A. Faure, J. Tennyson, V. Kokoouline and C. H. Greene, Rotational excitation of interstellar molecular ions by electrons. J. Phys. Conf. Ser. 192, 012016 [6pp], (2009).

[9] V. Kokoouline, A. Faure, J. Tennyson and C. H. Greene, Calculation of rate constants for vibrational and rotational excitation of the H_3^+ ion by electron impact. Mon. Not. R. Astron. Soc. 405, 1195 [8pp] (2010).

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