IAEA
International Atomic Energy Agency

INDC(NDS) - 0730
Distr. LP,NE,SK

INDC International Nuclear Data Committee

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

Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

14-16 March 2016

Prepared by

Bastiaan J. Braams, Detlev Reiter, Xavier Urbain, Viatcheslav Kokoouline,

Dirk Wünderlich and Hyun-Kyung Chung

March 2017

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form from
http://www-nds.iaea.org/publications
or sent as an e-mail attachment.
Requests for hardcopy or e-mail transmittal should be directed to
NDS.Contact-Point@iaea.org
or to:
Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

March 2017

INDC(NDS) - 0730
Distr. LP,NE,SK

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

Summary Report of the Third Research Coordination Meeting

IAEA Headquarters, Vienna, Austria

14-16 March 2016

Prepared by

Bastiaan J. Braams, Detlev Reiter, Xavier Urbain, Viatcheslav Kokoouline

Dirk Wünderlich and Hyun-Kyung Chung

Abstract

The Third 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 14-16 March 2016 at IAEA Headquarters in Vienna. Participants reported on the last 5 years of research activities during the period of the CRP and reviewed the current status of the database on atomic and molecular processes of H and He components in fusion plasmas. The proceedings of the meeting are summarized here. Participants' summaries and future work plans are also provided.

March 2017

TABLE OF CONTENTS

1. Introduction

In the divertor and near-wall region of magnetic confinement fusion plasma experiments processes involving neutral atoms, molecules and molecular ions are important. This applies for both: plasma spectroscopy but also the dynamics of the powerful plasma flows near strongly exposed surfaces. The primary plasma constituents are hydrogen and helium and their isotopes in atomic, ionic form and the molecular and molecular ion states. All relevant species may be in rovibrationally (molecular) or electronically excited (atoms, ions and molecules) states. For a complete description one needs cross-sections for collisions with electrons, collisions among the heavy particles, photon-induced and radiative processes and processes on the walls, all resolved with respect to rovibrational excited states and with respect to the hydrogen isotope (H, D, T).

The International Atomic Energy Agency (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 established in order to review, improve and publicly expose the database on atomic and molecular processes involving hydrogen and helium. Twelve research projects in the area of experimental and theoretical atomic and molecular physics as well as collisional-radiative modeling of fusion plasmas are represented in the CRP. The first Research Coordination Meeting (RCM) was held in 10-12 August 2011 and the second RCM in 3-5 July 2013. The third RCM was held on 14–16 March 2016 at IAEA headquarter in Vienna where ten experts participated. P. Krstic and X.-W. Ma could not attend this last RCM.

This report contains the proceedings of the meeting in Section 2 and discussions and conclusions in Section 3 and 4. The list of participants is provided in Appendix 1 and the meeting agenda in Appendix 2. Presentations are summarized in Appendix 3 and made available at https://www-amdis.iaea.org/CRP/HydrogenHelium/3RCM/.

2. Proceedings

The final research coordination meeting of the CRP on Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and their Isotopes in Fusion Plasma proceeded with a welcome by A. Koning, the new section head of the nuclear data section. It was followed by a presentation on meeting objectives of B. Braams, the scientific secretary. The agenda was adopted and three rapporteurs, D. Reiter, X. Urbain and V. Kokoouline were designated to lead discussions on databases, experimental and theoretical data.

The meeting proceeded with 5 presentations by R. Celiberto, D. Reiter, K. Sawada, D. Wünderlich, X. Urbain on the first day. R. Celiberto reviewed elementary processes and thermodynamic properties of hydrogen and helium plasmas and D. Reiter on the status of state resolved hydrogen cross section database at FZ Juelich. K. Sawada presented the most up-to-date collisional-radiative (CR) model of molecular hydrogen and D. Wünderlich evaluated vibrationally resolved reaction probabilities and their application in population models for H_2 and D_2. X. Urbain presented experimental data of state-to-state charge transfer involving hydrogen and helium ions at low to intermediate energies.

The presentation continued on the second day with theoretical data and data evaluation by O. Motapon, C. Jungen, A. Larson, V. Kokoouline and J.-S. Yoon. O. Motapon presented the MQDT approach of electron/molecular cation reactive collision: Extensive calculations for H_2^+ and isotopomers and C. Jungen presented calculations of electronically excited states of HeH^+ as intermediates of $He^* + H^+$ and $He^+ + H^*$ collisions. Å. Larson presented the collaborative work with A. Orel on charge exchange recombination reactions involving the H_2 and HeH systems. V. Kokoouline presented cross sections for rotational and vibrational (de)excitation of isotopologues of H_3^+ and HeH^+ ions. J.-S. Yoon reviewed evaluated cross sections for electron impact with H, He and their molecules.

After the presentations, participants were divided into two groups where one group reviewed the status of comprehensive databases on processes of H and He in fusion boundary plasmas and the other group reviewed the computational work and the currently most needed data to be produced.

On the last day, group discussions were summarized on topics of comprehensive database on processes of H and He in fusion plasmas, experimental data of processes involving HeH^+ and He_2^+ and a list of most urgently needed data that may be obtained by computational work. A short review of processes and data for negative ion beam generation was presented. Summaries of reviews are presented in the Section 3.

Finally participants agreed to publish a CRP report of each group in the Atoms journal and discussed the possibility of data evaluation activities in the near future.

3. Discussion on data status and data needs

3.1 Status review of comprehensive database on processes of H and He in fusion plasmas

There are 4 databases presented at this CRP: K. Sawada (Nagano), D. Wünderlich (IPP), R. Janev / D. Reiter (FZJ), R. Celiberto (Bari). While data in these databases have significant differences, there are also significant inter-dependencies due to data exchange and interaction through the A+M data unit activities (between IAEA, ORNL, ADAS, NIFS etc), so they cannot be regarded as fully independent in a future evaluation process.

These data are needed for fusion applications such divertor (fusion) plasma dynamics, fusion edge plasma spectroscopy (more detailed), ancillary (low T) technical plasmas, etc. The range of applications is so wide that the recommended data should span 4-5 orders of difference in key parameters, different plasma composition, density and temperature, spatio-temporal scales. This becomes a daunting task.

The processes relevant to these applications are categorized as follows:

- $e + H \rightarrow H^*, p, H^- +$ (electrons, photons)
- $p + H \rightarrow$ charge transfer, excited states
- $e/p/H + H^- \rightarrow$ collisions with H^-
- $e + H_2 \rightarrow$ electron-molecule collisions
- $p + H_2 \rightarrow$ proton-molecule collisions
- $H, H_2, H^- + H_2 \rightarrow$ heavy-particle collisions
- Photonic processes in H_2 (photon dissociation, photon ionization, line radiation)
- $e, H, H_2, H^- + H_2^+ \rightarrow$ …..
- $e, H, H_2, H^- + H_3+ \rightarrow$…..

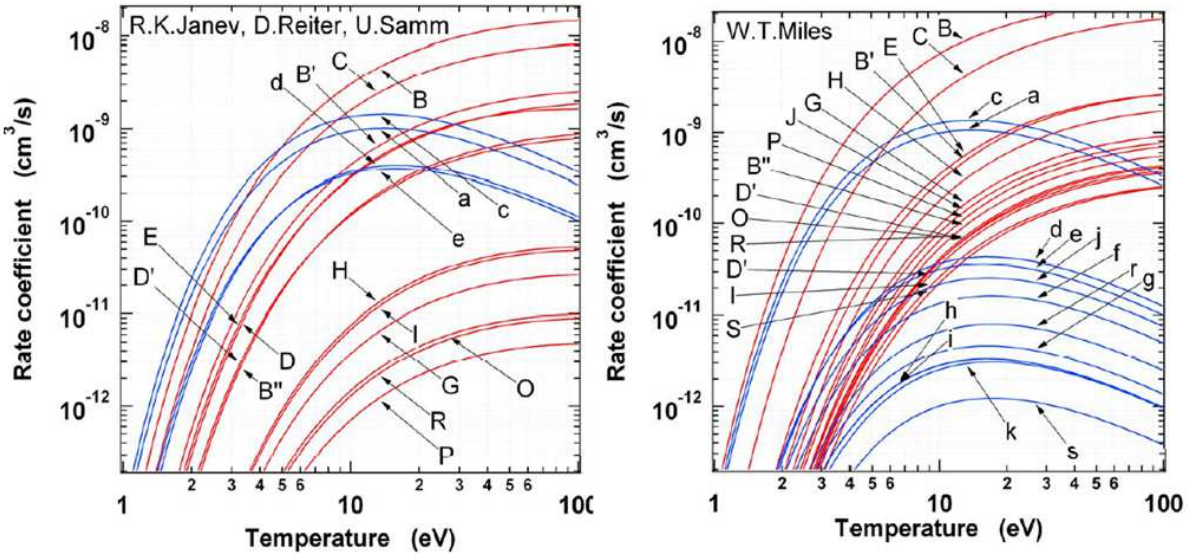
If all processes are fully state-resolved (H(n, l ,m), and H_2(N, v, J), and isotopes, isotopomeres, and He, He_2^+, HeH^+ etc) the data needs will be nearly endless. Therefore user communities should identify most sensitive sub-models and discrepancies, inconsistencies, in existing databases with respect to experimental data for single collision processes and prioritize the data needs.

The first priority, before any highly excited state process, is the vibrational distribution in the molecular ground state of $H_2(X\ ^1\Sigma_g^+, v)$ (T=0.5 – 20 eV) such as e, p, H, H_2 collisions on H_2(X, v) (v→v+1, v+2, etc) because of high v-sensitivity (in all presented databases) of processes involving H_2(X, v) and of the highest abundance of H_2(X, v), for low v values. Higher v states are less important in vibrational processes because of their typically very low population. In fusion, the vibrational distribution is mostly dominated by electrons, due to the very high ionization degree, while in atmospheric conditions, heaver particles dominate. Also surface processes influencing the H_2(X) vibrational spectrum may be relevant in fusion applications.

Also needed is the estimate from basic molecular physics to determine the relative importance of relaxation times of T_e (or eedf), T_{vib} or pdf(v), T_{rot} or pdf(v,J) as a function of (v, J) compared to timescales of interest in particular applications in order to further prioritize data needs in fusion research, which may, or may not be quite distinct from those in technical plasma applications.

A common plasma condition of interest is for electron temperature and energy, 0.5 -- 20 eV and densities n_e, n_p, n_{H2} of $10^8 - 10^{15}$ cm^{-3}. For beam heating of fusion plasmas, temperature range is 100 keV – MeV where there is no molecular component and the well-established high energy asymptotics. Mostly heavy particle collisions matter in this case.)

The second priority would be excitation/ionization cross sections to and from excited $H_2^*(\Lambda)$ or ionized $H_2^+(X)$, starting from the vibrationally resolved ground $H_2(X,v)$. The ground state $H_2(\Lambda,v)$ and $H_2(\Lambda,v,J)$ of singlet and triplet rotational-vibrational–electronical states start with the lowest N=2, N=3 states in united atom representation. Currently data evaluation is necessary for available data of this particular transition. For example, there is a significant discrepancy between data by Miles (J. Appl. Phys. 43, 678 (1972)) and by Janev (http://www.eirene.de/report_4105.pdf) .



The other issue is the data of isotopomers, for example, which reaction channels have an true isotope effect, i.e., which cannot simply be scaled if one uses ro-vibrational energy rather than v, J states of H_2, D_2, T_2, HD, HT, DT, and their ions. One such example is the DEA (dissociative electron attachment) process.

Finally, helium is an ubiquitous issue, since the main purpose of the divertor is to remove helium ash from the fusion plasma flame. Even for the e + He collisions, the full set of cross sections from R-Matrix or CCC calculations still has some issues with experimental evaluation and validation (see X.U. talk). For heavy particle collisions of p, He^{++}, He^+ + He (ground state, metastable state), theoretical data on charge exchange processes involving metastable or excited states are hardly available for experimental validation. Molecular fragmentation occurs at He_2^+ and HHe^+ at extremely low energies and for fusion relevance, formation and transport of He after molecular fragmentation should be verified.

For special applications (peripheral plasma systems with relation to fusion work, but not: fusion plasmas themselves), the following processes need to be understood:

For plasma sources, e.g. NBI sources

- e/p/H + H^- → …..
- e,H,H_2,H^- + H_2^+ → …..
- e,H,H_2,H^- + H_3^+ →…..

For planetary atmospheres, re-entry

- H,H_2,H^- + H_2 → …..

For NBI-heating, (CX, CX recombination on high Z), here: direct relevance for fusion plasma (spectroscopy)

- p + H → …..

3.2 Processes that may produce HeH^+ and He_2^+

For the formation of HeH^+ which later produce He + H, there is a very detailed ensemble of data acquired by photo ionizing H_2 with synchrotron radiation. H_2 is photo-ionized through Rydberg resonance. That is, the first field ionization of Rydberg states H_2 into a vibrational and rotational level right above threshold of HeH^+ formation. The cross-sections can be made available, parameterized for all the isotopomers. The other formation mechanism is H_2 in a vibrational level colliding with metastable He going through Penning ionization and rearrangement. This process has been well documented even for vibrational dependences. Another mechanism is that the ground state of H_2 colliding with metastable He forms HeH^+ by associative ionization (at sub eV energies) and there is no threshold. There exist also studies using thermal atoms for this process. Importance of metastable states has been well recognized for long, however their abundance, to make the above mentioned formation channels relevant for fusion plasmas, still needed to be fully established under divertor plasma conditions. It was noted that the singlet states converts to the triplet states very rapidly by super elastic collisions. In addition, the rearrangement process of H_2 + He^+ is worth investigating since He^+ may be an abundant species in fusion reactor in the (albeit narrow) transition layer between the recycling neutral He gas cloud and the main He^{2+} plasma component. The process is energetically favorable.

There are several mechanisms for the formation of He_2^+ as found in the dissociative recombination study of He_2^+ in the storage ring. When it is formed, it is in ~~the~~ highly excited states. After an effective cooling, it was measured that vibrationally excited states decay but rotationally excited states remain. Associative ionization between ground state of He and excited He also leads to He_2^+ and it is rather well understood. There is a threshold limit. In a normal He afterglow, He_2^+ is produced by three-body process (in millibar pressure plasma). All these mechanisms lead to very different vibrational distributions depending on dominant processes and plasma conditions. Their potential role in fusion plasmas still needs to be clarified.

3.3 Review of computational work, Fusion work most needed

Atomic and molecular physics theorists discussed possible collision processes to be studied related to fusion work. The list of possible processes is as follows:

- Vibrational excitation of H_2, state to state: not only the ground but also excited states as well
- Electron-impact ionization of H_2: several theoretical methods available for this study
- Dissociative ionization of HeH^+

  $e^- + HeH^+ \rightarrow 2e^- + p + He^+$
- Formation of HeH^+ : Cross sections have been measured

H_2^+ (v) + He → HeH^+ + H

- Formation of He_2^+
- Vibrational excitation, dissociative ionization of He_2^+

The H- beam:

- Cross sections for $H^- + H_2 \rightarrow H + H_2 + e^-$
- Cross sections for $H^- + H_2^+ \rightarrow H + H_2$

Particularly, there was an emphasis to produce a comprehensive data set for electron collisions with H_2, which should have been available already but is not. Modellers often need vibrationally resolved (rotationally averaged) cross-sections and sometimes use finely-resolved cross-sections (raw data) to be turned into a condensed form, case by case, of cross-sections for transport modelling. For plasma spectroscopic analysis, rotationally resolved cross-sections are critical to explain spectroscopic features. Theoretically, it is possible to treat a rotational structure separately from vibrational states and obtain a rotationally resolved cross-section.

It would be very useful to host detailed data in a publically exposed data repository so that they can be condensed as needed in an application. Also a guideline to integrate numerically over resonances (with corresponding width) or other detailed features to a condensed form would be necessary. It is noted that the finely-resolved cross-section for forward and their invers processes should be in detailed balance, even at asymptotic energy ranges; however, the averaged cross-sections may not satisfy the relationship of detailed balance and physically sound procedures for such cases have to be established.

Significant further information from experiments is needed to validate theoretical results.

3.4. Review of processes and data for negative ion sources and beam generation[-]

Cross-sections for electron collision excitation and de-excitation with molecular hydrogen are very important. However, necessary data are rather lacking in literature. There are only few vibrationally or rotationally resolved theoretical data. Even for excitation cross-sections from the ground state, there are contradictions between values from different data sources with large error bars. There are too few reliable data for most excited states of n=2 and n=3 and no reliable data at all for states with n>3. There are almost no reliable data for excitation between excited states nor for ionisation/dissociation from them.

Two classes of cross-sections for the formation of negative ions, H^- , are interesting. One class is the surface process and the other is volume process. For surface process, the surface with low work function is effective and a hydrogen atom or hydrogen molecule picks up an electron from the surface to form a negative ion. For volume process, highly (vibrationally) excited hydrogen molecule collides with an electron to form an intermediate excited hydrogen negative molecule H_2^{-*}, which dissociates to H and one H^-. Cross-sections for H^- formation are recently measured and available for relevant collision energy ranges.

There are several processes to destroy a negative hydrogen ion.

1. Electron stripping : $H^- + e^- \rightarrow H + 2e^-$
2. Mutual neutralization : $H^- + H^+ \rightarrow H + H^*$
3. Associative detachment : $H^- + H \rightarrow H_2 + e$
4. Non-Associative detachment : $H^- + H_x \rightarrow H + H_x + e$

For electron stripping, some data by Janev and Reiter are available but requires validation. The same holds true for photon detachment and its invers process: electron attachment. For mutual neutralization, H^- with H^+, H_2^+ and H_3^+, the uncertainty of the absolute rates and the branching ratios is

high. There may be a process of $H_2 + H^- \rightarrow 3\ H + e$, however, it is expected not to be a relevant channel. The atomic excited state distribution of outgoing channels is of interest. In addition, many different excitation processes of H* such as direct excitation, dissociative excitation, dissociative recombination do play a role in collision processes involving negative ions.

It is emphasized that the data needs for negative ion sources is that the plasma close to the H- generation zone is relatively cold (Te=1 eV), thus cross sections have to be known very accurately in the region close to the threshold energy, and hence in the lower energy range of the (exothermic) invers processes (this requirement is often not fulfilled by existing data that was created for application in much hotter or denser plasmas, e.g. fusion plasmas).

4. Conclusions

A final report of the CRP will be published as a special issue at the Atoms journal (http://www.mdpi.com/journal/atoms/special_issues/fusion_plasma), which is later published as a hard copy of APID (Atomic and Plasma-Material Interaction Data for Fusion) volume. B. J. Braams, X. Urbain, D. Reiter and V. Kokoouline were chosen as guest editors of the special volume.

It is recommended to organize a focused consultants' meeting on evaluation of specific data. The highest priority of evaluation is the data of molecular hydrogen, particularly vibrationally and/or rotationally resolved. Even processes involving electronic ground state as incoming or outgoing channels are lacking accurate data. Vibrational excitation data are critical while electron excitation of molecular hydrogen is desirable. Various relaxation channels through resonances should be investigated. Data for isotopes are available. Proton impact data of $p + H_2$ is available for direct vibrational excitation but their quality is debatable at least in some energy ranges. In fully ionized fusion plasmas vibrational population distribution seems to result from electron collisions. Photonic processes in H_2 such as cooling rates and spontaneous emission processes are understood at very crude level. Photonic dissociation and ionization of molecules are not well known either. For resonance lines (to the ground state) in terms of line trapping, probably only atomic hydrogen is of interest.

It is surprising but data of electron collisions with hydrogen atom is still needed for cases where H is initially in excited states. Data of processes involving states with the same n, but different angular momentum l are required in cases where they are not in thermal equilibrium such as in the low density case or in high energy hydrogen heating beams. Related to this problem which is important for line shape and intensity diagnostics, l-mixing by micro electric field may be investigated.

Data of $H^- + H_2$ is rather important for loss of negative ions. On the other hand, H^- + e/p/H process or radiative detachment, and photon induced process of H^- are less critical in terms of evaluation.

While H_2^+ is a short-living species in a typical fusion plasma environment, it may play an important role as an intermediate species to determine H_2 and H excited state populations, and hence also the dissociation degree in the neutral gas cloud. Particularly its presence is rather hidden in evaluating effective rates. On the other hand, H_3^+ could be important for laboratory/astrophysical plasmas, not for divertor plasmas, because its formation rates are small and destruction rates high, in the highly ionized plasmas (high ne/nH2 ratios) in divertors.

Appendix 1

List of Participants

Dr Asa Larson: Department of Physics; Alba Nova University Centre; Stockholm University, Roslagstullsbacken 21, 106 91 Stockholm, SWEDEN

Dr Xavier Urbain: Ecole de physique, Université catholique de Louvain, B-1348 Louvain la Neuve, BELGIUM.

Dr Ousmanou Motapon: Université de Douala – CEPAMOQ, Faculté des sciences, 237 Douala, CAMEROON.

Dr Christian Jungen: Laboratoire Aimé Cotton du CNRS, Université de Paris Sud, F-91405 Orsay, Cedex, FRANCE.

Dr Dirk Wuenderlich: Max-Planck-Institut für Plasmaphysik, Boltzmannstraβe 2, D-85748 Garching, F. R. GERMANY.

Dr Detlev Reiter: Forschungszentrum Jülich GmbH, Institut für Plasmaphysik (IPP) IEK-4, Leo-Brandt-Straβe 1, D-52428 Jülich, F. R. GERMANY.

Dr Roberto Celiberto: Department of Water Engineering & Chemistry, Polytechnic of Bari, Via Orabona 4, 70125 Bari, ITALY.

Dr Keiji Sawada: Faculty of Engineering, Shinshu University, 4-17-1, Wakasato, Nagano 380-8553, JAPAN.

Dr Jung-Sik Yoon: National Fusion Research Institute, Gwahangno 113, Yuseong-gu Daejeon, REPUBLIC OF KOREA.

Dr Viatcheslav Kokoouline: Department of Physics, University of Central Florida, Orlando, FL 32825, UNITED STATES OF AMERICA

Dr Bastiaan J. Braams: IAEA Atomic and Molecular Data Unit, P. O. Box 100, A-1400 Vienna, AUSTRIA.

Dr Hyun-Kyung Chung: IAEA Atomic and Molecular Data Unit, P. O. Box 100, A-1400 Vienna, AUSTRIA.

Agenda

Monday, 14 March **Meeting Room: C0343**

09:30 – 10:00 **Arjan Koning, Bas Braams**: Welcome, Introduction of Participants, Meeting Objectives, Adoption of Agenda.

10:00 – 10:45 **Roberto Celiberto**: Elementary processes and thermodynamic properties of hydrogen and helium plasmas.

10:45 – 11:15 *Break*

11:15 – 12:00 **Detlev Reiter**: Status of state resolved hydrogen cross section database at FZ Juelich.

12:20 – 14:00 *Lunch*

14:00 – 14:45 **Keiji Sawada**: Collisional-radiative model of molecular hydrogen.

14:45 – 15:30 **Dirk Wünderlich**: Evaluation of ro-vibrationally resolved reaction probabilities and their application in population models for H_2 and D_2.

15:30 – 15:45 *Break*

15:45 – 16:30 **Xavier Urbain**: State-to-state charge transfer involving hydrogen and helium ions at low to intermediate energies.

16:30 – 17:00 **All**: Discussion.

19:00 – … *Social Dinner (Gmoakeller, Am Heumarkt 25, 1030 Wien)*

Tuesday, 15 March

09:00 – 09:45 **Ousmanou Motapon**: Advances in the MQDT approach of electron/molecular cation reactive collision: Extensive calculations for H_2^+ and isotopomers.

09:45 – 10:30 **Christian Junge**n: Electronically excited states of HeH^+ as intermediates of $He^* + H^+$ and $He^+ + H^*$ collisions.

10:30 – 10:45 *Break*

10:45 – 11:30 **Åsa Larson (with Ann Orel)**: Charge recombination reactions involving the H_2 and HeH systems

11:30 – 12:10 **Viatcheslav Kokoouline**: Cross sections for rotational and vibrational (de)excitation of isotopologues of H_3^+ and HeH^+ ions.

12:15 – 14:00 *Lunch*

14:00 – 14:45 **Jung-Sik Yoon**: Evaluation of cross section for electron impact with hydrogen, helium and their combination molecules in fusion plasma.

14:40 – 15:30 **Roberto Celiberto**: Overview of the Phys4Entry chemical network

15:00 – 15:15 *Break*

15:15 – 17:00 **(A) Celiberto, Reiter, Sawada, Wünderlich, Yoon**: Status review of comprehensive database on processes of H and He in fusion plasmas.

(B) Motopon, Jungen, Larson, Kokoouline, Urbain: Review of computational work; future work most needed.

Wednesday, 16 March

09:00 – 09:40 **Reiter *et al.***: Status review of comprehensive database on processes of H and He in fusion plasmas.

09:40 – 10:00 U**rbain**: Processes that may produce HeH^+ and He_2^+

10:00 – 10:40 **Kokoouline *et al.***: Review of computational work; future work most needed.

10:40 – 11:00 *Break*

11:00 – 11:30 All: Miscellaneous topics

11:30 – 11:50 **Dirk Wuenderlich**: Review of processes and data for negative ion beam generation

11:50 – 13:00 ***Reiter et al****. Closing discussion*

13:00 *Close of Meeting*

Summaries by Participants

Elementary Processes and Thermodynamic Properties of Hydrogen and Helium Plasmas

R. Celiberto
Dipartimento di Ingegneria Civile, Ambientale, Edile, del Territorio e di Chimica
Politecnico di Bari (Italy) and Istituto di Nanotecnologia - CNR, Bari (Italy)

Non ideal effects, in high-density hydrogen plasmas, have been described. In particular, the ionization degree and the electrical conductivity, have been discussed at the light of the pressure ionization phenomenon. This is generated by the lowering of the ionization threshold of hydrogen atoms caused by the so-called self-energy term and by the Debye's potential, both entering in the Hamiltonian of the hydrogen atom and accounting for the collective effects of the screening charges.

A self-consistent model of non-equilibrium plasma, generated by a shock wave during the immersion of a space vehicle in Jupiter's atmosphere, has also been presented. The simulation included: a) the vibrational kinetics of H_2 molecules, b) a collision radiative model for H and He atoms, c) the plasma chemistry for dissociation and ionization, d) the Boltzmann equation for the calculation of the energy distribution function (eedf), e) radiation transport and f) the fluid dynamics equations for the description of the plasma flux. The main results, concerning gas-temperatures, molar fractions of atoms and molecules, dissociation and ionization processes and eedf as a function of the distance from the shock wave front, have been discussed.

Furthermore, elementary processes in hydrogen-helium plasma have been presented. In particular has been discussed the cross section calculation for the reaction $H + HeH^+ \rightarrow H_2^+ + He$ by using the Quasi-Classical Trajectory (QCT) method and compared with the quantum-mechanical Close Coupling (CC) method to assess the reliability of the QCT approximation. Results for vibrational an rotational processes, and comparison with the experiments have been discussed.

Theoretical calculations and experimental results for recombination of hydrogen atoms on tungsten surface were also presented. The Molecular Dynamics simulations, in a semi-classical formulation, has been discussed and the main results, represented by the recombination probability and the fraction of energy acquired by the translational and internal modes of the formed H_2 molecules, as well as by the surface, have been illustrated. Experimental measurements for the recombination coefficient have in conclusion been showed.

Finally, cross section calculations for the dissociation of He_2^+ molecular ion by electron-impact were presented. The R-matrix method, in connection with the adiabatic nuclei approximation, utilized in the work, was illustrated. The most relevant results, represented by the cross sections calculated as a function of the incident electron energy, and for processes starting from different vibration levels of the molecular ion, have discussed and interpreted at the light of the interplay between the vibrational wave functions and the vertical transition matrix.

Collisional-Radiative Model of Molecular Hydrogen

Keiji Sawada
Faculty of Engineering, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

We have constructed collisional-radiative models of H_2 and D_2 in which the electronic, vibrational, and rotational states are resolved. The levels are labeled by n, v and Λ, N, J. In these models, assuming Hund's (b) case, 4133 and 7817 levels for $n<7$ are included for H_2 and D_2, respectively.

Emission intensities of the molecules in plasmas are calculated as a function of the molecular density, the electron temperature and density, the vibrational and rotational temperatures in the ground electronic state. In order to test the newly developed models, we applied them to RF H_2/D_2 + He plasmas at Shinshu University. Electron temperature and density are determined from mixed helium atom emission intensities, and the vibrational and rotational temperatures are determined from the $d^3\Pi_u$ - $a^3\Sigma_g^+$ emission line intensities. Calculated intensities of the continuum $a^3\Sigma_g^+$ - $b^3\Sigma_u^+$ and $d^3\Pi_u$ - $a^3\Sigma_g^+$ band with these parameters well reproduce the experimental spectra. For other bands, we corrected the electron impact excitation rate coefficients from the electronic ground state in the models. As shown in Fig.1, the line intensities of the $E^1\Sigma_g^+$ - $B^1\Sigma_u^+$ and $e^3\Sigma_u^+$ - $a^3\Sigma_g^+$ bands are especially well reproduced. The models with the corrected rate coefficients can be used for the spectroscopic diagnostic of the input parameters by analyzing emission intensities of the above transitions.

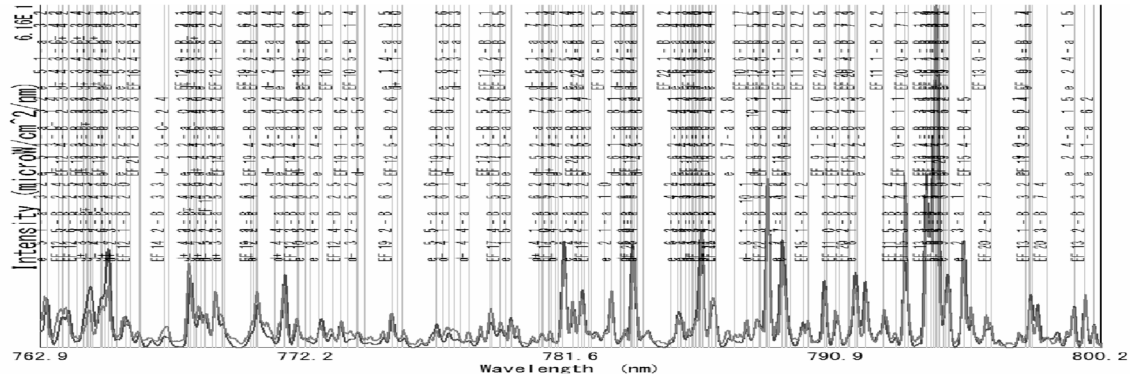


Fig.1 Spectra of D_2 (762.9 nm -800.2 nm). Experiment (gray) and calculation (black).

The models provide precise effective reaction rate coefficients for the molecular processes in plasmas. We have calculated the rate coefficients which are used in neutral transport codes.

Mutual neutralization in collisions of H^- with H^+ and He^+

Åsa Larson, Sifiso M. Nkambule and Ann E. Orel

Mutual neutralization is the reaction where oppositely charged ions collide and an electron is transferred resulting in formation of neutral fragments. Here, results from *ab initio*, fully quantum mechanical studies on mutual neutralization in collisions of H^- with H^+ and He^+ are presented. Total and differential cross sections are computed as well as final state distributions. The reactions are studies collisions of different isotopes of the cat- and anions. When possible, the calculated results are compared with measurements.

For mutual neutralization in collisions of H^+ with H^-, the calculated cross section and final state distributions agree well with measured ones. At low collision energies, the H(n=1)+H(n=3) channel dominates, while at higher collision energies, the n=2 channel becomes important. At low energies, the cross section is larger for collisions of isotopes with a large reduced mass, while at high energies the order is reversed. The differential cross section shows a dominance of backward scattering, which can be explained by the scattering amplitudes for the gerade and ungerade set of states being out of phase with each other.

Mutual neutralization in collisions of He^+ and H^- form molecular electronic states that have potential energies above the ground state potential of the HeH^+ ion. These are electronic resonant states and the potential energies, non-adiabatic coupling elements and autoionization widths of these states are computed by combining electron scattering calculations with structure calculations. The calculated total mutual neutralization cross section is larger than measured cross section at low energies, but it agrees with other measurements and previous theoretical computations at high collision energies. The inclusion of autoionization has a negligible effect on the total cross section, while the inclusion of

rotational couplings will increase the cross section for energies larger than 10 eV. The differential cross section shows a dominance of forward scattering, in agreement with other mutual neutralization reactions of other heteronuclear ions.

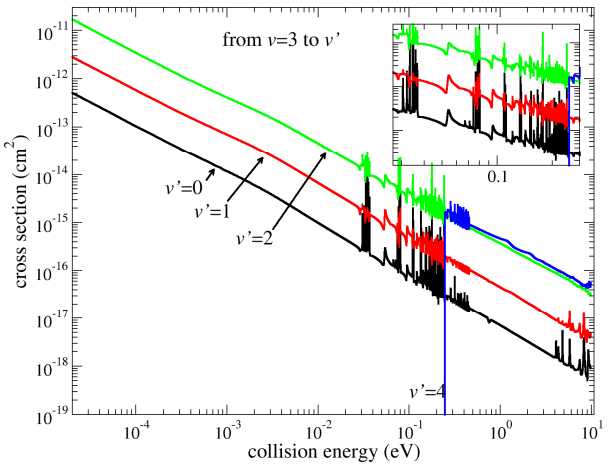
Cross sections for rotational and vibrational excitation of HeH^+ and H_3^+ ions

Viatcheslav Kokoouline
Department of Physics, University of Central Florida

Cross sections for rotational and vibrational excitation and de-excitation of the HeH^+ ion (and its isotopologues, $^{3,4}HeH^+$ and $^{3,4}HeD^+$) and the H_3^+ ion by an electron impact were calculated for collision energies between 0 and 5 eV. Cross sections were determined from scattering matrices, which were computed in a spirit of the multichannel quantum defect approach. The matrices for scattering from a particular rotational or/and rotational level rv to another one $r'v'$ were obtained from geometry-fixed scattering matrices $s(Q)$. To obtain $s(Q)$, in the case of HeH^+, the UK R-matrix code was employed. In the case of H_3^+ , the scattering matrices were constructed from quantum defects determined from *ab initio* calculations of Rydbgerg states of the H_3 molecule. Obtained cross sections exhibit Rydberg series of rotational and vibrational resonances. Examples of cross sections for vibrational (de)excitation starting from the initial vibrational level v_i=3 are shown in the figure below. If no detail about Rydberg series present in the cross sections is needed, one can average the cross sections over energy intervals between Rydberg resonances and produce a much smoother energy-dependence for such cross sections. The dependence can conveniently be represented by a simple fit formula

$$\sigma(E)=\frac{\pi}{k^2}P,$$

where k is the wave number of the incident electron, and the excitation probability P is zero if the electron energy E is smaller than the excitation energy $D_{v'v}=E_{v'}-E_v$ or P is a constant P_0 if $E>D_{v'v}$ (for de-excitation processes $D_{v'v}<0$). Therefore, the averaged cross sections are characterized by only three parameters $E_{v'}$, E_v and P_0. These parameters for collisions between HeH^+ and electrons are given in the table below for first six vibrational levels of HeH^+.



E_v (eV)	0	0.3612	0.6845	0.9696	1.2161	1.4229
	v_i=0	v_i=1	v_i=2	v_i=3	v_i=4	v_i=5
v_f=0		0.17	0.02	0.0057	0.0028	0.0012
v_f=1	0.16		0.27	0.035	0.0058	0.0021
v_f=2	0.018	0.25		0.31	0.048	0.016
v_f=3	0.0047	0.031	0.29		0.37	0.075
v_f=4	0.0021	0.005	0.044	0.36		0.5
v_f=5	0.0009	0.0017	0.013	0.069	0.48	

Advances in the MQDT approach of Electrons/molecular cation reactive collisions : Extensive calculations for H_2^+ and isotopologues

O. Motapon[1,2*], M. D. Epee Epee[1], F. Colboc[3], T. Tchakoua[1], J.Zs.Mezei[3, 8], N. Pop[4], K. Chakrabarti[3,5], S. Niyonzima[3,6], F. Argoubi[7], D. R. Backodissa Kiminou[3], M. Telmini[7]and I. F. Schneider[3,8]

1. LPF, UFD Mathématiques, Informatique Appliquée et Physique Fondamentale, University of Douala, P. O. Box 24157, Douala, Cameroon
2. University of Maroua, Faculty of Science, P.O. Box 814, Maroua, Cameroon
3. Laboratoire Ondes et Milieux Complexes, UMR 6294 CNRS and Université du Havre, 25, rue Philippe Lebon, BP 540, 76058, Le Havre, France
4. Department of Physical Foundation of Engineering, "Politehnica" University, BvVasileParvan No 2, 300223, Timisoara, Romania
5.Department of Mathematics, Scottish Church College, 1 & 3 Urquhart Square, Kolkata 700 006, India
6. Département de Physique, Faculté des Sciences, Université du Burundi, B. P. 2700 Bujumbura, Burundi
7. LSAMA, University El Manar, Tunis, Tunisia
8. Laboratoire Aimé Cotton CNRS-UPR-3321, Université Paris-Sud, Orsay F-91405, France
9. Institute of Nuclear Research of the Hungarian Academy of Sciences, P.O. Box 51, Debrecen H-4001, Hungary

We present the results of our recent MQDT based [1] computations of the Dissociative Recombination of H_2^+ and its isotopologues, and the competing processes.

On one hand, cross sections have been reported for rotational transitions (excitations and de-excitations) $N_i^+ \rightarrow N_i^+ \pm 2$ and $N_i^+ \rightarrow N_i^+ \pm 4$, with $N_i^+ = 0$ to 10, for electronic collisions energy varying from 10^{-5} to 0.3 eV for H_2^+[2], HD^+[3], D_2^+, HT^+ and DT^+. For the same systems and the same transitions, Maxwell *isotropic* rate coefficients have been presented for electronic temperatures up to a few hundreds Kelvin. A very good overall agreement is found between our results and the former computations using the Adiabatic-Nuclei-Rotation (ANR) approximation [4] for H_2^+ and HD^+, as well as with experiments [5,6] for HD^+. The cross sections, Maxwell isotropic rate coefficients of the dissociative recombination of H_2^+ and HD^+ have also been presented as a function of the initial rotational state. As well, the Maxwell *anisotropic* rate coefficients, derived from these cross sections in the conditions of the Heidelberg Test Storage Ring (TSR) experiment [5,6] have been compared with the experiments and found to agree very well. Owing to their accuracy, these data can be used in their present of fitted form in the modeling of the kinetics of the interstellar chemistry [7].

On the other hand, the extended form of our method, improved to consider two ionic states in the description of Dissociative Excitation [8-9], has been used to perform cross sections computations for Dissociative Recombination and Dissociative Excitation of H_2^+cations and their isotopologues (HD^+, HT^+, DT^+, D_2^+) with electrons with energy up to 13eV. Comparison with measurements and previous computations show an overall good agreement.

Finally systematic computations of Dissociative Recombination, Vibrational Excitation and De-excitation, Elastic Collisions, and Dissociative Excitation of H_2^+ and HD^+ have been performed in the above mentioned energy range. The cross sections and isotropic rate coefficients are available.

References

[1] A. Giusti, "A multichannel quantum defect approach to dissociative recombination", J. Phys. B **13**, pp. 3867-3894 (1980).
[2] M. D. Epee Epee *et al*, " Reactive collisions of very low-energy electrons with H2+: Rotational transitions and dissociative recombination ", MNRAS **455**, p. 276 (2016)
[3] O. Motapon *et al*, " Rotational transitions induced by collisions of HD+ with low energy electrons ", Phys. Rev. A **90**, p. 012706 (2014)
[4] A. Faure & J. Tennyson, J.Phys. **B 35**, p. 3945 (2002)
[5] D. Shafir *et al*, "Rotational Cooling of HD^+ Molecular Ions by Superelastic Collisions with Electrons", Phys. Rev. Lett. 102,

p. 223202 (2009).
[6] D. Schwalm *et al*, "Rotational Cooling of HD^+ by Superelastic Collisions with Electrons", J. Phys. : Conf. Ser. **300**, p. 012006
(2011).
[7] J. H. Black, "H_3^+ at the interface between astrochemistry and astroparticle physics", Phil. Trans. R. Soc. A **370**, pp. 5130–5141,
(2012).
[8] O. Motapon *et al*, "Electron molecular cation reactive collisions: from channel mixing to competitive processes", J. Phys.Conf. Ser. **300**, p. 012018 (2011)
[9] K. Chakrabarti *et al*, "Dissociative recombination of electrons with diatomic molecular cations above dissociation
threshold: Application to H_2^+ and HD^+", Phys. Rev. A **87**, p. 022702 (2013).

Evaluation of ro-vibrationally resolved Reaction Probabilities and their Application in Population Models for H_2 and D_2

Dirk Wünderlich and Ursel Fantz

Population models balance exciting and de-exciting reactions for excited states in atoms or molecules. In order to obtain small error bars of the results, the set of reaction probabilities included to such models has to be as complete and as accurate as possible. Especially in the case of molecules it is difficult to fulfill both requirements. Reason is the large number of excited states caused by the superposition of electronic, vibrational and rotational excitation. Even for the hydrogen molecule – the simplest existing neutral molecule – up to now huge uncertainties exist in the available cross sections for electron collision excitation.

The presentation introduces efforts made during the last years in order to improve the existing data base for H_2. Focus was laid on the step from vibrationally resolved population models toward ro-vibrationally resolved models, being of high relevance for plasma diagnostics. Due to the huge number of excited levels and interconnecting reactions, corona models (balancing only electron collision excitation from the ground state with spontaneous emission) are used instead of more complete collisional radiative models. Corona models have been constructed for the Werner ($C^1 \rightarrow X^1$) and Lyman ($B^1 \rightarrow X^1$) transitions in hydrogen and for the Fulcher transition ($d^3 \rightarrow a^3$) in hydrogen and deuterium.

Potential energy curves taken from literature have been prepared – taking in to account the adiabatic correction terms – to enable the calculation of Franck Condon factors and Einstein coefficients for hydrogen and deuterium. The semiempiric Gryzinski method was applied for calculating vibrationally resolved excitation cross sections. The cross sections have not been rotationally resolved and thus an additional process has been introduced to the models, thermalizing the rotational sublevels in the upper state of the three transitions.

The results of the corona models have been benchmarked versus measured spectra. The agreement in the position of the lines and the general structure of the emission bands is quite good. For the Werner and Lyman transition deviations in the band structure are seen that can be explained by excitation via cascades from energetically higher electronic states missing in the corona models.

In a next step, the models have been applied to spectra taken at an ICP discharge: the Werner, Lyman and Fulcher emission measured in wavelength intervals (e.g. the first four diagonal Fulcher bands) was scaled using the models to the emission of the full band. It was demonstrated that up to 21 % of the power coupled into the plasma is emitted into the VUV/UV range. Additionally, it is shown that the photon flux towards the surfaces is comparable to the ionic flux, while the atomic flux is by approximately one order of magnitude larger.

Although the presented corona models represent a valuable extension of the available set of evaluation tools, they are based on a crude procedure of ro-vibrationally resolving excitation cross sections that itself have large error bars. Full quantum mechanical calculations on such cross sections are necessary and highly desirable for improving the quality of population models for molecular hydrogen.

Electronic excited states of HeH^+ as intermediates of $He^+ + H^*$ and $He^* + H^+$ collisions

Ch. Jungen
Laboratoire Aime Cotton du CNRS, Batiment 505, Universite de Paris-Sud, F-91405 Orsay, France

More than 80 excited electronic states of the hydrohelium ion HeH^+ of $^{1;3}\sum^{+}, ^{1;3}\Pi, ^{1;3}\Delta, ^{1;3}\Phi$ and $^{1;3}\Gamma$ symmetry have been calculated ab initio up to n = 6 for internuclear distances R ranging from 0.5 out to 100 bohr [1]. The computations involve a configuration interaction (CI) treatment based on a home-made suite of programs that uses special basis sets designed for the representation of molecular Rydberg states. Except for the very lowest excited states the present energies are consistently lower than those obtained previously (available up to n = 4) [2], with an average lowering corresponding to several hundred cm^{-1}.

R-matrix calculations of low-lying Rydberg states of the hydrohelium molecular ion HeH^+ are also discussed, corresponding to $^1\Delta$ and $^3\Delta$ symmetry [3]. The calculations are restricted to the range $1 \leq R \leq 5$ bohr, but include states with principal quantum numbers $3 \leq n \leq 10$, up into an energy range which is not accessible to standard quantum chemical methods. The R-matrix code employed [4] is set up in spheroidal coordinates, which are well adapted to describe the motion of the two electrons in the dipolar two-center system.

HeH^+ is an effective one-electron system having an overall electronic structure similar to H_2^+. The interaction of the excited electron with the He^+ 1s core electron causes small singlet-triplet splittings to appear and *l*-mixing interactions to occur, that are not present in H_2^+. It is thus suggested that, for instance, charge-exchange collisions $\mathbf{He^* + H^+ \leftrightarrow He^+ + H^*}$ could be described by choosing the H_2^+ system as a starting point.

References
[1] M. Jungen and Ch. Jungen, Mol. Phys. 113, 2333 (2015).
[2] J. Loreau, J. Li_evin, P. Palmeri, P. Quinet, and N. Vaeck, J. Phys. B: At. Mol. Opt. Phys. 43, 065101 (2010).
[3] I. Bouhali, S. Bezzaouia, M. Telmini, and Ch. Jungen, EPJ Web of Conferences
[4] F. Argoubi, S. Bezzaouia, H. Oueslati, M. Telmini and Ch. Jungen, Phys.Rev. A 83, 052504 (2011)

Evaluation of Cross Section for Electron Impact with hydrogen/helium and Their Combination Molecules in Fusion Plasma

J.-S. Yoon
National Fusion Research Institute, Daejeon, Korea

Hydrogen and helium and their combination molecules are important molecules in fusion plasma and these molecules properties are studied recently. In this project, our main research object is to provide a more complete fundamental data set for electron collisions with hydrogen and helium and their combination molecules through evaluation of cross section including various processes such as ionization, excitation, recombination and attachment for electron impact with hydrogen and helium. The evaluation have been started based on previous evaluation research for H_2, D_2, HD [JPCRD 37(2), 913(2008) abd Rep. Prog. Phys. 73, 116401(2010)] and updated electron impact cross sections of vibrationally and electronically excited diatomic molecules. As a result, the electron-impact cross sections for some of the different processes for these molecules could not be reviewed in this final

result. This has left us with a partially incomplete picture of the subject and final evaluated recommended data are following:

1.Total and elastic scattering and momentum transfer cross sections
2. Rotational, vibrational and electronically excitation
3. Emission cross section
4. Dissociation
5. Ionization
6. Dissociative electron attachment

To obtain a real comprehensive picture, the following few problems have to be addressed in the near future:

1. Total electron-impact scattering cross sections (elastic + inelastic) have not been measured so far for both HD and D_2 molecules. Such measurements using the latest technology are required at all electron energies from 0 to 1,000 eV.
2. 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. These cross sections need to be measured again using a new technique.
3. No measurements for the appearance energies of HD^+, H^+ /HD and D^+ /HD are available. Also, total electron-impact ionization cross sections for HD molecules have not been reported in the literature.
4. The absolute dissociative electron attachment cross sections for HD and D_2 molecules at 300 K and at higher temperatures in the case of the 4 eV process have been measured earlier but have been found in uncertainty estimation. So, these need to be measured again. Also, no effort has been made to measure these cross sections at higher temperatures for the 8 and 14 eV processes.

Status of state resolved hydrogen/helium cross section database at FZ Jülich

Detlev Reiter

With the start of plasma operation at the W7X stellarator (Greifswald, Germany) and the accompanying plasma edge modelling activities at FZ Jülich the He cross section database as used in current edge transport codes has been re-evaluated. This is also regarded as an important step towards preparation of the first low activation phases when ITER starts plasma operation, likely with He plasmas. The current reference in these codes (EIRENE, DEGAS) for electron collisions is M. Goto, 2002, JQRST, which bases on the NIFS report: Y. Ralchenko: NIFS-DATA-59. With respect to heavy particle collisions involving He and He ions, only the resonant processes (charge exchange) seem to be relevant for edge transport modelling. Here the role of metastable n=2 states of neutral He atoms is unclear (no data, but scaling can perhaps be used). For neutral beam penetration into fusion plasmas the high energy asymptotics for a large number of processes involving He and its ions have been reconsidered and have been fixed in the EIRENE online database (www.eirene.de) on the basis of available cross sections found under https://www-amdis.iaea.org/.

Regarding the hydrogen database (involving atoms, molecules and their ions, as well as isotopomeres) there are various levels of detail in use in edge plasma transport codes, ranging from simple Corona rates, tabulated or fitted reduced collisional radiative, up to fully integrated CR models to retain the full multidimensional parametric dependency. In addition to these transport code specific datasets a state resolved cross section repository is maintained at FZJ under www.hydkin.de, for a much wider class of collision processes involving H, H^-, H_2, H_2^+, H_3^+ and their excited states, mainly for internal use but also publicly accessible. Here processes are currently grouped into 9 sub-categories:

1) electron collisions on H, H*(n), and a few also H*(nl) resolved
2) proton collisions on H, H*(n), and a few also H*(nl) resolved

3) e, p, H collisions on H^-
4) electron collisions on $H_2(N,v,J)$
5) proton collisions on $H_2(N,v,J)$
6) H, H^- and H_2 collisions on H_2
7) photonic processes in H_2
8) e, H, H- and H_2 collisions on H_2^+
9) e, H, H- and H_2 collisions on H_3^+

A number of additional cross sections in most of these categories have been added during the past few years (except 7).

With respect to 1) the nl resolved cross sections are available and apparently in good shape fully for n=2 and partially for n=3. Above n=3 only n resolved excitation, ionization and recombination cross sections are part of the database. The same applies to the invers (to radiative recombination) processes of initial (nl and n) state resolved photo-ionization of H atoms.

Processes in category 2 are mostly relevant only in the high collision energy range, except charge exchange, for which total , but only a quite limited amount of state resolved cross sections are available

In category 4 the issue is excitation and the various ionization, dissociation channels to and from electronic excited states of H_2, where significant discrepancies in databases used in fusion are still present. Only very limited information is available regarding vibrational resolved transitions, and the ro-vibrational (v,J) resolved cross sections are not considered in the present database. Most sensitive (and apparently largely unavailable, or uncertain) data might already be the v-v- transitions, already in the electronic ground state of H_2, because of the steep v dependence of many other processes in vibrational state v of the H_2 electronic ground state, such as negative ion formation or ion conversion reaction starting from $p+H_2(v)$.

Processes of category 5 are relevant in the high energy range only e.g. for neutral particle beams in fusion plasmas. Exceptions are proton induced v-v transitions. The cross sections for the latter are typically larger than those for corresponding electron impact collisions, but the rate coefficients are still significantly smaller at same temperatures.

Processes of category 6,7,8,9 have not further been upgraded very much in the past recent years in our database, because in fusion plasmas H- , H_2^+ and H_3^+ appear to remain tiny minority species under all relevant conditions. This is distinct from weakly ionized technical hydrogen plasmas, e.g. in linear plasma devices or negative ion sources, which are also relevant as ancillary systems in fusion. These ions, in particular H_2^+, may, however, be important short living intermediate states, so the balance between their formation and destruction should be correctly treated in edge plasma transport simulations. When using the present hydrogenic data repository www.hydkin.de one finds that e.g. H_3^+ becomes a relevant contributor as positive charge carrier only at very low ne/nH_2 ratios, not typically encountered unless a strongly recombining zone in a dense molecular cloud is considered.

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

E-mail: nds.contact-point@iaea.org
fax: (43-1) 26007
telephone: (43-1) 2600-21725
Web: http://www-nds.iaea.org