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IAEA Specialists' Meeting on "Review of the Status of Atomic and Molecular Data for Fusion Edge Plasma Studies"

Vienna, 11-13 September 1989

SUMMARY REPORT

Prepared by R.K. Janev

October 1989

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

This Report contains the Summary of the IAEA Specialists' Meeting on the "Review of the Status of Atomic and Molecular Data for Fusion Edge Plasma Studies" which was organized by the IAEA Atomic and Molecular Data Unit and held on September 11-13, 1989 in Vienna, Austria. The Meeting Proceedings are briefly described. Three Working Group Reports regarding the data status and data needs for fusion edge plasma modelling and diagnostics, as well as the Meeting conclusions, are also included in this Summary Report.

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1. INTRODUCTION

The motivations for organizing the IAEA Specialists' Meeting on the "Review of the Status of Atomic and Molecular (A+M) Data for Fusion Edge Plasma Studies" on 11-13 September 1989 in Vienna were twofold:

1) The understanding of plasma edge physics is aquiring an increasingly important role in the current large tokamak fusion research and, in particular, within the ITER conceptual design studies. A review of the A+M data status for edge plasmas from the point of view of the newest fusion research and ITER design needs was deemed necessary.

2) The IAEA A+M Data Unit is conducting a Co-ordinated Research Programme (CRP) on the A+M data for fusion edge plasmas (with twelve participating laboratories) which is entering its second year. The Meeting was an oportunity to review the results achieved by the participants during the first year of the programme and to up-date the priorities of the CRP.

The objectives of the Meeting were set along the above motivations, with a particular attention to the ITER design needs and the corresponding adjustments of the CRP tasks. The edge plasma physics, in which the A+M processes are of crucial importance, emerged as one of the most important research areas in the current world fusion programme. The plasma edge region, which defines the boundary conditions for the dynamics of the entire magnetically confined plasma, plays a decisive role in determining the gross energy confinement time, the plasma purity control, and the power and particle exhaust from a fusion reactor. Knowledge of the physical processes in the edge plasma is a key not only for understanding the observations on the current large tokamaks (e.g. enhanced confinement regimes, edge localized balooning modes, recycling, edge radiation, etc), but also for the design of an efficient impurity control system, a system for power and helium exhaust, and for improving the overall plasma performance of a fusion machine. The gas phase atomic and molecular processes in this plasma region determine the neutral particle transport, radiation power rates, the energy balance (and the temperature) at the edge, and, thereby, the intensity of various plasma-surface processes. The A+M processes are also the basis for most of the diagnostics of the edge plasma.

The programme of the Meeting was organized (see Appendix 1) so as to reflect the role of A+M processes in the critical issues of the current fusion research and reactor design, including review of both the data needs and the data status for the all important classes of processes. The data needs for the following fusion issues were considered: modelling of impurity and neutral particle transport in the plasma edge, edge plasma radiation losses (viability of a radiative edge), hydrogen recycling and helium exhaust, edge plasma diagnostics, and some others. The status of all A+M processes involved in the above areas was analyzed, with emphasis on: electron impact processes for the edge plasma hydrogen and impurity ions, atoms and molecules, collision processes between edge plasma heavy-particle constituents, and spectroscopic data for all plasma ege atomic (ionic) and molecular species. Besides the reviews on the data status, most of the participants also reported original, recently obtained data on specific processes.

The Meeting was attended by 23 participants and one observer (see Appedix 2).

2. MEETING PROCEEDINGS

The Meeting was opened by Mr. V.A. Konshin, Director of the IAEA Division of Physical and Chemical Sciences. Then the work of the Meeting proceeded in the following sections:

Section 1: Atomic and molecular data needs for modelling and diagnostics of tokamak edge plasmas,

Section 2: Data status and new results for electron-impact inelastic processes in tokamak edge plasmas,

Section 3: Data status and new results for ion-atom(molecule) collision processes,

Section 4: Ion(atom)-molecule inelastic and reactive collisions,

Section 5: General discussion of the data status and data needs,

Section 6: Formulation of Meeting Conclusions and Recommendations (including discussions in three working groups and a plenary session).

Section 1 started with an overview of the physics aspects of ITER design, presented by Dr. D. Post, Head of the Physics Group of ITER Team. Dr. Post highlighted the atomic physics issues in ITER conceptual design work, including their reflection in the recently suggested design- and performance-related R&D tasks in support to ITER. Particular attention in Dr. Post's talk was devoted to the A+M data needs for the power and particle exhaust for ITER, which is one of the major critical issues in the further ITER design work.

Dr. R. Hulse presented an exhaustive review on the impurity transport modelling in core and edge plasmas. The role of specific atomic processes in this transport was discussed in detail. A sensitivity analysis of impurity transport results on the accuracy of particular processes was carried out, which demonstrated that the transport in the edge plasma is highly sensitive to the accuracy of atomic data.

Dr. D. Reiter discussed in detail the required atomic and molecular database for modelling the neutral gas transport in edge plasmas by 3-D Monte Carlo codes (such as EIRENE and DEGAS). Making use of the full potential of these codes, and a proper characterization of the source terms for the plasma fluid equations provided by these codes, require knowledge not only of the total cross sections but also of the energy and angular distributions of reaction products. Adequate data formatting and data needs for the higher velocity moments were also stressed by Dr. Reiter.

Dr. P. Stangeby presented a detailed analysis of the impurity production and transport mechanisms in presently operating tokamaks. It was stressed that while the inference of impurity influx rates based on measurements of the absolute intensities of CI, CII, BeI etc. lines at the edge has become an important technique in edge impurity studies, the accuracy of "photon efficiency" numbers appear to be uncertain to a factor of two or more. Such uncertainties have significant consequences on the predictions of impurity content in the central plasma, radiated power, shielding properties of the plasma edge, etc.

Dr. A. Galkowsky reviewed the atomic processes entering in the source terms of a 2-D multifluid model for describing the transport in a divertor hydrogen- helium plasma. A detailed analysis of the required atomic database (including multistep processes) was presented along with specific results of extensive multifluid code calculations regarding the helium exhaust problem. The atomic physics required for a divertor plasma model, which describes the electrons by the Boltzmann equation and the ions within the fluid approximation, was discussed by Dr. R. Marchand. It was demonstrated that in the divertor region, under the conditions of fast ionization, the electron distribution function is not Maxwellian. A proceedure for a simple estimate of non-coronal rates was outlined.

A general review on the atomic and molecular processes underlying the edge plasma diagnostic methods was presented by Dr. H.-W. Drawin. The basic physics and its relation to observed quantities was elucidated for most of the currently used diagnostic techniques. The A+M data needs for various plasma edge diagnostics were analyzed in detail.

The current spectroscopic investigations of the tokamak edge plasmas were reviewed by Dr. A. Pospieszczyk. In this talk particular attention was paid to the atomic database required for the Li-beam based spectroscopy of the edge plasma as well as of the impurity influxes of both atoms and molecules. A better quantitative understanding of the latter is strongly needed. The corresponding atomic database required for diagnostics of a radiatively cooled plasma edge mantle was also discussed.

Section 2, devoted to the spectroscopic and electron impact database for the plasma edge, Dr. S. Trajmar presented an extensive review on the electron-impact excitation processes involving plasma edge atomic and molecular species. Both generic plasma species (hydrogen, helium, "common" and metallic and diagnostic beam atoms (Li, inert gas atoms) were included in the data status analysis. Particular attention was devoted to the data for dissociative excitation processes of molecular hydrogen, including the angular and energy distributions of dissociation products.

Dr. H. Tawara presented an overview of the database for electron-impact processes of hydrocarbon molecules, $C_k H_n$. The available data for direct ionization, dissociative excitation and ionization, particle (ion or atom) production and other impact-induced fragmentation processes were presented. Important gaps in the database for this class of plasma edge molecular impurities were identified. The defficiencies are particularly large for the partial cross sections and energy/angular distributions of products. It was stressed that under plasma edge conditions ($C_k H_n$ are usually produced on the walls of a plasma device), the hydrocarbons may have higher internal energy (e.g. vibronic excitations) than in normal laboratory conditions and, therefore, their collision cross sections may be significantly different from those measured in laboratory experiments.

Dr. I. Cadez reported on electron-impact ionization measurements of several molecular systems (H_2O, CH_3OH) and discussed the recent advances in the experimental studies of dissociative electron attachment on molecular hydrogen.

The database for electron-impact ionization of multiply charged ions was reviewed by Dr. P. Defrance. Apart from the common impurity (including metallic) ions in the plasma edge, Dr. Defrance analyzed also the database from ions from diagnostic probe beams (inert gast atoms).

Dr. W.L. Wiese presented a comprehensive review on the spectroscopic database for the plasma edge constituents. The data on the transition wavelengths, energy levels and transition probabilities for all plasma edge atoms and their ions was thoroughly discussed from the point of view of completness and quality.

The data status for the heavy particle collision processes taking place in the edge plasma region (Section 3) was discussed in three review talks. Dr. R. Phaneuf presented an exhaustive survey on the charge transfer database for impurity ion collisions with H, H_2 and He. Apart from the data for individual collision systems, scaling relationships for the charge exchange cross section (with respect to collision energy and ionic charge state) were discussed. Dr. Phaneuf reported new results for several specific charge exchange reactions obtained in a series of recent merged beams experiments.

Dr. V. Abramov reviewed an extensive database for the processes involving carbon atoms and ions from the point of view of its application in the ITER and OTR design problems. The database includes all relevant processes of carbon ions with other edge plasma constituents. Dr. Abramov also provided information on the status of atomic collision experiments with the ATOS aparatus at the Kurchatove Institute.

Dr. W. Lindinger presented a review on the ion-neutral reactions involving atomic and molecular hydrogen at near thermal energies. particular attential was paid to the cycle of hydrocarbon molecule reactions. A comprehensive survey of reaction rate coefficients for near-thermal ion-molecule reactions was presented.

Drs. H. Winter and H. Tawara discussed the influence of metastable states in the projectile ion beams (C^{q+}, O^{q+} and N^{q+}, $q \leq 2$ beams) on the electron capture from atoms and molecules. The charge exchange cross sections with ionic species in metastable states may be drastically different (higher) from those with ground state ions. Dr. H. Winter discussed the methods for determination of the metastable ion beam fraction and derivation of the cross sections for the individual beam fractions.

Dr. P. Krstic described a theoretical model for calculation of electron capture in slow-molecule collisions which also includes the vibrational states of the molecule. The model allows for generalizations to include the dissociative electron capture channel. The model was successfully applied to the $H^+ + H_2$ collision system.

In Section 4, which was devoted to the inelastic and reactive ion/atom-molecule collisions, Dr. F. Linder reviewed the data on ro-vibrational transitions and particle interchange reactions in the $H^+ + H_2(D_2)$ system, charge transfer reactions (including the dissociative channel) in low-energy molecule collisions, Dr. F. Linder reviewed the data on ro-vibrational transitions and particle interchange reactions in the $H^+ + H_2(D_2)$ system, charge transfer reactions (including the dissociative channel) in low-energy inert atoms and H_2, N_2, O_2, CO and CO_2 molecules. Particular attention in these analyses was paid to the resonant processes, the role of vibrational states and to the energy and angular distributions of reaction products.

The database for particle interchange reactions between edge plasma constituents (projectiles: $H^+(D^+,T^+)$ He^+, He^{2+}, C^+, O^+ Fe^+, Ni^+, Cu^+, Co^+, H_2^+, HD^+, D_2^+; target species: He, H_2, HD, D_2, CO, OH, O_2, CO_2, $C_k H_n$) was presented by Dr. R.K. Janev together with the initial results of an evaluation effort for about 50 reactions. This evaluation is being performed by the IAEA A+M Data Unit and will include about 100 particle interchange reactions.

In Section 5, the Meeting participants had a general discussion on the A+M data status and A+M data needs in the fusion research and then splitted into three Working Groups to discuss in detail more specific items and to formulate the Meeting Conclusions and Recommendations. The Working Groups Reports are given in the next Section of this Report, while the Meeting Conclusions and Recommendations are given in the last section.

3. WORKING GROUP REPORTS

3.1. Working Group Report on Atomic and Molecular Data Needs for Diagnostics and Modelling of Reactor-Grade Fusion Edge Plasmas

H.W. Drawin (Chairman), V.A. Abramov, R.A. Hulse, R.K. Janev
R. Marchand, and A. Pospieszczyk.
(Drs. D. Post, and P.C. Stangeby could not attend).

INTRODUCTORY REMARKS

The information on atomic and molecular (A+M) data in Plasma Diagnostics is necessary for the following purposes:

- to identify the atomic and molecular species using spectroscopic measurements (identification of spectra),

- to measure the plasma electron densities, the electron and ion temperatures and the densities of atomic and molecular species as a function of plasma facing materials, of externally imposed boundary conditions (e.g. application of ergodic limiters, etc) and of gross plasma parameters (e.g. as a function of confinement time, filling gas, ...), using spectroscopic methods, eventually in connection with other methods.

The information on A+M data in the field of Plasma Modelling is necessary for the following reasons:

- to interpret diagnostic data,

- to construct theoretical models and to evaluate these models in connection with the analysis of experimental data,

- to predict impurity effects such as radiation cooling, screening of the scrape-off layer against penetration of impurities,

- to predict and analyse wall erosion and re-deposition of wall-eroded material.

With the exception of some particular cases (see section - D), the atomic and molecular data needed for diagnostics are essentially the same as those needed for modelling.

The working group has discussed the data needs for edge and divertor plasma diagnostics and modelling. It has identified the dominant processes which take place in such plasmas, and it has identified processes and elements for which insufficient knowledge of the data still exist. They are listed and commented below. A new aspect is that due to the relative low temperatures and relative high electron densities in edge and divertor plasmas, multi-step processes become important for neutral and weakly ionized species. The consequence is that collision cross sections for the lower lying excited states must be known with some reliability.

A. SPECTROSCOPIC DATA

For the purpose of spectra identification, the wavelength tables for neutral molydenum and tungsten, and their lower ionization stages ($z < 15$), should be completed and up-dated.

It would be most useful to have photographs of molecular emission spectra for the prominent molecules H_2, D_2, T_2, HD, TD, OH, OH^+, OD, OD^+ CO, CO^+, C_2, C_2^+ and C_xH_y, $(C_xH_y)^+$, (with $x \leq 3$, $y \leq 8$), where H stands for the isotopes H,D and T. The spectra should be taken under tokamak edge plasma conditions, since the excitation conditions in such plasmas are very different from the ones in usual molecular gas discharges. The spectra should be accompanied by wavelength tables and an indication of the intensities of the prominent lines or bands.

B. COLLISION CROSS SECTIONS FOR ATOMS AND IONS

1. Hydrogen

1.1. Electron collisions

There still exist uncertainties and discrepancies in the cross-section data for excitation and ionization from the excited states. The same holds for the excitation cross-sections for the ground state atom for energies from threshold to 20 times threshold energy.

1.2. Proton collisions

Excitation and charge exchange cross-sections for collisions with excited hydrogen atoms are not well known for energies below 20 keV.

It is desirable to remove these uncertainties urgently.

2. Helium

2.1. Electron collisions

Excitation and ionization cross-sections for electrons colliding with excited helium atoms are still not sufficiently well known. Of particular interest are data for the He I 2^3S and 2^1S metastable states. Of interest are also the cross-sections for transitions between excited triplet and singlet levels for which the data are not well known.

2.2. Proton collisions

Excitation and charge exchange cross-sections for collisions between protons and excited helium atoms are not well known. Since the charge exchange collisions become more resonant with increasing principal quantum number n they could influence the level populations.

2.3. Charge exchange collisions with impurity ions

It would be of interest to have a set of charge exchange cross-sections for quasi-resonant collisions of helium with ions of the prominent impurities C^{z+}, O^{z+} and eventually Be^{z+} and B^{z+}. These collisions which populate excited levels of the (z-1) times ionized atoms could be used for diagnostic purposes when a Li-probing beam (see below) is replaced by a He-probing beam, provided the cross-sections are sufficiently large. It would be interesting to undertake the corresponding studies.

3. Lithium

Lithium atomic beams are currently used as probing beams for diagnostic purposes. In order to calculate the attenuation of beam intensity, it is desirable to include multi-step processes. Therefore the cross-section database should be completed by including excitation, ionization and charge exchange processes of excited Li-atoms with the plasma constitutents.

4. Other low-Z elements

The working group identified as the most important species the following elements:

Be, B, C and O.

4.1. Electron collisions

There is significant body of information on the electron-impact excitation and ionization cross-sections for the ground-state ions of above species based mostly on theoretical calculations. The accuracy of the excitation cross-sections of neutral and singly ionized Be is insufficient (uncertainty of a factor of two). Experimental data for excitation of these ions are, however, rather limited (see WG 2 Report).

For multi-step models excitation and ionization cross-sections involving the lower lying excited levels are needed for the neutral atoms and the first two ionization stages. Of particular interest are collisions involving the metastable levels: Be I 2s 2p $^3P^o$, $2p^2$, ^3D, BI $2s2p^2$ ^4P, CI $2s^2$ $2p^2$ ^1S, $2s^22p^2$ $^3P^o$, $2s^2$ $2p(^2P^o)$ 3s $^3P^o$, 2s $2p^3$ $^3D^o$, CII $2s2p(^3P^o)$ 2p ^4P, OI $2p^6$ ^1D, $2p^5$ 3s $^5S^o$, $2p^5$ 3s $^3S^o$.

4.2. Proton collisions

Charge exchange and excitation cross-sections are needed for the lower lying excited states of the neutral atoms.

5. Metals

The following elements are of interest for the present and future "reactor-grade" fusion plasmas:

Ti (Z=22)
Cr (Z=24), Fe(Z=26), Ni(Z=28), (Cu(Z=29))
Mo (Z=42)
W (Z=74)

5.1. Electron collisions

The electron collision cross-sections for ionization of ground state atoms and ions of Ti, Cr, Fe, and Ni are virtually complete.
This is not the case for Mo and W.

There is a lack of data for the excitation cross-sections for the neutral atoms (with the exception of Fe) and the first ionization stages of all elements in their ground state. Priority should be given to fill the gaps.

The level structrue of Mo and W in the neutral, low and medium ionization states is so complicated that it will be difficult to formulate a realistic and reliable multi-step model based on individual cross-section data. Rather, one should try to construct an atomic model on a more general basis by using scaled ionization and recombination coefficients, for instance. It is difficult to formulate any further-going recommendations.

C. COLLISION CROSS-SECTIONS FOR MOLECULES AND MOLECULAR IONS

Introductory remarks

It is not yet clear how important molecular species are in the edge plasma region. By viewing onto carbon limiters or carbon tiles, spectra of C_2, CO, CH(D) and other hydro-carbons have been identified. These spectra were emitted under stationary and stable plasma conditions. It seems that molecular H_2 (D_2) has not yet been identified with unambiguousness. Also OH has not been seen yet. However, one should not conclude that these molecules are absent or that their density is so low that their influence can be neglected. Electronic transitions in atomic hydrogen, for instance, lead to spectral lines in a relative narrow frequency band, i.e. the photon density per frequency unit is high and the spectral lines are easily measurable. Electronic transitions in the H_2 molecule lead to rotational-vibrational electronic bands whose individual spectral lines are week compared to the line intensities of corresponding electronic transitions in the hydrogen atom for the same excitation conditions (equal densities and temperature). Hence, it could be that the individual molecular line intensities are too weak to be easily detectable though the molecular densities need not to be negligible compared to the atomic density.

Since molecules influence the plasma state, the radiation losses, the particles and energy fluxes and the plasma-wall interaction in general, the members of the working group recommend that spectroscopic and cross-section data should be made available for a restricted number of molecules. These are:

H_2, HD, D_2, T_2, DT
OH, OD, OT and their ions
CO, CO^+
C_x H_y with x=1,2,3; $y \leq 8$ and H replaced partly or completely by the isotopes D, T.

The hydro-carbons C_x H_y are formed by interaction of the plasma with carbon containing plasma facing components. The hydro-carbon chemistry probably plays an important role in the wall erosion process.

For diagnostic purposes and for modelling the following data are needed.

1. Spectroscopic data

- see Section A -

2. Cross-sections for electron collisions

Electron collision cross-sections are needed for:

- direct excitation of electronic states
- direct ionization
- dissociation
- dissociative excitation
- dissociative ionization.

Since it is impossible to take into account in the models the individual rotational and vibrational states, it is recommended that the cross-sections are weighted over rotational and vibrational state distributions typical for tokamak edge plasma conditions. These could be different from those in usual gas discharges.

In order to test the influence of multi-step processes it would be useful to have the cross-sections also for collisions with some prominent lower lying excited electronic states, in particular for H_2 (D_2, HD,...).

3. Cross-sections for proton (deuteron, triton) collisions

Proton collision cross-sections are needed for:

- dissociation
- charge exchange
- particle interchange.

To permit a multi-step treatment it would be useful to have data involving the lower lying excited electronic states (in particular H_2, D_2, HD,...) for the following processes:

- electronic excitation,
- direct ionization,
- dissociative excitation,
- dissociative ionization.

As for the electronic collisions, the cross-sections should be weighted over rotational and vibrational state distributions, typical for tokamak edge plasmas.

D. COLLISION COEFFICIENTS AND HIGHER VELOCITY MOMENTS

For pratical applications the collision coefficients $\langle \sigma v \rangle = \langle \sigma v_{rel} \rangle$ are needed.

Monte Carlo calculations (and kinetic calculations in general) require knowledge of the following velocity moments (for neutrals only)

$$\langle \sigma v_{rel} \rangle \, , \, \langle \sigma v_{rel} , v_{p,e} \rangle \, , \, \langle \sigma v_{rel} , v_{p,e}^2 \rangle$$

Calculation of these quantities requires the integration of:

$$F(0, \infty) = \int_{v=0}^{\infty} f\ (v')\ dv'$$

For the Monte-Carlo calculations it is essential to know the velocity distributions of reaction products as function of pre-collision velocities.

The data for H, H_2 and He, including multi-step processes, are most urgently needed. Polynomial fits, similar to those in the book of Janev et al (Springer, 1987), would be an adequate representation of the data.

3.2. Report of Working Group on the Status of Spectroscopic and Electron Impact Data Bases

S. Trajmar (Chairman), H. Tawara (Co-chairman),
W. Wiese, I. Cadez, P. Defrance

1. Spectroscopic data base

The principal spectroscopic quantities are the wavelengths of spectral lines and their classifications, the atomic energy levels and molecular potential energy curves and the transition probabilities. For most species of interest to fusion edge plasmas, the wavelength and atomic energy level data are quite complete and of high quality, while there are more gaps in the molecular data and transition probabilities, and the quality of the latter is often quite low. Table 1 provides a summary of the current spectroscopic data status, both with respect to completeness and quality of the data. It shows that the principal data needs exist in the following areas:

a) Atoms and ions: some of the transition metals (for example Ni), the heavy noble gases and heavy metals (Ta and W). Also, the data on transition probabilities need to be greatly improved in quality.

b) Molecules, including molecular ions: all species mentioned in recent IAEA (and other) summary reports, except

H_2, HD, D_2, O_2 and CO, H_2^+, O_2^+ and CO^+.

Many data are critically evaluated and compiled in a series of books and reports. These are listed in the recent review by Janev et al (Nuclear Fusion, 29, 109 (1989)).

2. Electron collision data base

a) Introduction

Electron collision processes involving atomic, molecular and ionic species play an important role in edge-plasma physics. From the point of view of plasma behaviour and diagnostics, the important species are: H, He, Ne, Ar, C, O, Li, B, Be, Si, Cu, Al, Ti, Cr, Fe, Mo, Ni, Zn, Ta, W, H_2, CO, N_2, O_2, H_2O, and hydrocarbon molecules as well as their ions and H_3^+. In addition to the ground state species in some cases (He, ions) the metastable states and for H_2 and other molecules the vibrationally excited molecules also have to be considered. The highest priorities are H_2, H_2^+ H_3^+, and the hydrocarbons.

b) Electron impact excitation of neutral atoms and molecules

Under electron impact excitation we consider elastic scattering, momentum transfer, excitation (rotational, vibrational and electronic, including various dissociative channels), and total electron scattering. Tables 2 and 3 summarize the status of atomic and molecular cross section data, respectively. (The case of hydrocarbons is discussed separately in section d).

Elastic scattering, momentum transfer and total electron scattering cross sections are available for all species over a wide energy range with satisfactory accuracy. Rotational excitation cross sections can be

Table 1: Status of Spectroscopic Data

Species	Wavelengths Coverage*	Wavelengths Quality**	Energy Levels Coverage	Energy Levels Quality	Transition Probabilities Coverage	Transition Probabilities Quality
(a) Atoms and moderately charged ions:						
1. H, He, He^+	1	A^+	1	A^+	1	A^+
2. Li, Be, C, O, Ne	1	A^+	1	A^+	1	A–B
3. Fe	1	A^+	1	A^+	2	B–C
4. Al, Si, Ar. Ti, Cr, Ni	1	A^+	1	A^+	2	B–C
5. Kr, Xe, Zr, Mo, Ta, W	2–3	A^+	2–3	A^+	2–3	B–D
(b) Molecules:						
H_2, HD, D_2, O_2, CO, H_2^+, O_2^+, CO^+	1	A^+	1	A^+	2	A–B
All other species of interest	3	–	3	–	3	–

* Coverage: 1 = Quite complete
2 = Substantial gaps in the data
3 = Little or no data available

** Quality : A = High accuracy (A^+ means much better than ± 3 %)
B = Good accuracy, normally uncertainties smaller than ± 10 %)
C = Accuracy within ± 25 %
D = Accuracy is factor of two or worse

Table 2. Summary of Experimental Atomic Excitation Cross Section Data

Species	Elastic	Excitation	σ^M	σ_{TOT}	Opt.
H	h	h	h	h	h
He	h	h	h	h	h
Ne, Ar, Kr, Xe	h	m	h	h	m
O	m	m	-	-	l
C	-	-	-	-	-
Li	m	m	m	h	m
Cu	m	l	m	-	m
Si, Be, Al, Ti *Cr, Fe, Mo*	-	-	-	-	l
Ni, Zr, Ta, W	-	-	-	-	-

h, m and l refer to high, medium and low degree of data availability. Opt. designates optical excitation functions.

Table 3. Summary of Experimental Molecular Excitation Cross Section Data

Species	Elastic	Excitation				σ^M	σ_{TOT}	Opt.
		Rot.	Vibr.	El. D.	El. C.			
H_2	h	m	h	m	m	h	h	m
CO	h	(m)	h	l	l	h	h	m
N_2	h	(m)	h	h	m	h	h	m
O_2	h	-	m	h	l	h	h	m
H_2O	h	(m)	m	-	l	h	h	m
CO_2	h	(m)	h	-	l	h	h	m

h, m and l have the same meanings as in Table I. El. D. and El. C. refer to electronic discrete and continuum state excitations, respectively. Opt. refers to optical excitation functions.

directly measured only for H_2 by the present experimental techniques and obtained by unfolding from the shape of the elastic scattering feature (with some assumptions) for other simple molecules. Sufficient information is available for H_2 but not for more complex species. Vibrational excitation cross sections are reasonably well covered in the important low-energy range except for O_2 and the hydrocarbons. There are serious gaps in the data concerning electron impact excitation of electronic states of molecules. Cross sections for many discrete state excitations are missing or limited in energy ranges. Cross section data at low impact energies and the role of resonances at these energies need to be investigated. The situation for the excitation of continuum electronic states which lead to dissociation in general, and especially to dissociation into neutral ground state fragments, is unsatisfactory. Much more work is required concerning the kinetic energy distribution of all dissociation fragments (including all neutral and charged species). The emphasis should be on H_2, H_2^+ and H_3^+ and the hydrocarbons.

Electron collision cross sections for metastable He and certain ions are also needed.

The status of theoretical calculations are in good shape as far as atomic species are concerned. Excitation and ionization cross sections for any atom (in any ionization state) can be calculated with accuracy which is satisfactory for most modelling and diagnostic purposes. The same can not be said for molecules for which the theoretical calculations are more complicated and much less reliable. The methods and approximations of theory should be checked against experiments to establish their validity.

c) Electron Impact Ionization of Natural Atoms and Molecules

Electron impact ionization cross sections for most of the atoms have been measured and can be calculated quite reliably.

The situation is more complicated and less satisfactory for molecules. In this case the following remarks are made:

1) Total ionization cross sections should be known to the accuracy $\leq \sim 15\ \%$ for the ground state molecules of interest: H_2, D_2, CO, CO_2, C_2, C_mH_n, H_2O. The reasons for the present disagrements should be clarified in order to achieve this task. Deuterated (tritiated) species are important to be studied as well.

2) Some partial cross sections exist and should be rechecked and extended in addition to (1). Parallel checks in different laboratories are welcome.

3) Angular and energy distributions of ions from dissociative ionization are generally poorly known. The present status of the experimental techniques allows the determination of these functions and this work should be done in near future.

4) Ionization cross sections for excited particles and fragment neutral molecular species are of extreme importance and they are generally unknown. For some cases ($H_2(v)$ for instance) they were obtained by simple calculations but, generally, the experimental determinations are needed. It is a long-term task and this work is related to the development of the particular target sources.

5) Vibrationally excited hydrogen (H_2, HD, D_2) is certainly present in edge plasmas and the dissociative attachment (DA) process for these molecules should be further studied in detail. The strong dependence of the DA cross sections on ro-vibrational excitation allowed the development of the diagnostic technique for $H_2(v)$ population determination. This diagnostic technique may be applied in independent experimental studies of the $H_2(v)$ production and interaction with other partners. Due to the high DA cross sections for high v, dissociative attachment should be included in the list of dissociative processes of importance for plasma modelling.

d) Hydrocarbon data

Production mechanisms of hydrocarbons from graphite-covered fusion devices are quite complicated. Very little is known on molecular species present near edge region. Mass spectroscopic (laboratory) observation under proton bombardment on graphites shows that CH_4 is the most dominant and that fairly large amount of C_2H_m(m=2,4,6) and C_3H_n(n=4,6,8) are produced. Through a survey based on this finding, the present situation on AM data can be summarized as follows (see Tables 4 and 5):

1) Substantial data are available only for CH_4.

2) Total ionization cross sections for various hydrocarbons seem to be reasonably well established.

3) Partial ionization cross sections (for production of H^+, H_2^+, $C_mH_n^+$) are limited and, moreover, the data are scattered, in particular at low energies.

4) Total and partial hydrocarbon dissociation cross sections are known only for a few hydrocarbon molecules and they are not reliable.

5) Energy and angular distributions of products (ions, atoms, molecules, radicals) are only little known.

6) Dissociation sections vary significantly depending on the internal energy of the parent molecule.

7) Internal energy states of dissociation products have to be known.

8) Great care should be exercised when laboratory data are applied to plasma modelling and diagnostics.

9) Cross sections of photon emissions for molecular bands and for ions are still scarce.

10) More systematic measurements are needed for hydrocarbons other than CH_4.

e) Electron Impact Excitation of Atomic and Molecular Ions

Electron impact excitation cross sections for ions have been determined only in very few cases and mainly for singly charged species. At the present time one must rely on calculated data. Recent developments concerning ion sources (both for singly and multiply charged species), merging beam and storage ring techniques indicate great possibilities in this area.

f) Electron Impact Ionization of Multiply Charged Ions

Electron impact ionization is the dominant mechanism for ion production in plasma. Multiply charged ions exist in the edge plasma especially at low charge states, according to the low electron temperature (< 500 eV).

Reviews and compilation of recommended cross sections for electron impact ionization of ions have been published between 1982 and 1987. Many experimental and theoretical results have been produced after these publications. Ion species relevant to fusion edge plasma are reviewed here.

Investigated atomic species are: C and O (impurities), Ne and Ar (diagnostics) and metallic ions (Ti, Cr, Fe, Ni). Only ions with ionization potential lower than 500 eV are collected.

Table 4: The present status of A+M data for hydrocarbons by electron impact

	CH_4	CH_3	CH_2	CH	C_2H_2	C_2H_4	C_2H_6	C_3H_4	C_3H_6	C_3H_8
Elastic	o				o		o			o
Inelastic	o				Δ		Δ			Δ
Excitation										
Dissociation										
Total	o						o			o
Partial										
Ionization										
Total	o	o	o		o		o		o	o
Partial	o	Δ	Δ		Δ		o			
Photon Emission	o				o	o	o			

o: fairly good
Δ: available but large uncertainties

Table 5: The present status of A+M data for hydrocarbon ions by electron impact

	CH_4^+	CH_m(m=1,2,3,5)
Ionization	Δ	
Dissociation	Δ	
Recombination	o	o

o: fairly good
Δ: available but large uncertainties

Experimental data show:

1) Evidence for individual resonant excitation followed by double autoionization (REDA) processes for C^{3+} and O^{5+},

2) presence of metastable states: their population may be of order of 100 % in some cases.

The theory is generally in good agreement with experiment for ground state or excited states ions, although there are some exceptions (in the Ni homonuclear sequence for instance). For many electron systems, calculations must include direct processes and indirect (excitation-autoionization) and also include branching ratios for radiative decay and autoionization of doubly excited states.

The role of metastable excited states in the plasma is related to:

1) the lowering of the effective ionization potential for a particular ion. The shift is order of a few eV for complicated systems and is maximum for helium-like ions ($\approx$ 300 eV for C^{4+}).

2) Cross sections are larger for metastable than for the ground state, according to classical scaling laws. Again, the effect is maximum for helium-like ions (an order of magnitude).

Future needs are:

1) The experimental work must be pursued: many data are missing: Cr^{q+}, Fe^{q+}, Ni^{q+} for $q < 5$; Fe^{7+}, Fe^{8+} and other atomic species: Al, Si, Ti, Mo, W ...

2) A particular attention must be given to the presence of metastable states (possibility of "on-line"-population estimation). Additional question: does the observed metastable population reflect the true population in the plasma?

3) Existing theory must be applied for all mentioned cases. Question: can the reported discrepancies between theory and experiments be explained?

g) Conclusions

The principal needs on spectroscopic data are to fill the data gaps on the heavier elements and molecular species of interest, and to substantially improve the transition probability data.

The large body of electron collision cross section data which is required for the understanding of edge-plasma behaviour can not be generated by experimental work alone. The large number of species, collision processes and the wide range of impact energies simply overwhelm the experimental capabilities. Some of the measurements are extremely difficult, time consuming or simply impossible. Theoretical calculations utilizing larger computers could produce the necessary data in most cases but their reliability has to be checked against measured cross sections. Clearly a joint experimental/theoretical approach is required. Benchmark measurements should be carried out and used to check out theoretical models and approximations. The measurements then should be complemented by calculated data.

Modellers should give guide by narrowing down the data requirement based on the importance of the particular data on the plasma behaviour or on its value in plasma diagnostics.

3.3. Report of Working Group on the Status of the Database for Heavy Particle Collisions in the Plasma Edge

R. Phaneuf (Chairman), F. Linder, W. Lindinger, R. Krstic, V. Piksaikin and J.J. Smith

1. Relevant species

The number of possible combinations of reactants for collisions between heavy particles in the edge plasma is enormous. As a first step in assessing which reactions will be most important, it is instructive to categorize the species present in the edge plasma in terms of their relative abundances. The categories listed below are presented in order of decreasing relative abundance. Included are species most often present in current devices, as well as those expected in D-T fusion reactors.

a) Primary plasma constitutents:

H^+, D^+, T^+, H, D, T

H_2, D_2, T_2, HD, HT, DT

H_2^+, D_2^+, T_2^+, HD^+, DT^+, HT^+

He, He^+, He^{2+}

H^-, D^-, T^-

b) Dominant impurities:

C^{q+} (q=0-6), O^{q+} (q=0-8)

c) Metallic impurities:

Fe^{q+}, Ni^{q+}, Cr^{q+}, Ti^{q+}, Be^{q+}, Mo^{q+}, W^{q+} (q=0-10)

d) Molecular impurities:

C_mH_n, C_m, CO, O_2, CO_2

$C_mH_n^+$, C_m^+, CO^+, O_2^+, CO_2^+

e) Diagnostic species:

He^{q+} (q=0-2), Li^{q+} (q=0-3), Ne^{q+} (q=0-10)

2. Classes of data

a) Total cross sections: (integrated over angles, product states),
b) Partial cross sections: (for specific product states),
c) Product distributions: (differential in product kinetic energy and/or angle, particularly important for neutral products),
d) Reactant states: (e.g. metastable states, vibrational/rotational states)
e) Reaction rate coefficients: (maxwellian or other velocity distribution)

3. Collision processes

In general, in the temperature range of interest in the plasma edge, 0.1 eV < T < 500 eV, only heavy-particle collision processes that are resonant or exothermic will have sufficiently large cross sections or rate coefficients to play a significant role. Endothermic processes having threshold energies ranging from several eV to tens of eV, such as excitation and ionization, have maximum cross sections at energies of tens of keV, and will have negligibly small cross sections at edge-plasma energies. The relative importance of a process in the edge is also determined by the relative abundances of the reactants. For example, a process involving two primary constituents will be more important than one involving one primary constituent and an impurity, which will in turn be more important than one involving two impurity constituents. A survey of edge-relevant processes based on the above criteria follows. It is understood that where they are not specified, the isotopes D and T may be substituted for the chemical symbol H. The symbol M is used to designate any of the metallic impurities listed in the previous section. Long-lived excited or metastable states may also play an important role in the edge, since collision processes involving such states may have large cross sections. The role of excited levels becomes increasingly important at higher densities, where times between collisions may become less than radiative lifetimes.

a) Charge exchange:

i) H^+ + H, H_2, He, H^-, C_mH_n, CO O_2, C, O, Li, O_2
Total and state-selective cross section data are available for most of these reactions. The data on product distributions and well-characterized reactant states is very sparse.

ii) C^{q+}, O^{q+}, He^{q+}, M^{q+} + H, H_2, He (M-metal)
Total cross-section data are available for all C^{q+} and O^{q+} charge states, and for Fe^{q+} + H, H_2 for q > 2. Partial cross-section data are available for approximately half of the C^{q+} and O^{q+} cases. No state selective data are available for the metal ions, and a semi-empirical scaling formula is all that is available for the total cross sections for q > 4 (accuracy within a factor of 2).

iii) H_2^+, $C_mH_n^+$, CO^+ O_2^+ + H, H_2, He
Cross-section data are available for some of these reactions involving molecular ions, but they have not been surveyed or compiled.

iv) Li^{q+}, Ne^{q+} + H, H_2, He
Total and partial cross-section data are available for some of these reactions, but they have not yet been surveyed or compiled.

b) Particle interchange reactions:

i) H^+, D^+, T^+ + H_2, D_2, T_2, HD, HT, DT

ii) He^+, He^{2+} + H_2, D_2, T_2, HD, HT, DT

iii) H^+, D^+, T^+ + C_mH_n, CO, O_2, CO_2

iv) H_2^+, D_2^+, T_2^+, HD^+, HT^+, DT^+ + H, D, T, He, H_2, D_2, T_2, HD, HT, DT

v) C^+, O^+ + H_2, D_2, T_2, HD, HT, DT

vi) M^+ + H_2, D_2, T_2, HD, HT, DT

vii) $C_mH_n^+$, CO^+, CO_2^+, O_2^+, HeH^+, HeD^+, HeT^+ + H, D, T, H_2, D_2, T_2, HD, HT, DT, He

viii) M^+ + C_mH_n, CO, O_2, CO_2

Total and/or partial cross-section data are available for some of these reactions, as well as data for reactions in which the initial vibrational state of the molecular ion is specified. Surveys and compilations of data for these reactions are incomplete at this time. The most comprehensive data available are those for reactions involving hydrogenic ions and molecules.

c) Energy Transfer Collisions:

i) Momentum transfer
ii) Rotational/vibrational excitation
iii) Excitation transfer (internal)
iv) Electronic excitation, ionization, dissociation

Data exist for some of these processes at energies relevant to the edge plasma, particularly for atomic and molecular hydrogen neutrals and ions. Fine-structure transitions are the most important of the internal electronic excitation transfer reactions. Electronic excitation, ionization and dissociation reactions are endothermic and are not important heavy-particle reactions at the low temperatures prevailing in the edge plasma because of their negligibly small cross sections.

4. MEETING CONCLUSIONS AND RECOMMENDATIONS

The three day discussions and presentations of the Meeting participants regarding the A+M data needs and A+M data status for fusion edge plasma studies can be summarized as follows:

1) Atomic and molecular processes taking place in the plasma edge region of present-day large tokamak experiments are a major factor determining the plasma edge conditions (plasma properties, parameters, dynamics) and thereby influence the overall plasma performance. Knowledge of quantitative characteristics of these processes is critical for modelling and diagnostics of edge plasmas, interpretation of experimental observations, and prediction of plasma behaviour and properties. Design of the next step fusion devices (such as ITER, NET, OTR, FER, etc), particularly the impurity control and power and particle exhaust system, is essentially determined by the plasma edge atomic physics.

2) Due to the low plasma temperatures, high plasma and neutral gas densities, and presence of molecular species, the range of spectroscopic and collisional properties of edge plasma constituents is extremely wide. The range of collisional processes is particularly expanded due to the fact that the edge plasma is in a collisional-radiative regime (collisions of excited species important).

   The current large tokamak experiments and the ITER design activity have revealed significant gaps in the A+M data base for the plasma ege studies. These gaps are particularly important for the processes involving low charge state ions of metallic impurities (Be, B, Ti, Fe, Ni, Cr, V, Mo, W), for the processes involving excited (electronic and ro-vibrational) states of basic edge plasma neutral constituents (H, H_2, He), for the collisional and spectroscopic properties of molecular edge plasma impurities (particularly the hydro-carbons), and for the angular and energy distributions of reaction products. The required accuracy for the dominant A+M processes in the plasma edge (from both modelling and diagnostic point of view) is $\lesssim$ 10-15%.

3) The status of spectroscopic and electron impact databases for the basic edge plasma constituents (H, H_2, He) and common impurities (C,O) is in a satisfactory form, except for the collision processes involving excited states. The collisional database for metallic impurities and the spectroscopic database for the high-Z impurities (Mo,W) is rather fragmentary and less reliable. Very sparce are also the data for electron-molecular impurity collision processes, particularly for hydro-carbons (with exception of CH_4). The information regarding the product energy and angular distributions is either incomplete (as for H_2, H_2^+) or missing (other molecular species). The electron-impact processes with ro-vibrationally excited molecules is also rather sparce.

4) Most important heavy-particle collision processes in the plasma edge are those which are either exothermic or resonant. Charge exchange, particle exchange and fine-structure transition processes may belong to the above categories. The charge exchange database is virtually complete for the H, H_2 and He neutral colliding with C^{q+}, O^{q+} and Fe^{q+} ($q \gtrsim 3$). The data for other metallic impurities in low charge states is very fragmentary. Particle exchange reactions involving hydrogenic species are available but in most cases from only one or two sources. Critical evaluation of these data is, therefore, difficult. Dissociative particle exchange reactions are also poorly documented, particularly for hydrocarbons. Information is also missing about the influence of plasma environement on both electron- and heavy-particle-impact processes with complex molecules (such as hydrocarbons), which under plasma conditions may have different internal energy content (ro-vibrational or electronic excitations) with respect to laboratory experiment conditions.

5) Given the new emphasis and shifts in the A+M data needs for edge plasma studies (increased interest in Be, B and metallic impurities, Li-, He-, and Ne , diagnostic beams, inclusion of processes involving excited species in modelling codes, required information on reaction product angular and energy distributions, all processes of hydro-carbons and metallic carbides, etc), some more intensified data production activity would be desirable to fill in the existing gaps in the database. It has been recommended that adjustments in the research programmes of the participants in the IAEA Co-ordinated Research Programme on "Atomic and Molecular Data for Fusion Edge Plasmas" are made accordingly, whenever possible.

6) In order to involve a larger number of experts in the plasma edge A+M data compilation and evaluation process, the Meeting participants have suggested preparation of a number of review articles for the most important classes of collision processes in the plasma edge. The reviews should be prepared by the middle of 1990 and be published in vol. 2 of the Nuclear Fusion Supplement Series on "Atomic and Plasma Surface Interaction Data for Fusion".

IAEA Specialists' Meeting on "Review of the Status of Atomic and Molecular Data for Fusion Edge Plasma Studies"

11-13 September 1989, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, September 11

9:30 - 9:45 : Opening: V.A. Konshin — Room C07-VI

Section 1: Atomic and Molecular (A+M) Data Needs for Modelling and Diagnostics of Tokamak Edge Plasmas

Chairman: H.-W. Drawin

9:45 - 11:00:
- D. Post: Atomic physics issues for ITER power and particle exhaust
- R. Hulse: Atomic and molecular data needs for impurity transport modelling

11:00 - 11:20: Coffee break

11:20 - 12:00: D. Reiter: Atomic and molecular data needs and formats for neutral gas transport models

12:00 - 14:00: Lunch

Section 1: Continued

Chairman: D. Reiter

14:00 - 15:40:
- Stangeby: On A+M data needs for plasma edge studies in present tokamaks
- A. Galkowski: Helium exhaust problem and A+M data needs
- R. Marchand: Atomic processes in Boltzmann simulation of divertor plasmas

15:40 - 16:00: Coffee break

16:00 - 17:00:
- H.-W. Drawin: A+M data for edge plasma diagnostics
- A. Pospieszczyk: A+M data for spectroscopic edge plasma diagnostics

Tuesday, September 12

Section 2: Data status and new results for electron-impact inelastic processes in tokamak edge plasmas

Chairman: R. Phaneuf

9:00 - 10:45: S. Trajmar: Electron-impact excitation of atoms and simple molecules of interest to fusion edge plasma studies

H. Tawara: An overview of hydrocarbon data

I. Cadez: Measurements of electron-impact ionization cross sections for molecules

10:45 - 11:00: Coffee break

11:00 - 12:00: P. Defrance: Electron-impact ionization of multiply charged ions

W. Wiese: Spectroscopic data for the plasma edge constituents

12:00 - 14:00: Lunch

Section 3: Data status and new results for ion-atom (molecule) collision processes in tokamak edge plasmas

Chairman: F. Linder

14:00 - 15:40: R. Phaneuf: Charge exchange collisions in the plasma edge: Data status and new results

H. Tawara: Electron capture by C^+, N^+, O^+ ions at low energies: influence of metastable ion beam states

H. Winter: Electron capture in low energy ion-atom/molecule collisions in the presence of metastable ion beam fractions: C^{q+}, O^{q+} - He, H_2 (q=1,2)

15:40 - 16:00: Coffee break

16:00 - 18:00: V. Abramov: ITER/OTR-relevant database on elementary processes involving carbon ions

W. Lindinger: Ion-neutral-reactions at near thermal energies, involving atomic and molecular hydrogen

P. Krstic: Charge exchange calculations for ion-molecule systems

Wednesday, September 13

Section 4: Ion (atom) - molecule inelastic processes and particle interchange reactions

Chairman: H. Tawara

9:00 - 11:00: F. Linder: Ion-atom/molecule collisions at low eV energies

R. Janev/J. Smith: Database for particle-interchange reactions

V. Piksaikin: Ongoing and planned A+M activities at Obninsk

11:00 - 11:15: Coffee break

Section 5: General discussion on the data status and data needs

11:15 - 12:15: General discussion

Formation of Working Groups on:

WG1: A+M data needs for modelling and diagnostics of reactor-grade fusion edge plasmas (Room: C07-53)

WG2: Status of the electron-impact collision data and the spectroscopic database (Room: C07-55)

WG3: Status of the heavy-particle collision data (Room: C07-VI)

12:15 - 14:00: Lunch

Section 6: Formulation of Meeting Conclusions and Recommendations (Room: C07-VI)

Chairman: R. Janev

14:00 - 16:40: Parallel sessions of Working Groups. Preparation of Working Group Reports

16:40 - 17:00: Coffee break

17:00 - 18:00: Adoption of Meeting Conclusions and Recommendations

Specialists' Meeting on "Review of the Status of Atomic and Molecular Data for Fusion Edge Plasma Studies"

11-13 September 1989, IAEA Headquarters, Vienna

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