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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

2nd IAEA Research Co-ordination Meeting on

"Atomic and Molecular Data for Plasma Edge Studies"

17-19 June 1992, Vienna, Austria

SUMMARY REPORT

Prepared by R.K. Janev

February 1993

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

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ABSTRACT

The proceedings and the results of the 2nd IAEA Research Co-ordination Meeting on "Atomic and Molecular Data for Plasma Edge Studies", held on June 17-19, 1992 at the IAEA Headquarters in Vienna, are briefly described. The present report also includes the summaries of the data status assessments for the relevant A+M plasma edge processes, prepared by two Working Groups of the Meeting, as well as a set of proposals and recommendations for future work. The Progress Reports on the work performed by the research groups participating in the IAEA Co-ordinated Research Programme on this subject are appended to this Summary Report.

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Appendices

1. INTRODUCTION

The 2nd Research Co-ordination Meeting (RCM) on "Atomic and Molecular Data for Plasma Edge Studies" (June 17-19, 1992, IAEA Headquarters, Vienna) was organized as part of the activity within the IAEA Co-ordinated Research Programme (CRP) on the same subject which was carried out during the period 1988-1992. The objectives of the Meeting were to review the work performed by the CRP participants in the period since the last RCM in 1989, assess the present status of the atomic and molecular (A+M) data for plasma edge modelling and diagnostics, summarize the overall achievements of the CRP, and discuss the form and content of the final CRP document.

The Meeting was attended by seven (out of eleven) chief scientific investigators of the CRP constituting projects, and six observers (four of them with contributions). The List of Meeting Participants is given in **Appendix 1**.

After the opening remarks given by the Head of IAEA A+M Data Unit and the adoption of Meeting Agenda **(see Appendix 2)**, the work of the Meeting proceeded in the following sessions:

1) Spectroscopic and electron-impact collision data for plasma edge constituents
2) Heavy particle collision processes - I
3) Heavy particle collision processes - II
4) Atom-ion and ion-surface collision processes
5) Summary of the CRP accomplishments and form of the final CRP document
6) Status of A+M databases for plasma edge studies
7) Meeting conclusions

The highlights of the meeting presentations (meeting sessions 1-4) are given in the next section of this Report. The results of the data status assessment study of meeting Working Groups (meeting sessions 5 and 6) are presented in Section 3. The meeting conclusions and recommendations regarding the A+M data status and needs for plasma edge studies are given in Section 4, while the discussions on the content and structure of the final CRP document are given in Section 5. The Progress Reports on the individual research project within the Co-ordinated research programme are reproduced in **Appendix 3**.

2. HIGHLIGHTS OF MEETING PRESENTATIONS

In the session on spectroscopic and electron-impact collision data for the palasma edge constituents, **Dr. W.L. Wiese** presented a detailed review of the recent work in the National Institute for Standards and Technology (NIST, Gaithersburg) on establishment (or completion) evaluated spectroscopy databases (wavelengths, energy levels, oscillator strengths, transition probabilities) for the light atoms and ions (up to Z=10) present in the tokamak edge plasmas. The new NIST data evaluation effort is based on the recent (and expected in the near future) extensive R-matrix and configuration interaction calculations (R-MATRIX and CIV 3 codes) undertaken within the international Opacity Project, and on the advanced recent experimental data (mainly for comparison and consistency checks). It is expected that this activity will considerably improve the accuracies in the spectroscopy data for the ions above the B-like isoelectronic sequence, the current data uncertainties for which are about 25-50%, or larger. The data for the OII ion, so far missing in the NIST evaluated spectroscopy database, will also be provided by the end of 1993. **Dr. A.Ya. Faenov** described the content of the spectroscopic database for multiply charged ions already established at VNIIFTRI (Mendeleevo, Moscow Region), and the ongoing experimental and theoretical work, both at VNIIFTRI and in other associated institutions, directed on extending and improving this database. Dr. Faenov emphasized the high sensitivity of the data to the experimental methodology, and the paramount experimental difficulties to obtain accurate spectroscopic data for the high-Z elements.

In the part on electron-impact collision processes of the first meeting session, **Prof. F. Brouillard** (University of Louvain-la-Neuve) reported on the results of crossed beams experiments recently performed in his laboratory for the electron-impact double ionization of C^+, N^+, O^+, F^+, Ne^+, H^-, C^-, O^- and CO^- ions, and for the single ionization of CO^+. The energy range investigated is from the threshold to several keV. The future plans of this laboratory include cross section measurements for the dissociative electron-impact ionization channels of CH^+ and CO^+. This information (presently missing) is essential for the successful modelling of the transport of carbon in the plasma edge.

Prof. E. Salzborn (Giessen University) presented a comprehensive review of the single- and multiple ionization processes in electron-ion collisions. The review addressed the physical mechanisms of the processes, experimental methods for cross section measurements and the available (experimental) results of interest to plasma edge studies. A substantial portion of the experimental database for these processes has been generated by the Giessen group in the period covered by the present CRP, including the electron-impact single- and multiple ionization data for Li^{q+}, Ne^{q+}, Ar^{q+}, Xe^{q+}, Cu^+, Cs^+ and W^{q+} ions of direct relevance to fusion. The data for W^{q+} ions are of particular importance for the divertor modelling (and plasma radiative cooling) studies.

The progress report of **Dr. S. Trajmar** (Jet Propulsion Laboratory, Passadena), containing the recent results of his group on electron-impact excitation of helium atoms ($1^1S \rightarrow n\,^1P$, n=2-6, transitions) and electron-impact ionization of metastable inert gas atoms, has been presented by **Dr. H. Tawara**. Dr. Tawara reported also on the compilation and evaluation work performed at the Data and Planning Centre of the National Institute for Fusion Science (NIFS, Nagoya) which includes: ion production cross sections in electron collisions with CO, CO_2, H_2O (with an analysis of energy and angular distribution of reaction products), excitation and line emission cross section from the electron-impact dissociative recombination cross sections for HO^+, H_2O^+ and H_3O^+ (D_3O^+). Dr. Tawara emphasized the strong dependence of these cross sections on the internal energy (vibrational or other type of excitation) of the target.

In the meeting session on heavy particle collision processes **Prof. E. Salzborn** (Giessen University) reported on their recent experimental results for electron detachment and double ionization in collisions of H^- with a large number of gaseous targets, including inert gas atoms. He has also showed the results of cross section calculations of the Lebedev Institute group (Moscow) for these processes, which are in good agreement with experimental data.

Interesting saturation properties of the neutralization efficiency of various gaseous neutralizers were reported. **Dr. T. Shirai** (JAERI, Naka) presented the work at JAERI on the parametrizartion of recommended cross sections from the ORNL Redbook vol. 1 (Report ORNL-6086/VI, 1990) for the heavy particle collisions involving H, H_2, He, Li and their ions. The analytic function to which the recommended cross sections are fitted has a rather simple polynomial form (with up to 10 fitting parameters) and tends to have a monotonic asymptotic behaviour. Only a limited number of cross sections have so far been parametrized, demonstrating the adequacy of adopted analytic expression. **Prof. R.K. Janev** (IAEA, A+M Data Unit) presented theoretically based cross section scaling relationships for the single- and double-electron loss processes in collisions of multicharged ions with helium. Universal scaled semi-empirical cross section expressions (vs. scaled energy) for these processes were presented, valid (to within 10-30%) in the entire energy range of interest in fusion applications. Similar cross section scaling was presented also for the process of transfer ionization. **Prof. F. Brouillard** (Univ. of Louvain-la-Neuve) reported new experimental cross sections (using an "animated" crossed beams technique) for the ion-pair formation processes in collisions of $H^*(3s)$ with inert gas atoms. The results of recent cross section measurements in this laboratory for associative ionization in D(1s) + $D^*(2s)$ and $H^*(2s)$ + $H^*(2s)$ collisions were also presented. This work will be extended to the H^* + He and H^* + H_2 collisions.

Prof. N.N. Semashko (Russian Scientific Centre "Kurchatov Institute", Moscow) presented preliminary results for the reaction $H_2^+ + H_2^+ \rightarrow 2H^+ + 2H$ in the 10-20 eV energy range. The cross section for this reaction is shown to be large (on the order of 10^{-16} cm^2). Prof. Semashko presented the plans of the "Kurchatov Institute" group for investigation of other particle rearrangement and dissociative reaction channels in this collision system, as well as for experimental investigation of collision processes of Ga^{q+} (q=1-3) ions with electrons and hydrogen atoms and molecules. In a very interesting presentation, **Dr. V.A. Abramov** (Kurchatov Institute) demonstrated the role of charge exchange processes in collisions of hydrogen atoms and multiply charged plasma impurity ions in the formation and properties MARFES plasma instabilities occuring in the near-separatrix plasma region.

Prof. F. Linder (Univ. of Kaiserslautern) presented a comprehensive review of the ion-molecule reactions in edge plasmas, including his evaluations of the available data information and the recent cross section measurements performed by his group. Prof. Linder emphasized the problems in the evaluation of ion-molecule reaction cross sections from different literature sources which are associated with the diversity of experimental techniques used and their inherent uncertainties (including sometimes the unspecified internal energy state of reactants). The new results reported in this presentation included: particle rearrangement in $H^- + D_2$ collisions (with vibrationally resolved final reaction channels and information on the angular distribution of reaction products), rotational excitation in $H^- + H_2$ collisions, and dissociative electron capture in $He^+ + H_2$ collisions (including energy-angular distributions of the H^+-product).

Prof. H. Winter (Technical University, Vienna) presented the results of extensive studies performed in his group on both ion-atom and ion-surface collisions. Part of the investigations of ion-atom collision processes in this group are related to the establishment of an atomic collision data base required for Li-beam plasma edge diagnostics. The recent work along this line of research includes state selective and total electron capture cross section measurements for the Li(2s) + H^+, He^{2+}, Ne^{2+}, $(C,N,O,Ne)^{6+}$ collision systems. Prof. Winter discussed also the collisions of O^+ ions with H_2 and He from the point of view of the role of metastable ion beam fractions in the electron capture process in these collision systems. He presented new cross section data for the O^+ + He electron capture collisions. In the part of Prof. Winter's presentation devoted to ion-surface collisions, emphasis was given to the interaction of highly charged ions with surfaces and to the recent advances in the understanding of associated physical processes. Prof. Winter presented a large amount of results on the secondary electron emission coefficient for collisions of multiply charged ions (up to Ar^{16+}, I^{25+}) with surfaces, which show a strong enhancement of the electron yield with increasing the ionic charge.

Dr. J. Yao (Chinese Nuclear Data Centre, Beijing) reported on the systematic theoretical investigations of light ion (H and He isotopes) reflection from the Be, B, C, Al, Si, Ti, Fe, Ni, Cu, Mo, W and Au surfaces in the projectile energy range from 10 eV to 100 keV and angles of incidence from 0° to (step 5°) 75°. The particle (and energy) reflection calcualtions have been performed by using the PANDA-P code based on a bipartition model solution of the Boltzmann transport equation. Analytic fit expressions for the reflection coefficients (including dependence on the incidence angle) were also presented.

3. WORKING GROUP REPORTS

3.1. Report of the Working Group on the Status of Spectroscopic and Electron-Impact Collision Data for Edge Plasma Constituents

Members of the Working Group

W.L. Wiese, E. Salzborn (co-chairmen), V.A. Abramov, J. Botero
R.K. Janev, Yubo Qiu, H. Tawara

1. Edge Plasma Constituents

The composition of edge plasmas in currently operating tokamaks is subject to frequent changes, caused by the specific objective of each particular experiment. Testing of various options of the impurity control system, power and particle exhaust system, optimization of the divertor performance, experimentation with various plasma facing materials to achieve better overall plasma performance, all lead to a highly variable impurity content of the edge plasmas, both in terms of the chemical composition and relative abundance of impurities. One way to reduce this variability is to take the ITER edge plasma as typical for the next-step fusion devices, allowing for the back-up material options for the plasma facing components (as the principal sources of plasma impurities). In any D-T based fusion reactor the hydrogen and helium isotopes will be the dominant plasma edge constituents, and the diagnostics and burning control scenarios may require a delibarate introduction of specific impurities, other than those released from the plasma facing components (PFC). Based on these considerations, and allowing for plasma edge temperatures in the range between ~ 1 eV and 500 eV, the composition of the edge plasmas of a reactor level fusion device would be (besides the electrons) as follows:*

*** This list should be complemented by the one in the Section 3.2.**

a) Primary species
- H, D, T atoms and ions,
- H_2, D_2, T_2, DT, H_3, D_3, T_3, D_2T, DT_2 and thier ions,
- He atoms and ions,

b) Atomic impurities
- Be, C, O atoms and ions,
- B, Si, Ti atoms and ions (if B-, Si-, Ti-doped carbon is used for PFC's),
- Fe, Cr, Ni atoms and ions,
- Mo, W, Ga (Ta, Cu) atoms and ions (in some divertor concept options),
- V atoms and ions (in high safety reactor concepts),

c) Molecular impurities
- C_n H_m and their ions (for carbon based PFC's),
- H_2O, CO, CO_2 and their ions,
- Be-, B-oxides and carbides,

d) Diagnostic and burning control species
- Li, Ne, (Si), Ar, Kr atoms and ions.

Notes: (1) If Be is used on all PFC's, O is drastically reduced in the edge volume.
(2) Kr may be used also for radiative divertor plasma cooling.

2. Spectroscopic data

The availability and quality of the spectroscopic data (energy levels, wavelengths, and transition probabilities) for the fusion plasma constituents has been recently reviewed by Wiese [1]. For the low-Z elements, the database is satisfactory, both in terms of completness and acccuracy. With increasing Z, the spectroscopic data become increasingly sparce and their accuracy drops rapidly. For high-Z impurities (such as Mo and W) in higher charge states, even the energy level spectrum is not well documented. Below we give some more specific comments on the data base status and the prospectives of its development.

2.1. Atomic Species

a) Low-Z impurities ($Z \leq 10$). The basic spectroscopic information for the ions with $Z \leq 10$ is available and has the adequate accuracy. (For instance, the uncertainties in atomic transition probabilities for He- and Li-like ions are well below 10%, and for Be- and B-like ions below 15-20%). The most comprehensive sources of evaluated spectroscopic data for these elements are still the NIST (ex-NBS) Standard Reference Data publications, [2-5], and for the energy levels and wavelengths of Be ions a valuable sourcce is the more recent evaluation by Odintsova and Striganov [6]. Recently, Kelly [7] also published a very comprehensive evaluation of the wavelengths for all the elements up to Kr.

b) Medium-Z impurities ($10 < Z \leq 30$). The volume of required spectroscopic information increases drammatically with Z, while their availability and accuracy decrease significantly. As stated above, the uncertainty of the information on transition probabilities of He- and Li-like ions is of the order of 10%, it increases to about 25% for the Be- and B-like ions, and becomes between 25 and 50% (or larger) for C-like and higher isoelectronic sequencies. The available spectroscopic information for the elements in this Z-range is collected and evaluated in the following publications: Refs. [7-9] for the wavelengths, Refs. [10-12] for the energy levels, and Refs. [13-15] for transition probabilities. Since the most important metallic impurities (such as Fe, Ti, Ni) fall on this Z-range, it should be emphasized that the available data information decreases with increasing the charge state and becomes increasingly less reliable. This situation, however, begins to change due to the organized international activity on generation spectroscopic and collisional data within the OPACITY and IRON projects. The information from these large theoreticcal projeccts, generated by the most sophisticcated presently available computational codes, still needs to be collected and critically evaluated. Experimental benchmark studies should be undertaken to check the reliability of the spectroscopic information generated by these projects.

c) High-Z impurities ($Z > 30$). The spectroscopicc data for these elements is rather sparce and, generally, of low accuracy. Most of the available information is contained in Refs. [8] (wavelengths), [2,16] (energy levels) and [15] (transition probabilities). We note that the spectroscopic data for tungsten, even moderately ionized, are particularly limited.

2.2. Molecular Species

The spectral data information for the diatomic plasma edge molecular species (such as H_2, CO, O_2, CH) is available, at least for the ground and low-lying electronic states [17,18]. For the poly-atomic molecules (e.g. heavier hydrocarbons), however, the data situations is quite insatisfactory.

3. Electron Collision Processes

The data base for electron-impact processes involving plasma edge ions, atoms and molecules has recently been surveyed in a series of review articles collected in vol. 2 of "Atomic and Plasma-Material Interaction Data for Fusion" (1992) and in the Topical issue of Physica Scripta, T.37 (1991). The data for He-atoms, and Be-and B-atoms and ions have been thoroughly compiled and critically assessed by the participants of two recent IAEA Consultants' Meetings (see IAEA Reports INDC(NDS)-253/N2 (for the He-data) and INDC(NDS)-254 (for Be- and B-impurities)). Below we give some more details on the data status for electron collision processes.

3.1. Neutral atoms and molecules

Rather comprehensive information on the elastic and inelastic electron collision processes with plasma edge neutrals is compiled and evaluated in the reviews [19-22]. Ref. [20] concentrates on the elastic and momentum transfer processes, Ref. [19,21] provide critical assessments for both elastic scattering and excitation, while Ref. [22] is devoted exclusively to the processes of hydrocarbons (including also their ions). Experimental elastic scattering and momentum transfer data are available for some low-Z neutrals (H, Li, O), for all inert gas atoms and all molecules in the plasma edge (except for some hydrocarbons). These are no such data for Be, B, C and the intermediate- and high-Z plasma edge neutrals. The experimental data base for excitation of plasma edge neutrals is approximately in a similar shape, with the exception of a limited amount of excitation data for Be, O, Al, Ti, Cr, Fe and Mo. Theoretical calculations with methods of a varying level of sophistication are available (except for the heaviest impurities), but their accuracy cannot be assessed in the cases where no experimental cross section measurements exist. The data for electron-impact non-dissociative ionization are available for all the plasma edge atomic and molecular neutrals [23,24], except for certain hydrocarbons. It should be stressed that the data for dissociative electron-molecule excitation and ionization are rather incomplete, and that only a small part of the existing data is of sufficient accuracy. Particularly scarce is the information on the energy and angular distribution of dissociated products (which, however, is very important in the particle transport modelling studies).

3.2. Ionized Species

The most recent review and data assessment of electron-ion collision processes has been done by G. Dunn [25]. This review includes both atomic and molecular ions, and all major inelastic processes (excitation, ionization, radiative and dielectronic recombination, as well as dissociative channels of these processes in the case of molecular ions). Information on electron-impact ionization processes is also available in Ref. [23]. Comprehensive data reviews and assessments for the electron-impact excitation, ionization and dielectronic recombination of metallic ions can be found in Ref. [24]. A number of evaluated data sets for these processes, involving Ti, Cr, Fe and Ni ions, are also presented in Ref. [24].

The data base for all electron-impact processes of light impurity ions ($Z \leq 10$) is satisfactory in terms both of completeness and accuracy (uncertainties usually below 25%). For medium-Z ions, only the single-ionization data base is complete, but its accuracy begins to decrease. For C^{q+}, the ionization cross section are known only for $q=1$-3. The excitation and dielectronic recombination cross sections for the impurity ions with $10 < Z \leq 30$ are available to a much lesser extent, particularly for the multielectron open-outer-shell ions. The data base for these processes for the most abundant plasma impurities in this Z-range (Fe, Ni, Ti) is, however, fairly satisfactory (see Ref. [24]).

The data information for electron-impact collision processes involving high-Z metallic ions (Ga, Mo, Ta, W) is extremely sparce. For instance, the single-electron ionization cross sections are known only for the singly charged Ga and W ions. The excitation and dielectronic recombination data for these ions are also rather fragmentary. Evidently, a strong effort has to be made in order to improve this situation. (The participants have been informed that the Kurchatov Institute is planning ionization cross section measurements for Ga^{q+}, q=1-3). It should be noted that the existing computational methods for providing information on inelastic electron-impact collisions involving high-Z ions, also encounter serous difficulties, owing to the necessity of adequate description of strongly pronounced relativistic effects in these systems. (For the low- and medium-Z ions, these difficulties are absent, and a configuration-interaction approach is quite acceptable).

The data base for the singly ionized molecular ions is fairly good, as far as the total cross sections are concened (see[25]). For many collision systems, however, various dissociative reaction channels still remain unresolved, and only composite reaction cross sections are available (e.g. cross sections for ion or neutral production, etc). The information on the angular and energy distributions of dissocative reaction products is still extremely fragmentary, even for the diatomic molecular ions. The available electron collision data for the hydrogen ions are collected and reviewed in Ref. [22].

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3.2. Report of the Working Group on the Status of the Data Base for Heavy Particle Collisions in the Plasma Edge

2. IAEA Research Coordination Meeting on
"Atomic and Molecular Data for Plasma Edge Studies"
June 17 - 19, 1992, IAEA, Vienna, Austria

Members of the Working Group

F. Linder, H. Winter (co-chairmen),
F. Brouillard, K. Katsonis, N.N. Semashko, T. Shirai, Yao Jinzhang

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. Furthermore, reactions needed for modelling negative ion source kinetics in view to development of future high energy neutral heating beams have been partly covered.

1.1 Primary plasma constituents

H, D, T and their positive and negative ions
H_2, D_2, T_2, HD, HT, DT and their positive ions
He, He^+, He^{2+}

1.2 Dominant impurities

Be^{q+} (q=0-4), B^{q+} (q=0-5), C^{q+} (q=0-6), O^{q+} (q=0-8)

1.3 Metallic impurities

Fe^{q+}, Ni^{q+}, Cr^{q+}, Ti^{q+}, Mo^{q+}, Ga^{q+}, W^{q+} (q =1-10)

1.4 Molecular impurities

C_mH_n, C_m, CO, O_2, CO_2, H_2O, B- and C hydrides, Be- and B oxides and -carbides, and their ions

1.5 Diagnostic species

Li^{q+} (q=0-3), Ne^{q+} (q=0-10), Si^{q+} (q=0-13), Ar^{q+} (q=0-18)

2. Collision Processes

Its worth repeating that in the temperature range of interest in the plasma edge ($0,1 \leq T_i \leq 500$ 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 thus have negligibly small cross sections at edge-plasma relevant 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, and so forth. A survey on 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 or other atomic 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 considerably larger cross sections than for the respective ground states. The role of excited levels becomes increasingly important at higher densities, where times between collisions may become shorter than the related radiative lifetimes.

2.1 Electron transfer

(i) $H^+ \rightarrow (H, H_2, He, H^-, Li, C_mH_n, CO, O_2, C, O, H_2O)$

Total cross section data are available for most of these reactions, but generally not at low collision energies. Data on product distributions and well characterized reactant states are also very sparse.

(ii) $(He^{q+}, Be^{q+}, B^{q+}, C^{q+}, O^{q+}, M^{q+}) \rightarrow (H, H_2, He)$

Total cross sections are available for all He^{q+}, C^{q+} and O^{q+} charge states, and for $Fe^{q+} \rightarrow (H, H_2)$ for q›2. Partial cross section data are available for approximately half of the C^{q+} and O^{q+} cases, but again generally not at low energies. Almost 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) $(H_2^+, C_mH_n^+, CO^+, O_2^+, H_2O^+) \rightarrow (H, H_2, He)$

Cross section data are available for some of these reactions involving molecular ions, and their compilation has been started in the data centers.

(iv) $(Ne^{q+}, Si^{q+}, Ar^{q+}) \rightarrow (H, H_2, He)$

Total and partial cross sections are available for some of these reactions, and their compilation has been started in the data centers.

(v) $Li \rightarrow (H^+, He^{q+}, Be^{q+}, B^{q+}, C^{q+}, O^{q+}, Ne^{q+})$

Compilation of recently measured total and partial cross sections has been started.

2.2 Heavy particle rearrangement reactions (including associative and dissociative processes)

In the following list of collision systems, it is understood that all possible isotopic combinations of H, D and T are to be considered, e.g. (H^+, D^+, T^+) → (H_2, D_2, T_2, HD, HT, DT), etc.

(i) (H^+, He^+, He^{2+}) → H_2

(ii) (H^*, H_2^*, He^*) → (H, H_2, He)

(iii) (H_2^+, H_3^+) → (H, H_2, He)

(iv) (H^+, He^+, He^{2+}) → molecular impurities (C_mH_n, CO, etc.)

(v) (Be^+, B^+, C^+, O^+, Ne^+, Si^+, Ar^+, M^+) → H_2

(vi) ($C_mH_n^+$, CO^+, O_2^+, CO_2^+, H_2O^+, HeH^+) → (H, H_2, He)

(vii) M^+ → molecular impurities (C_mH_n, CO, etc.)

(viii) (H^+, H_2^+) → H_2^+

Total and/or partial cross section data are available for some of these reactions, the most comprehensive of which being those for reactions involving hydrogenic ions and -molecules.
Data on energy and angular distributions of the reaction products are still very sparse.
The importance of studies with well-defined reactant states has been recognized and some data are available for reactions in which the initial vibrational state of the molecular ion is specified.
Surveys and compilations of data for the reactions listed above are incomplete at this time, although some progress has been made recently in the data centers. Several articles which have been prepared within the present CRP and which will be published in the Nucl. Fusion A&M Suppl. vol. II, are dealing with these processes.

2.3 Energy and momentum transfer collisions

(i) Elastic Scattering

(ii) Rotational/vibrational excitation

(iii) Internal-excitation transfer

Data exist for some of these processes at energies relevant to the plasma edge, particularly for atomic and molecular hydrogen neutrals and ions. Cross sections and swarm coefficients for these species have been critically evaluated in the energy range 0,1 eV - 10 keV by Phelps (J.Phys. Chem. Ref. Data **19**(1990)653).
Energy transfer processes involving vibrationally excited H_2/D_2 molecules, both in the gas phase and in collisions with metallic surfaces, have been discussed by Cacciatore et al. (Nucl. Fusion A&M Suppl. vol. II (1992), in press).
Concerning internal electronic excitation transfer, fine-structure transitions are the most important processes. Electronic excitation, ionization and dissociation in heavy-particle collisions are less important processes in the edge plasma because of their small cross sections at edge-relevant energies.

2.4 Surface collisions

Whereas reliable data are already compiled on some plasma-wall interaction processes as physical sputtering and particle reflection - cf. the related chapters in Atomic and Plasma-Material Interaction Data for Fusion, Nucl. Fusion Suppl. vol. I (1991) - information of other processes e.g. relevant for edge-plasma modelling as particle-induced electron emission is still rather scarce. Within the present CRP, a considerable amount of new informations on the latter processes has been gained, in particular regarding electron emission due to impact of slow highly charged ions on metallic surfaces. Such data might become useful for estimating the possible influence of low-Z impurity ion bombardment at the first wall in view to the adjustment of the electron temperature gradient in the plasma edge, which in turn is of great interesat for overall plasma stability and -energy confinement.

3. Classes of data

3.1 Total cross sections - integrated over angles and product states.

3.2 Partial cross sections - for specific product states.

3.3 Product distributions - differential in product kinetic energy and/or angle, particularly important for neutral products.

For informations of types 3.1 - 3.3, in addition to ground states also specified excited states (metastable and for abundant species also short-lived electronically excited states) are of interest.

3.4 Reaction rate coefficients - to be calculated from the cross sections by assuming Maxwellian or other velocity distributions.

Proposals for "Conclusions and Recommendations"

1. The energy range important for fusion edge plasma studies falls into a longstanding gap between the well established techniques for beam studies at keV energies and swarm studies at thermal energies. There is a strong need for more measurements with low-energy beams. In principle, the experimental techniques are now available, but substantial efforts are needed in their application.
2. Further development of scaling laws appears desirable, but it seems doubtful whether they can successfully be extended down to collision energies in the eV range, in particular if molecular systems are considered. Under these conditions, one needs full dynamical calculations based on accurate potential energy surfaces, i.e. substantial efforts are also required on the theoretical side.
3. The role of excited states in collision processes relevant to fusion edge plasmas must again be emphasized. More experiments are needed with well defined reactant states (both for ions and neutrals, electronically and rovibrationally excited).
4. Beyond total cross sections and rate coefficients, post-collision energy and angular distributions of the products are needed for kinetic modelling of the edge plasma. Such data are missing in most of the cases and their measurement is urgently needed.
5. More efforts for determining precise total yields and electron energy distributions for slow highly charged ion-induced electron emission from relevant first wall materials are recommended.

4. MEETING CONCLUSIONS AND RECOMMENDATIONS

The presentations at the plenary meeting sessions, the data status analyses of the two working groups, as well as the data needs considerations related to the next-step fusion experiments, have led to the following general conclusions and recommendations regarding the current status and required future work on atomic and molecular data for fusion plasma edge studies:

1) The spectroscopic data base for the primary plasma edge constituents and for the light and medium-Z plasma impurities can be considered as satisfactory. The recent results generated within the OPACITY Project (and those expected) should significantly increase and improve the spectroscopic data base for all atomic impurities with $Z \leq 26$. The data base for high-Z impurities (Ga, Mo, Ta, W), however, is extremely inadequate, and a dedicated effort is required to improve this situation. The ongoing IAEA Co-ordinate Research Programme on the medium- and high-Z impurities is a good step in that direction. The spectroscopic data base for the diatomic plasma edge molecular species is, generally speaking, adequate for most of the current plasma edge studies. For the polyatomic molecular impurities (e.g. heavier hydrocarbons), the data are still fragmentary. However, there have not been, so far, explicit requests from the fusion community for establishing a systematic spectroscopic data base for these molecular species.

2) The data base of electron-impact collision processes for the primary plasma constituents and for the low-Z plasma impurities can be considered as satisfactory, as far as the processes involving ground state species are concerned. With the exception of H, the electron-impact processes involving excited atomic, molecular or ionic plasma edge species are rather poorly documented. Detailed calculations of the radiative plasma edge cooling would require the cross section knowledge for all the electron-impact processes involved in a collisional-radiative model, at least for He, H_2 and the major plasma edge impurities (Be, B, C, O, hydrocarbons, and some other impurities, depending on the selection of plasma edge cooling concept and the plasma facing materials). While general efforts, like the present CRP, are helpful in improving the

overall data situation for the plasma edge studies, concerted data generation efforts would be required for establishing the required complete data bases for selected plasma-edge-cooling impurities (such as Kr, for instance). Again, it is expected that the results of the ongoing OPACITY Project should significantly improve the general data situation for the low- and medium-Z impurities.

The electron-impact collisional data base for high-Z impurities is in a very poor shape and dedicated data generation efforts (such as the above mentioned IAEA CRP) are required. It should be emphasized that the data base for electron-molecule (molecular ion) collision processes is still inadequate even for the dominant plasma edge molecular constituents. The missing information is mainly related to the dissociative processes, and includes the channel-selective cross sections and the energy (angular) distribution of reaction products. This information is urgently required both for the modelling and diagnostic plasma edge studies.

3) The data base for heavy particle collisions of plasma edge constituents includes a very large number of collision processes, but only a limited number of them have sufficiently large reaction rates to compete with the rates of dominant electron-impact processes. These are the elastic, momentum and energy transfer, and (quasi-)resonant processes. For plasma edge modelling purposes (particularly for modelling of neutral particle transport, hydrogen recycling in the divertor region and helium removal), the most urgent recent requests from the fusion community include data for the elastic and momentum transfer processes in ion-neutral and neutral-neutral collisions, and data for all resonant and quasi-resonant electron capture and energy transfer processes. While there is a limited experimental information for the elastic collisions of plasma edge ions and neutrals (particular those in molecular form), the necessary theoretical methods for elastic cross section calculations in this energy range are well established (the classical and semi-classical scattering theories). However, the application of theoretical methods relies on accurate knowledge of interaction potentials at all internuclear distances, both for the ground and excited state interacting particles. The knowledge of these interaction potentials, particularly for the excited states, is presently rather limited. The interference between the elastic and inelastic channels becomes important even for moderately charged ions at the energies above a few hundred eVs. The problems

associated with the interaction potentials and channel interference become even greater when molecular species are involved. The present forum recommends that the Agency undertakes an organized action for establishing an accurate elastic scattering and momentum transfer data base for the most important plasma edge ion-neutral and neutral-neutral collision systems.

The energy transfer processes in ion-neutral and neutral-neutral collisions associated with fine-structure or ro-vibrational transitions are also not sufficiently well documented for the all dominant plasma edge heavy constituents. This information will play an essential role in the modelling of edge plasma cooling in cold dense gas divertor concepts, and is also important in several plasma edge diagnostic schemes. Since it would be unrealistic to expect that the required information can be generated experimentally, systematic calculations with the most sophisticated existing (or further developed) theoretical models (benchmarked with experimental data) are suggested. For the primary plasma edge constituents, useful information of this kind has already been collected and generated by the part of atomic physics community involved in the development of hydrogen negative ion sources. For modelling the plasma edge cooling, as well as for plasma edge diagnostics, infomration on state selective ccapture in neutral-multiply charged impurity ion collisions is required. This information is presently limited to collisions of hydrogen atoms with fully stripped He, Li, Be, B, C and O ions. For incompletely stripped ions and other plasma edge neutrals, even the information on total electron capture is incomplete. Unfortunately, for the incompletely stripped ions with $q \leq 4$ prevailing in the plasma edge, the existing electron capture cross section q-scaling relationships cannot be applied (except for the excited target states). At very low plasma edge temperatures (e.g. in a cold dense gas divertor), particle interchange reactions may become an important factor in neutral particle transport and overall edge plasma kinetics. The data base for these reactions is still not complete and shows large uncertainties. The internal energy state of the reactants, which is a sensitive function of the plasma conditions, has a strong influence on the rate coefficients of these processes. The above mentioned data uncertainties reflect to a large extent the uncertainties in the reactants internal energy in different experiments. In general, the knowledge of ro-vibrational state distribution of molecular species involved in low-energy heavy particle collisions is very important for an accurate treatment of edge plasma kinetics. At present, however, the data base for the inelastic and particle rearrangement processes involving ro-vibrationally excited molecular species is extremely modest.

Finally, the particle-surface interaction processes are an inextricable part of the edge plasma modelling and diagnostic codes. Although these processes have not been the main subject of the present Meeting, it should be mentioned that for plasma edge temperatures below ~ 20 eV, the characteristics of these processes (particularly those involving multiply charged ions and molecular species) are very poorly documented. A much stronger research effort is required to improve the data base for these processes.

4) The generation of atomic and molecular data for fusion plasma edge studies has been considerably increased recently, and the contribution of the present Co-ordinated Research Programme to this increase is significant. Despite the important defficiencies of the existing data base, the overall data situation is much better today than it was at the beginning of this CRP. It is important that the newly generated or improved data, including those from the present CRP, be incorporated in the corresponding plasma edge modelling and diagnostic codes. The Agency could play an important role in this data transfer process.

5) Specific Recommendations to the IAEA

In view of the above conclusions regarding the status of the atomic and molecular data base for fusion plasma edge studies, as well as having in mind the termination of the present Co-ordination Research Programme in the near future, it is strongly recommended that the Agency undertakes the following actions:

a) The work on the collection and evaluation of atomic and molecular data for plasma edge studies should be continued by the IAEA A+M Data Unit and by the international Atomic Data Centre Ntwork;

b) Initiation of a new Co-ordinated Research Programme focussed on establishment complete purpose-oriented A+M data bases for specific plasma edge issues (e.g. for hydrogen recycling and helium exhaust);

c) Establishment of specific task force groups, composed by members of the Data

Centre Network and external Agency consultants (or Research Contractors), to create a number of small (but essential) data bases, such as:

- data base for elastic and momentum transfer ion-neutral and neutral-neutral collisions,
- data base for hydrocarbons,
- data base for a radiative-collisional code for molecular hydrogen.

d) Establishment of a mechanism for efficient transfer of fusion relevant data generated within the OPACITY Project into the Agency's plasma edge data base.

c) The Agency should also find efficient ways for communicating the data information generated or evaluated within the present CRP, to the fusion users.

5. FINAL CRP DOCUMENT

The results obtained within the present CRP have been published by the CRP participants in the journal literature, in vol. 2 of the IAEA series on "Atomic and Plasma-Material Interaction Data for Fusion" (1992), and are summarized in **Appendix 3** to the present Report. Having, however, in mind the importance of the plasma edge region for the overall plasma performance of next-step fusion devices, as well as the significant role of atomic and molecular processes in determining the properties of edge plasmas, the meeting participants shared the opinion that a more comprehensive presentation of the existing data information for all radiative and collision processes taking place at the plasma edge, supplemented with the background physics and an overview of the current research of these processe, would be useful not only for the plasma edge modellers, but also to the broader fusion and atomic physics communities. This point of view defined the form of the "final CRP document" as a collection of extensive reviews on the physics (described briefly) and data base for specific classes of collision processes of plasma edge species, to be published in book format. The idea of "comprehensivness" has resulted in a significant extension of the scope of presentation and the list of contributors beyond the present CRP. In order that this infomration reach the broader physics community, it has been suggested that the book be published by an external publisher. The content of the book (with the contributors) is given below.

ATOMIC AND MOLECULAR PROCESSES IN MAGNETIC FUSION EDGE PLASMAS

Table of Contents

*** To be contacted for acceptance to contribute.**

Note: The authors may include other co-authors in the preparation of their contribution.

Appendix 1

2nd IAEA Research Co-ordination Meeting (RCM)
"Atomic and Molecular Data for Plasma Edge Studies"

17 - 19 June 1992, IAEA Headquarters, Vienna, Austria

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Appendix 2

2nd IAEA Research Co-ordination Meeting (RCM)
"Atomic and Molecular Data for Plasma Edge Studies"

17 - 19 June 1992, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

WEDNESDAY, June 17

09:30 - 09:45 - Opening **(Meeting Room: A-07-42)**
- Adoption of Agenda

Session 1: Spectroscopic and Electron-Impact Collision Data for Plasma Edge Constituents

Chairman: F. Linder

09:45 - 10:25 W.L. Wiese: Spectroscopic data for light plasma impurities.
10:25 - 11:00 A.Ya. Faenov: Spectroscopic data and studies at VNIIFTRI.

11:00 - 11:15 **Coffee break**

11:15 - 11:50 F. Brouillard: Electron-impact ionization of ions.
11:50 - 12:25 E. Salzborn: Ionization processes in electron-ion collisions.

12:25 - 14:00 **Lunch**

Session 1: Cont'd

14:10 - 15:00 H. Tawara: Collision data for H_2O, CO and CO_2 edge plasma impurities.
15:00 - 15:45 S. Trajmar: Cross sections for electron impact excitation cross sections of He and for electron collision processes involving excited atoms (presented by H. Tawara).

15:45 - 16:00 **Coffee break**

Session 2: Heavy Particle Collision Processes - I

Chairman: F. Brouillard

16:00 - 16:40	E. Salzborn:	Atomic processes in plasma neutralizers for negative ion based NB injectors.
16:40 - 17:20	T. Shirai:	Analytic expressions for the collision cross sections of H, H_2, He and Li atoms and ions with atoms and molecules.
17:20 - 18:00	R.K. Janev:	Cross section scaling relationships for heavy-particle collision processes.

THURSDAY, June 18

Session 3: Heavy Particle Collision Processes - II

Chairman: H. Winter

09:00 - 09:45	F. Brouillard:	Charge exchange and associative ionization with excited atomic hydrogen.
09:45 - 10:30	N.N. Semashko:	Simultaneous dissociation of molecular hydrogen ions in low-energy collisions.
10:30 - 10:45	**Coffee break**	
10:45 - 11:30	F. Linder:	Beam studies of ion-molecule collisions at edge-relevant energies.
11:30 - 12:15	V.A. Abramov:	The role of atomic processes in formation of MARFES.
12:30 - 14:00	**Lunch**	

Session 4: Ion-Atom and Ion-Surface Collision Processes

Chairman: V.A. Abramov

14:00 - 14:45	H. Winter:	Recent ion-atom/ion-surface collision-related data relevant for plasma edge balance and diagnostics.
14:45 - 15:30	Yao Jinzhang:	Reflection coefficients for light ions from solid surfaces.
15:30 - 15:45	**Coffee break**	

Session 5: Summary of the CRP accomplishments and form of the final CRP document

Chairman: R.K. Janev

15:45 - 16:30	Summary reports on the results achieved to-date within individual CRP projects. (Brief reports from project Principal Scientific Investigators)
16:30 - 17:30	Discussion of the form, content and structure of final CRP document.
17:30 - 17:45	Formation of Working Groups for assessment of the status of A+M data for plasma edge studies.

FRIDAY, June 19

Session 6: Status of A+M data bases for plasma edge studies

09:00 - 12:00 Parallel Working Group Sessions:

A) Working Group on Spectroscopic and Electron-Impact Collision Data
(Meeting Room: A-07-41)

B) Working Group on Heavy Particle Collision Processes
(Meeting Room: A-07-42)

WG tasks:

a) Assess the data availability and further data needs in the respective fields;

b) Prepare a short Working Group Report on the data situation.

12:00 - 14:00 **Lunch**

14:00 - 15:45 **Session 6: (Contd.)**

15:45 - 16:00 **Coffee break**

Session 7: Meeting Conclusions

Chairman: R.K. Janev

16:00 - 17:30
- Discussion and adoption of Working Group Reports
- Formulation and adoption of Meeting conclusions

17:30 - **Adjourn of the Meeting**

Appendix 3

Progress Reports on the CRP Research Projects

Progress Report on The Determination of Atomic Spectroscopy Data for Fusion Edge Plasma Studies

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A. Introduction

At NIST, our work to provide additional, as well as more accurate, spectroscopic data for fusion edge plasmas proceeded at in two directions:

1) We provided new spectroscopy data of very high accuracy through experiments and calculations. For example, by performing very sophisticated atomic structure calculations involving several thousand interacting configurations, we obtained highly accurate transition probabilities for prominent lines of C III and O V. Also, we carried out an extensive laboratory study of the Pt I and II spectra to establish new, very precise wavelength standards throughout the ultraviolet region of the spectrum.
2) We continued the critical evaluation and compilation of spectroscopic data for neutral spectra or low stages of ionization of light elements that are of principal interest in magnetic fusion research, such as Li, Be, B, C, and O.

B. Theoretical Work

We have performed extensive multiconfiguration calculations for a number of prominent lines of C III, O V and N I. This work was partly prompted by pronounced discrepancies among recently published, sophisticated theories as well as with advanced experiments. In the case of N I our results agree closely with another very recent multiconfigurational approach, as well as an emission experiment, also performed at NIST, in which relative emission data wete scaled to accurate atomic lifetime data.

The agreement between these three approaches suggests that our new transition probability data for N I are accurate to within 10%.

For C III and O V ions of the Be-sequence, we have performed very detailed multiconfiguration calculations were done in the dipole length and velocity representations and the agreement achieved between these two approaches was typically within 0.1%. Agreement with other advanced calculational data is excellent. We therefore estimate that these new data are accurate to within one percent.

C. Laboratory Work

We have done an extensive high-precision study of the wavelenght positions of about 3,000 lines of Pt I and Pt II, and have published both an atlas and a comprehensive table of these lines. The wavelengths, which have been determined with an average uncertainty of ±0.002 Å, provide convenient laboratory wavelength standards throughout the ultraviolet, from about 1000 Å to 4000 Å. Therefore, by using a platinum reference lamp it will be possible to measure precisely any line shifts of impurity lines in plasmas and obtain accurate values for Doppler shifts due to plasma motion.

D. Spectroscopic Data Evaluations

A comprehensive evaluation of the energy levels and wavelengths of singly ionized oxygen is nearing completion. This will be the first new tabulation of these quantities since the energy level and multiplet tables done at NBS in the 1930s and 40s. The new tables will contain many revisions and also substantial expansions of the earlier data. Also, atomic transition probabilities are compiled for all spectra of the elements C, N, and O. These tables will update and significantly expand the 1966 NBS tables on these elements. We expect that they will contain about 10 times more material than the earlier tables and the typical uncertainties of the data will be about ± 10% as compared to a range of ±(25-50)% in the earlier compilation. For numerous prominent lines, accuracies in the range of 1-3% may be reached. Thus the advance in both quantity and quality against the earlier table is expected to be substantial.

CROSS SECRTIONS FOR ELECTRON-IMPACT EXCITATION OF He AND FOR ELECTRON COLLISION PROCESSES INVOLVING EXCITED ATOMS

S. Trajmar

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Our activities during the recent year have been concentrated in two areas:

1) Measurement and calculation of electron-impact excitation cross sections for He
2) Measurement and calculation of cross section for electron collisions with excited atoms.

Differential and integral cross section for the $1^1S \rightarrow 2^1P$ and $1^1S \rightarrow (3^1P + 3^1D + 3^3D)$ excitation processes in He were measured at 30, 50 and 100 eV electron energies. First-order many-body theory (FOMBT) was used to calculate differential and integral cross sections for excitation of the n^1P (n=2, ...6) levels in He in the impact energy range of threshold to 500 eV and a simple scaling law was derived from the n=2, ...6 results that provides differential and integral cross sections for excitation of all levels with n≥6.[1] Differential and integral cross sections for excitation of the n^3S, n^1S and n^3P (n=2,3) levels in He were also measured at 30,50 and 100 eV and calculated at impact energies ranging from 30 eV to 500 eV.[2] In these two papers extensive comparisons are made with previous experimental and theoretical data. A secondary standard for normalizing inelastic electron scattering cross sections in terms of differential cross sections for excitation of the 2^1P level in He was proposed.[3]

Electron collisions with excited atoms play an important role in many partially ionized systems. Particularly important are collisions with metastable rare gases because of:

a) their prominence in many practical systems
b) the large cross sections associated with many of these processes
c) long life time of these species
d) large energy stored in these species

We have surveyed and summarized electron collision cross sections in this area[4] and initiated laboratory programs to measure some of these cross sections. Presently, work is in progress for measuring electron impact ionization cross sections for metastable Ne, Ar, Kr and Xe.[5,6] Work is also in progress for measuring and calculating electron collision cross sections for short-life excited atoms. In the inital work ^{138}Ba (...$6s^2\ ^1S$) is excited by laser to the ...$6s6p\ ^1P_1$ level and then deexcitation and further excitation differential cross sections are measured. These cross sections are also calculated using the unitarized distorted wave approximation.[7]

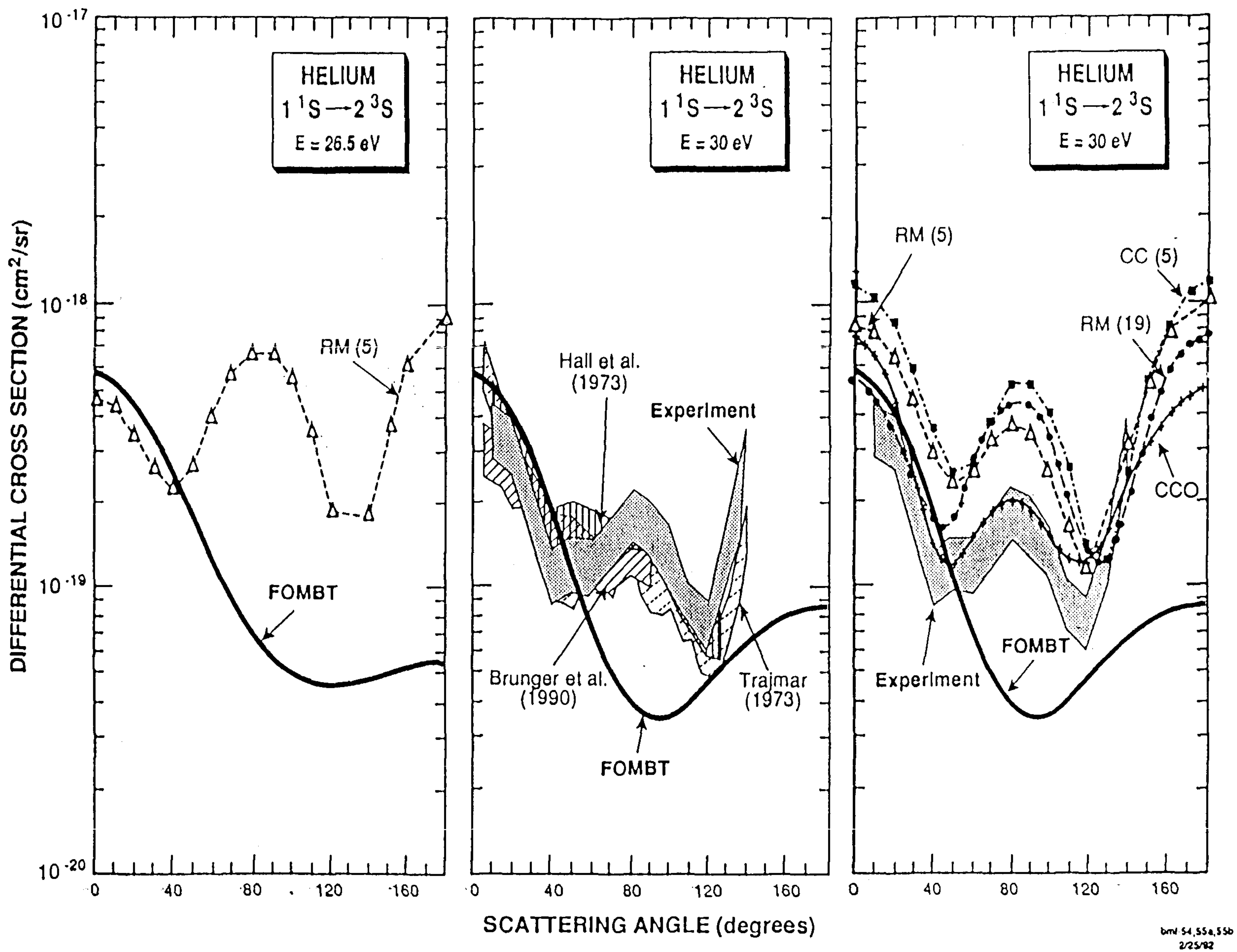
TABLE I. Summary of cross section measurements for excitation of the n^3S, n^1S and n^3P (n=2,3) levels in He.

Reference		Levels	Type	Energy[a] Range (eV)	Angular Range (deg)
St. John et al.	1964	$3\,^3S, 3\,^1S, 3\,^3P$	Q	60, 100, 200	–
Jobe – St. John	1967	$2\,^3P$	Q	Tr – 450	–
Vriens et al.	1968	$2\,^3S, 2\,^1S$	DCS, Q	100-225; 400	5–20
Moussa et al.	1969	$3\,^3S, 3\,^1S, 3\,^3P$	Q	50–6000	–
McConkey-Woosley	1969	$3\,^3P$	Q	24–300	–
van Raan et al.	1971	$3\,^3P$	Q	20–1500	–
Opal–Beatty	1972	$2\,^3S, 2\,^1S, 2\,^3P$	DCS	82, 200	30–150
Rice et al.	1972	$2\,^1S$	DCS, Q	26.5–81.6	10–80
Brongersma et al.	1972	$2\,^3S, 2\,^1P$	Q	19–24	–
Croocks et al.	1972	$2\,^3S$	DCS	40-70	25-150
Hall et al.	1973	$2\,^3S, 2\,^1S, 2\,^3P$	DCS, Q	29.2, 39.2, 48.2	10-125
Trajmar	1973	$2\,^3S, 2\,^1S, 2\,^3P$	DCS, Q	29.6, 40.1	3–138
Suzuki–Takayanagi	1973	$2\,^3S, 2\,^1S, 2\,^3P$	DCS	50–500	20–120
Skerbele et al.	1973	$2\,^3S, 2\,^1S$	DCS	300–500	0–20
van Raan et al.	1974	$3\,^3P$	Q	100–1000	–
Chutjian-Srivastava	1975	$2\,^3P$	DCS,Q	60, 80	5–136
Chutjian–Thomas	1975	$3\,^3S, 3\,^1S$	DCS,Q	29.2, 39.7	5–136
Dillon–Lassettre	1975	$2\,^1S$	DCS	200–700	7.5–35
Dillon	1975	$2\,^3S$	DCS	200–500	7.5–35
Showalter-Kay	1975	$3\,^3P$	Q	60	–
Pichou et al.	1976	$2\,^3S, 3\,^3S$	DCS	Tr–23.4	30–120
Yagishita et al.	1976	$2\,^3S, 2\,^3P$	DCS	50–500; 200	5–120
Joyez et al.	1976	$2\,^3S, 2\,^1S, 2\,^3P$	DCS	Tr–20.2	6–120
Huetz et al.	1976	$2\,^3S$	DCS	Tr-23	120
van Zyl et al.	1980	$3\,^1S$	Q	50–2000	–
Phillips - Wong	1981	$2\,^3S, 2^1S, 2^3P, 2^1P$	DCS	Tr-24	40-90
Johnston–Burrow	1983	$2\,^3S$	Q	20.35	–
Spence et al.	1983	$2\,^3S, 2^1S$	Q	Tr-23	–
Sakai et al.	1989	$2\,^3S, 2\,^1S$	DCS	200–1000	0–16
Brunger et al.	1990	$2\,^3S, 2\,^1S, 2\,^3P$	DCS	29.6,40.1	2–90
Sakai et al.	1991	$2\,^3S$	DCS	200, 500; 200-800	0–12; 0

[a] Tr stands for threshold.

Summary of Electron-Impact Cross Section Measurments on Excited Atoms

Type	Species	References
DCS	He (2^3S)	Muller-Fieder *et al.* (1984)
	Na ($3^2P_{3/2}$)	Zuo *et al.* (1990); Vuskovic *et al.* (1989b); Jiang *et al.* (1990b, 1991a, 1991b)
	Ba (5^3D), (5^1D), (6^1P)	Register *et al.* (1978)
Opt. Ex. F.	He (2^3P)	Mityureva and Penkin (1975); Gostev *et al.* (1980b); Rall *et al.* (1989).
	Ne (3^3P_2), (3^3P_0)	Mityureva and Penkin (1975)
	Ar (4^3P_2), (4^3P_0)	Mityureva and Penkin (1989)
	Ar (4^3P_2 + 4^3P_0)	Mityureva *et al.* (1989)
	Kr (5^3P_2 + 5^3P_0)	Mityureva *et al.* (1989b)
	Xe (6^3P_2 + 6^3P_0)	Mityureva *et al.* (1991)
	Na ($3^2P_{3/2}$)	Stumpf and Gallagher (1985)
	Tl ($6^2P_{3/2}$)	Shafranyosh *et al.* (1989)
Ionization	H ($2s^2S$)	Dixon and Harrison (1971); Dixon *et al.* (1975); Defrance *et al.* (1981)
	He (2^3S), (2^1S)	Long and Geballe (1970); Dixon *et al.* (1976)
	He (2^3S + 2^1S)	Dixon *et al.* (1973); Fite and Brackmann (1963); Vriens *et al.* (1968); Koller (1969); Sherer-Izmi and Botter (1974)
	Ne (3^3P_2 + 3^3P_0)	Dixon *et al.* (1973)
	Ar (4^3P_2 + 4^3P_0)	Dixon *et al.* (1973)
	Na ($3^2P_{3/2}$)	Vuskovic (1991)
	Ba (5^3D), (5^1D), (6^1P)	Trajmar *et al.* (1986)
	Sr (4^1D_2)	Aleksakhin and Shafranyosh (1974)
	Mg (3^3P_2 = 3^3P_0)	Shafranyosh *et al.* (1991)
Total	He (2^3S)	Neynaber *et al.* (1964)
	He (2^3S), (2^1S)	Wilson and Williams (1976)
	Ar (4^3P_2 + 4^3P_0)	Celotta *et al.* (1971)
	Na ($3^2P_{3/2}$)	Bhaskar *et al.* (1977); Jaduszliwer *et al.* (1980 and 1985)


HELIUM
1 ¹S → 2 ³S
E = 26.5 eV
RM (5)
FOMBT
HELIUM
1 ¹S → 2 ³S
E = 30 eV
Hall et al. (1973)
Experiment
Brunger et al. (1990)
Trajmar (1973)
FOMBT
HELIUM
1 ¹S → 2 ³S
E = 30 eV
RM (5)
CC (5)
RM (19)
CCO
Experiment
FOMBT
DIFFERENTIAL CROSS SECTION (cm²/sr)
10⁻¹⁷
10⁻¹⁸
10⁻¹⁹
10⁻²⁰
0
40
80
120
160
SCATTERING ANGLE (degrees)
bml 54,55a,55b
2/25/92

IAEA Co-ordinated Research Programme
on "*Atomic and Molecular Data for Plasma Edge Studies*"

IAEA Research Agreement No. 5521/CF
"ELECTRON IMPACT IONIZATION OF ATOMIC AND MOLECULAR IONS"
Chief Scientific Investigator: Dr. E. Salzborn
Giessen University, Germany

Results obtained within this IAEA Research Agreement include:

I. Design, construction and successful tests of a complex experimental facility for measurements of absolute cross sections for single and multiple ionizaton of multiply-charged ions by electron impact.
The main components of the apparatus comprise: 10 GHz ECR-ion source for the production of multiply-charged ion beams; ion-optical devices for ion charge-state analysis, beam transport and focussing; high-intensity and high-energy electron guns ($\leq$ 1000V/450mA and $\leq$ 5000V/100mA, respectively); channeltron- and channel-plates-based detectors for single particle counting; computer-controlled data collection and analysis.
The apparatus is fully operational.

II. Measured absolute cross sections include:

Single-ionization ($\sigma_{q,q+1}$):

Li^{2+}, Ne^{q+} (q = 1,2,3,4), Cu^{1+}, Br^{q+} (q = 1,...,9), Ag^{1+}, In^{3+}, Sn^{4+}, Sb^{5+}, Te^{6+}, I^{7+}, Xe^{q+} (q =5,6,8,9,10), Cs^{1+}, Ba^{q+} (q = 1,2,3), La^{q+} (q = 1,2,3), Ce^{q+} (q = 1,2,3,4), Eu^{1+}, Tm^{1+}, W^{q+} (q = 1,2,3,4)

Double-ionization ($\sigma_{q,q+2}$):

B^{1+}, Ne^{q+} (q = 1,2,3,4), Ar^{q+} (q = 2,3,5,6), Cu^{1+}, Br^{q+} (q = 1,...,8) Ag^{1+}, In^{3+}, Sn^{4+}, Sb^{5+}, Te^{6+}, I^{7+}, Xe^{q+} (q = 8,10), Cs^{1+}, Ba^{q+} (q = 2,3), La^{q+} (q = 1,2), Ce^{q+} (q = 1,2,3,4), Eu^{1+}, Tm^{q+} (q = 1,2)

Triple-ionization ($\sigma_{q,q+3}$):

Ne^{1+}, Br^{q+} (q = 1,2,3,4), Xe^{q+} (q = 8,9,10), La^{2+}, Ce^{q+} (q = 1,2)

Quadruple-ionization ($\sigma_{q,q+4}$):

Br^{q+} (q = 1,2,3), Xe^{8+}

The present measurements expand the available data basis for electron-impact ionization cross sections by more than 30 per cent, 150 per cent and 50 per cent for single-, double- and triple-ionization, respectively.

III. A breakthrough could be achieved by the development of a novel energy-scan-technique which allows, for the first time, to resolve narrow resonances in the cross sections due to *resonant* ionization mechanisms; e.g. resonant excitation double-autoionization (REDA); resonant excitation auto-double-ionization (READI); resonant excitation triple/quadrupole autoionization (RETA, REQA).

Energy-scan measurements performed include:
Single ionization ($\sigma_{q,q+1}$):
B^{2+}, C^{3+}, N^{4+}, O^{q+} (q = 4,5), F^{6+}, Xe^{q+} (q = 1,2,3,4, 5,6), Cs^{1+}, Ba^{q+} (q = 1,2,3), La^{q+} (q = 1,2,3), Eu^{1+}, Tm^{1+}
Double ionization ($\sigma_{q,q+2}$):
Cs^{1+}, Ba^{q+} (q = 1,2), La^{q+} (q = 1,2), Ce^{q+} (q = 1,2,3), Tm^{1+}
Triple ionization ($\sigma_{q,q+3}$):
Ce^{1+}.

Co-ordinated Research Programme on "Atomic and Molecular Data for Fusion Edge Plasmas"

Report on the results obtained or expected in Louvain-la-Neuve on IONISATION AND REARRANGEMENT PROCESSES OF IONS AND ATOMS 1989 - 1993

F. BROUILLARD

1. ELECTRON IMPACT IONISATION OF MULTIPLY-CHARGED IONS

Cross sections for single and double ionisation of Ar^{7+} have been measured over the ranges 100-3000 eV and 550-3000 eV, respectively (ref. 1).

New measurements of the cross ection for single ionisation of Ar^{9+} have also been carried out, between 600 and 3000 eV to complete earlier measurements (ref. 2) but have not been published. They are however available in the Ph. D. thesis of S. Rachafi (ref. 3).

From mid 89 to mid 91, a new crossed electron-ion apparatus was built, capable of reaching higher energies (20 keV) and equiped with a purely mechanical beam sweeper. This apparatus will be used in 92 and 93 for measurements with $Ar^{8+,9+,10+}$, $Ne^{9+,10+}$ (internal ionisation) and C^{5+}, N^{6+}, O^{7+} (hydrogenlike ions).

A theoretical study has also been performed of the ionisation of Helium-like ions (ref. 4).

2. ELECTRON IMPACT IONISATION OF SINGLY CHARGED IONS.

Double ionisation cross sections have been measured for C^+, N^+, O^+, F^+ and Ne^+ from threshold to 2500 eV (ref. 5 and 6). Similar measurements have been carried out for CO^-, O^- and CO^-, to be published. A remeasurement was also done of the double ionisation of H^- (ref. 7).
Single ionisation of CO^+ was measured (ref. 8). Further measurements of single and double ionisation cross sections will be carried out in 92-93.

3. H^- PRODUCTION IN EXCITED HYDROGEN-RARE GAS COLLISIONS.

The in 1989 undertaken study (ref. 9) of the reaction

$$H(3\ell) + X \rightarrow H^- + X^+$$

has been continued, with an improved experimental method, to lower energy (300 eV) and to include helium as a target. Results are in course of publication (ref. 10) but are available in the doctoral thesis of B. Al Samour (ref. 11).

4. ASSOCIATIVE IONISATION OF EXCITED ATOMIC HYDROGEN.

Merged beam measurements have been carried out on the reactions :

$$H(1s) + H(2s) \rightarrow H_2^+ + e$$

$$D(1s) + D(2s) \rightarrow D_2^+ + e$$

The cross sections have been measured down to 0.005 eV CM-energy and show pronounced, different, structures (ref. 12 and 13).
The doubly excited channel :

$$H(2s) + H(2s) \rightarrow H_2^+ + e$$

has also been investigated (ref. 14).

New measurements will be done in 92-93 on the reactions

$$H(3\ell) + H(1s) \rightarrow H_2^+ + e$$

$$D(3\ell) + D(1s) \rightarrow D_2^+ + e$$

and possibly on :

$$He + H(2s) \rightarrow HeH^+ + e$$

$$H_2 + H(2s) \rightarrow H_3^+ + e$$

5. ELECTRON TRANSFER IN POSITIVE ION-NEGATIVE ION COLLISIONS.

The transfer ionisation reaction

$$He^{++} + H^- \rightarrow He^+ + e + H^+$$

has been investigated over the broad energy range 0.2-130 eV (ref. 14 and 15).

A new experimental set-up has been deviced to improve the accuracy of the measured absolute cross sections. It extends to merged beams the sweeping method that was previously developed for crossed beams and that avoids the need of measuring the geometrical form factor.

This new set-up will be used in 92-93 to measure the cross-sections, below 2 keV, of reactions as :

$$Ne^{4+,5+,6+,\ldots} + H^- \rightarrow Ne^{3+,4+,5+} + H$$
$$Ar^{4+,5+,6+,\ldots} \quad \ldots$$

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IAEA Co-ordinated Research Programme on
"Atomic and Molecular Data for Fusion Edge Plasmas"

Research Agreement: Theoretical Studies of Low-Energy Electron-Molecule Collisions
Institution: Dept. of Chemistry, California Inst. of Technology, Pasadena
Chief Scientific Investigator: Prof. V. McKoy

Report on Activities*

1. **Computational Method.** A multichannel close-coupling method, based on the Schwinger variational principle, has been developed for the study of elastic and inelastic low-energy electron-molecule collision processes. The formulation of the method allows for a general molecular target geometry, inclusion of the target polarization effects due to the interaction with incident electron, and all relevant electronic excitations. Some characteristic features of the Schwinger multichannel method are:
   - (i) the trial function used in the variational principle need not satisfy scattering boundary conditions (which are imposed on the unperturbed Green's function instead);
   - (ii) the N-electron wavefunction is expanded in Cartesian Gaussian orbitals (which permits analytical evaluation of most of the matrix elements involved);
   - (iii) the method can be applied to arbitary polyatomic molecules, the only limitation factor being the computer time.

The computationally intensive step in the cross section calculations are the "primitive" two-electron (containing the inter-electron interaction $1/r_{12}$) for all Gaussian orbitals. Evaluation of these integrals is well suited for distributed processing, presently available in the multiple-instruction-multiple-stream machines.

*** Prepared by R.K. Janev on the basis of the progress report given at the 1st RCM of this CRP (September 1990)**

2. Collision systems studied

The following collision systems and processes have so far been studied with the above method:

1) e-N_2: Excitation of $A^3\Sigma_n^+$, $B^3\cap_g$, and $W^3\Delta$ states
   Data information: total cross sections from threshold to 30 eV; differential cross sections at E=15 and 20 eV.

2) e-O_2: Excitation of $^1\Delta_g \rightarrow b^1\Sigma_g^+$ transition.
   Data: total cross section from threshold to 20 eV; differential cross section at E=4.5 eV.

3) e-H_2O: $\tilde{X}\ ^1A_1 \rightarrow {}^3A_1$ ($3a_1$-$3sa_1$) transition.
   Data: differential cross sections at E=12,15,20 and 30 eV.

4) e-CH_4: Excitation $^3T_2$ ($1t_2 \rightarrow 3a_1$) transition.
   Data: differential cross sections at E=12,15 and 30 eV.

5) e-C_2H_6: Elastic scattering (static-exchange only).
   -C_3H_8: Data: differential cross section at E=10 eV.

6) e-SiH_4: Elastic scattering (static-exchange only)
   Data: differential cross section at E=5 eV;
   momentum transfer cross section ($E \leq 30$ eV);
   total elastic cross section ($E \leq 30$ eV).

Plans for the near future include:

Electron-impact excitation and dissociation of H_2O, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_6 and C_3H_8.

Summary Report on Research Coordination Program on "Atomic and Molecular Data for Plasma Edge Studies"

subtitle : Compilation and evaluation of AM data involving atomic/molecular hydrogens and some hydrocarbon molecules

H.Tawara
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Nagoya 464-01, Japan
(June 18, 1992)

My principal objective in this RCP is to survey the present status of atomic and molecular data in hydrogen and hydrocarbon molecules which are the most relevant to fusion edge plasma studies, to compile and evaluate them, and, furthermore, to find new work necessary for their application to fusion research. Following the extension of the program, I have also tried to do similar work on the most common impurities in all plasma devices, namely H_2O, CO and CO_2 molecules.

The present activities are thus divided into three parts :

1) Data for hydrogens[1)]
There are a large number of investigations reported. But serious discrepancies are observed in some cases. It is found that, in particular, data for ion and neutral hydrogen atoms produced through dissociation or ddissociative ionization, that is, their (partial) production cross sections and energy distributions, are divergent among different authors.
2) Data for hydrocarbons[2-3)]
Through the present survey, we strongly feel that more systematic measurements are necessary among hydrocarbon molecules to get consistent, reliable data in electron collisions. So we have remeasured total electron scattering cross sections from various hydrocarbons (C_mH_n : m=1,2,3) and found generally good agreement with those previously determined. For the first time, we could observe the isomer effect, namely scattering of electrons is different among molecules with different configurations with the same numbers of atoms (C_3H_6 ; propene and cyclopropane)[4)]. Now we are going to remeasure dissociative (total and partial) ionization cross sections using our new apparatus.
3) Data for common impurities[5)]
As these impurities are also important in space science and astrophysics, a series of measurements had been reported previously. But the general situation of data seems to be similar to those above mentioned in 1) and 2), indicating that some data are still in serious disagreement with each other. Also the survey has been made on high energy proton/hydrogen

collisions which seem to be relevant to those in NBI processes[6].

Concluding remarks

Through the present survey on electron impact data for various molecules near the plasma edges, we have found the following general remarks common to all these molecules relevant to plasma edges :

1) Cross sections for dissociation products are not always reliable probably because their collection is not complete due to their relatively large energy gained through dissociation.
2) Most of cross sections for molecules and molecular ions are strongly dependent upon their internal energy, namely the excited states, and then they are varied sometimes by more than an order of magnitude. This is quite important in plasma research as a significant fraction of these molecules present near the edges are likely to be in highly excited states.
3) Cross sections for collisions of the state-selected molecules are very few and more systematic studies should be performed.
4) The energy distributions of products, which are important in getting information of their penetration into plasmas, are still unreliable.
5) Data for photon emission, which are most convenient in plasma diagnostics, are also sometimes in serious disagreement with each other. This is probably due to improper detector calibrations and corrections to the life-times of the excited states of molecules.

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Electron stripping cross sections for light impurity ions in colliding with atomic hydrogens relevant to fusion research

IAEA Co-ordinated Research Programme on
"Atomic and Molecular Data for Fusion Edge Plasmas"

Research Agreement: Measurements of electron impact ionization cross sections for molecules
Institution: Institute of Physics, Belgrade, Yugoslavia
Chief Scientific Investigator: Dr. I. Cadez

Report on Activities*

The principal subject of the experimental investigations undertaken under this Research Agreement was the measurement of ionization cross sections for the plasma edge molecules by electron impact, with emphasis on the hydrocarbons. Partial (dissociative) and total ionization cross section measurements have been performed for CH_4, C_2H_4, C_2H_6, n-propane and some alcohols. The comparison with the results of other measurements, when available, shows good agreement in the energy region below the cross section maximum, but significant differences in the region around the cross section maximum and above. In the case of CH_4, these differences are on the level of 20-30%, for ethan they are within 10-20%, and for propane are significantly larger.

The total and dissociative electron-impact ionization cross sections for H_2O have been remeasured in the energy range from threshold to 200 eV. These data are in good agreement with the majority of previous measurements except with the results of Srivastava, which for energies above 100 eV are significantly higher (up to factor fo two).

The dissociative electron attachement on $H_2(v)$ formed on and released from material surfaces, has also been studied within this project.

*** Prepared by R.K. Janev on the basis of the progress report given at the 1st RCM of this CRP (September 1990)**

Ion-Atom/Ion-Surface Collision-Data for Plasma Edge Kinetics and Diagnostics

Contributions to IAEA-CRP on A&M Data for Fusion Edge Plasmas (1989-92)

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Summary Report

1. Relevance for Edge Plasma Kinetics and Diagnostics

Cross section data of relevance for edge plasma diagnostics with "active" Li beams have been produced, covering single electron capture in collisions of Li atoms in both their ground and excited states with typical multicharged edge plasma-resident impurities. The corresponding absolute cross sections are incorporated into a data base which already covers inelastic collisions of Li atoms with electrons and protons, and can be made available to all groups interested in the application of active Li beams for edge plasma diagnostics. Furthermore, attention has been given to electron capture in collisions of slow C^{q+} and O^{q+} (q = 1, 2) with H_2 and He, with particular emphasis on the role of metastable initial projectile states. Finally, for edge plasma modelling the possible influence of electron emission from the inner surface of first wall materials due to impact of slow, highly charged impurity ions is being considered.

2. Active Li Beam Edge Plasma Diagnostics (Li-CXS)

In three recent publications the working principles and capabilities of active Li beam plasma edge diagnostics have been demonstrated. Space - and time - highly resolved measurements of both impurity ion densities /1/ and -temperatures /2/ in the tokamak edge plasma are now possible by means of Li-CXS (Li beam - activated charge exchange spectroscopy), given the necessary atomic collisions data (cf. part 1). Methods for precise, rapid data evaluation from such measurements have been presented in /3/. They are rather promising for detailed experimental studies on impurity ion transport in tokamak edge plasmas. For example, a better judgment on the applicability of forced impurity radiation cooling of the plasma edge may become possible in this way.

3. Single Electron Capture by Multicharged Ions from Li(2s) and (aligned) Li(2p)

Photon-spectroscopical studies have been carried out on single electron capture into $He^{+}(4\ell)$ states in He^{2+} - Li(2s) collisions /4/, and also on state-selective single electron capture in X^{6+} (X = C, N, O, Ne) - Li(2s) collisions /5/, because of their particular interest for Li-CXS. Ref. /5/ also covers equivalent data for Ne^{q+} (q = 7 ÷ 9) - Li(2s) collisions. Measurements for B^{q+} (q = 3, 5) have recently been finished anddata will be introduced in the Li-CXS data base referred to in part 1.

Detailed studies on electron capture in He^{2+} - Na(3p) collisions have been carried out by means of translational energy spectroscopy and dye laser excitation of Na target atoms /6/, serving as a forerunner to similar studies with Li(2p), since absolute cross sections for the latter processes are urgently needed for modelling active Li beam compositions in connection with Li-CXS. These studies have recently also been made with aligned Na(3p) target atoms /7/, considering the basic interest in such collision processes. Measurements have recently been started for He^{2+} - Li(2p) /8/ because of the reasons already explained.

4. More-Electron Transitions in Single Electron Capture from Li(2s)

If impurity ions with complex structure collide with e.g. Li(2s), a single electron capture can be accompanied by other electronic transitions (e.g. a change of core state) in the projectile. Such two-electron transitions have recently been studied in considerable detail for collision systems as C^{2+} - H_2, Ar and Ne^{2+}/Ar^{2+} - Li(2s)/Na(3s)/K(4s) /9/.

5. C^{q+}/O^{q+}-H_2/He Collisions - the Role of Metastable Projectile States

We have investigated in some detail the role of metastable primary ion states in collisions of slow C^{q+} and O^{q+} (q = 1, 2) with H_2 and He /10,11/. Corresponding absolute total cross sections have already been published for C^{q+} (q = 1, 2) - H_2/He in /12,13/, and for O^+ - He in /14/. Whereas in all of these collision systems the composition of the primary ion beams turned out to be of great influence, particularly interesting results have been obtained for O^+ - He collisions, where total cross sections for single electron capture into the $O^+\ {}^2D^o$ and ${}^2P^o$ metastable ions turned out much smaller than for $O^+\ {}^4S^o$ ground state ions, despite the highest energy defect for the last reaction. This unexpected behaviour has been explained /14/ by an efficient suppression of electron capture into either metastable ion state due to a competing, collisionally induced inelastic transition into the companion metastable primary ion state.

6. Recent Advances in Slow MCI-Surface Collisions

Extensive studies have been conducted on multicharged ion-induced electron emission from clean metal surfaces, involving total electron yield determination from measured electron emission statistics ("ES") /15/. In conjunction with measurements of the ejected-electron energy distributions, in particular spectroscopy of the comparably fast, but relatively scarce electrons resulting from Auger decay of transiently formed projectile inner shell vacancies /16/, an almost quantitative judgment on the probable importance of these processes for the charge balance in tokamak edge plasmas can now be made. Recently, we have extended such ES measurements to the so far highest primary ion charge states (e.g. Ar^{16+}, J^{25+} /17/) involved in multicharged ion impact on clean metals.

Acknowledgments

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IAEA Co-ordinated Research Programme on
"Atomic and Molecular Data for Fusion Edge Plasmas"

Research Agreement (No. 5473/CF): "Investigation of atomic collision processes in eV - keV energy range"
Institution: Russian Research Centre "Kurchatov Institute", Moscow, Russia
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Report on Activities*

The investigations of heavy-particle atomic collisions under this project included:

1. Charge exchange cross section measurements in slow collisions of multiply charged plasma edge impurity ions with atomic hydrogen;
2. Experimental study of dissociative processes in the mutual collisions hydrogen molecular ions at low energies.

Below we give a brief description of the investigations and the obtained results.

1. Hydrogen atom-multicharged ion charge exchange collisions

The investigations were performed on the aparatus ATOS used earlier for charge exchange cross section measurements involving inert gas multicharged ions. The use of non-inert gas multicharged ions in the present studies has required certain modifications and improvments of the aparatus, the most important of which are:

a) Improvment of the vacuum conditions. This has been achieved by introducing in the experimental chamber sputterless getters to collect the residual gases at the room temperature.
b) A special analyzer-detector has been designed, manufactured and introduced in the measurement system to allow for coincidence cross section measurements.

With this up-graded version of the aparatus, the charge exchange cross section in collisions of C^{3+} ions with hydrogen atoms were measured in the energy range from 1.5

to 700 eV/amu. The obtained results are in good agreement with those of the Oak Ridge group, and extend them to lower energies. The results have been published in Sov. Phys.-Plasma Physics **17** (No.5) 576 (1991) (Russian Edition).

2. Rearrangement and dissociative processes in $H_2^+ + H_2^+$ collisions

The investigation of these processes have been performed on the experimental aparatus DIVO, described in the IAEA report INDC(CCP)-224/GA (Vienna, 1984). The experimental set-up allows for coincidence measurements of various rearrangement and dissociative reaction channels of the colliding system. In the case of $H_2^+ + H_2^+$ slow collisions, the following reaction channels are possible:

$H_2^+ + H_2^+ \rightarrow$	$H_2^+ + H + H^+$	-2.65 eV	(1)
$\rightarrow$	$H + H^+ + H + H^+$	-5.30 eV	(2)
$\rightarrow$	$H_2 + H^+ + H^+$	-0.82 eV	(3)
$\rightarrow$	$H_3^+ + H^+$	+3.58 eV	(4)

Cross section measurements are presently in progress for the dissociative channel (2) in the energy range from threshold to 20 eV. The preliminary results of these measurements have been reported at the 2nd RCM of this CRP (June 17-19, 1992, Vienna). It is planned that these measurements will be finished by the end of 1992. The cross section for the reaction channel (4) will also be measured in the nearest future (in the energy range below 25 eV).

The plans for 1993 include cross section measurements for the $Ga^{q+} + H$ (q=1-3) charge exchange collisions in the energy region below 1 keV/amu, as well as electron impact ionization of Ga^{q+} (q=1-3) ions in the energy range from threshold to 25 eV.

IAEA Co-ordinated Research Programme on
"Atomic and Molecular Data for Fusion Edge Plasmas"

Research Contract: Theoretical cross section calculations for heavy particle collision processes in the plasma edge.

Institution: Institute of Physics, Belgrade, Yugoslavia

Chief Scientific Investigator: Dr. P.S. Krstic

Report on Activities*

1. Ion-Atom collision processes

The adiabatic method with hidden potential energy crossings in the complex plane of internuclear distance has been employed to study the collision dynamics of inelastic processes in hydrogen atom-fully stripped ion systems. The excitation, ionization and charge exchange processes in the H(n) - H^+, He^{2+}, Be^{4+}, B^{5+} systems have been studied in the energy range 0.2 - 25 keV/amu (typically), with n=1-3 for H^+ and He^{2+}, and n=1,2 for Be^{4+} and B^{5+}. The calculations include a large number (typically above hundred) of coupled adiabatic molecular states. The results of these calculations compare favourably with the experimental data and the results of extensive multi-state coupled-channel (AO-, or Mo-based) calculations, when these are available. Similar cross section calculations are now in progress for the H + Li^{3+} system. The results of these studies have been published in four publications.

2. Ion-molecule collisions

The electron capture process in the low energy H^+ + H_2 collisions has been theoretically studied within an "effective" two-(electronic) state model with inclusion of relevant vibrational states. The coupled equations have been solved numerically. The obtained results agree well with those based on a multi-channel close-coupling treatment.

*** Prepared by R.K. Janev on the basis of annual progress reports for this Research Contract.**

A more ambitious study of ion-diatomic molecule low-energy collision processes has been undertaken by employing the trajectory surface hopping model in conjunction with the infinite-order sudden approximation. The adiabatic energy surfaces are obtained by the diatomic-in-the molecule (DIM) model.. The system of coupled equations for the transition amplitudes is formulated for a number of selected electronic states of the three-atomic system and the pertinent vibrational states. This system has been solved numerically in the above mentioned approximations for the $H^+ + H_2$, D_2, T_2 systems at collisions energies below 1 keV (CM). The calculated total charge exchange cross sections agree well with the experimental data, when available. The cross sections for the population of different final $H + H_2^+$ (v) channels have also been calculated, as well as the corresponding differential cross sections for $E \leq 20$ eV (CM). The latter also agree with the experimental data, except for large scattering angles.
The work will be continued to improve the description of collision dynamics and to include collisions of He^+ and He^{2+} with hydrogen (isotopic) molecules.

IAEA Co-ordinated Research Programme (CRP) on "Atomic and Molecular Data for Fusion Edge Plasma Studies"

Summary Report of the Kaiserslautern Group

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The contribution of our group to the above CRP consists of two parts: (i) a review of the existing database for ion–molecule collision processes relevant to fusion edge plasmas; (ii) experimental studies on selected collision systems to generate new data. A brief description is given in the following. Plans for future work along these lines are indicated.

1. Review article

A review article has been prepared [1] which gives a survey on the existing database for ion–molecule collision processes relevant to fusion edge plasmas. In view of the enormous number of possible combinations of reactants, the scope of the article had to be limited. As a first step, we decided to consider hydrogen and helium species, which form the main plasma constituents.

The energy range of interest in edge plasma studies is approximately 1 – 200 eV. Accordingly, the data have been mainly collected from low energy beam experiments. The experimental methods used are briefly discussed and characterized with respect to their strengths and weaknesses.

The survey of data has been divided into the following categories: (1) reactive collisions; (2) energy transfer collisions; (3) negative ion collisions. Besides total cross sections, the survey also includes more specific data classes (state–selective cross sections, product distributions, etc.) which are needed for edge plasma modelling.

Several conclusions can be drawn from this review. Although only hydrogen and helium – the most elementary constituents of the edge plasma – are considered, there are still significant gaps and, in some cases, large uncertainties in the database for edge relevant energies. Even for very fundamental processes such as charge transfer in $H^+ + H_2$ and $He^+ + H_2$, the data are in a quite unsatisfactory state. With the existing experimental techniques, it should be possible to aim at a 10 % confidence level of the cross section data. However, considerable efforts are still needed to reach this goal.

On the other hand, it must be realized that the full range of cross section data, which is required for the understanding of the edge plasma, cannot be obtained from experimental work alone. A joint experimental/theoretical approach is clearly necessary. The experimental measurements are normally restricted to a limited range of experimental parameters. Once the theory has been checked against the experimental results, the full picture and the complete set of data can be derived from the theoretical calculations.

Another aspect is the range of collision systems and processes. Also in this respect are the experiments often confronted with serious limitations. It is necessary that theoretical methods are developed and tested against experiment for certain benchmark systems. Once this is done, the methods can be extended and applied to systems and processes which are difficult to access experimentally. The hydrogen and helium systems treated in the present review should be particularly suitable for this purpose. One has to keep in mind, however, that molecular collision systems are far more complex than ion–atom systems. In particular for collision energies in the eV range, one needs full dynamical calculations based on accurate potential energy surfaces. It is clear that this requires substantial efforts on the theoretical side.

For a number of processes treated in the present review, a strong dependence on the initial reactant state is observed. This aspect clearly demands particular attention in edge plasma modelling, both concerning the initial state population and the cross section behaviour of the reactants. Systematic studies with state–selected reactants have only begun a few years ago and, within the scope of the present review, the only existing measurements are those for the H_2^+ molecular ion. Corresponding measurements for the H_2 neutral molecule in well defined excited states are not available at the present time.

The general conclusion from this review is that the present state of the database concerning ion–molecule collision processes at low energies (about 1 – 200 eV) cannot be regarded as satisfactory. There are important deficiencies in several respects. Substantial efforts from both experiment and theory are still needed to provide a sufficienty complete and reliable database for edge plasma modelling.

2. Experimental studies

a) Experimental technique

In our experiments, we use the crossed beam (CB) technique. A mass and energy selected ion beam is crossed at right angles with a supersonic nozzle beam of the target gas. Both beams are well collimated and can be made nearly monoenergetic. The kinematically well defined conditions permit measurements with high resolution in energy and angle. The product analysis is performed using a rotable detector which allows mass and energy analysis of the product ions. The energy resolution is generally sufficient to perform state resolved measurements. In favourable cases, individual rotational transitions can be resolved.

The CB technique has reached the state that it is now possible to carry out measurements down to collision energies in the order of 0.1 eV, so that the full energy range relevant to edge plasma studies can be covered. All types of processes (elastic, inelastic, reactive) can be studied with this method, and all classes of data needed for edge plasma modelling can be obtained. These include product and state specific differential cross sections, angle–integrated partial cross sections for individual product states, and total cross sections summed over all product states. Thus, the measurements provide both a very detailed and a complete picture of the collision processes. It must be realized, however, that these measurements are very time consuming so that, in practice, the number of such studies will be limited.

It is important to stress that cross sections have to be determined in absolute units in order to be useful in practical applications. There are several possibilities for obtaining absolute cross sections in CB experiments. The most direct and therefore most attractive method consists of using simple ion–atom scattering systems as secondary standards. Examples of such systems are H^+ + He, He^+ + He, and H^- + He. These systems are well known both experimentally and theoretically; they are easy to handle experimentally and are therefore conveniently used for this purpose. In our experimental studies related to the present CRP, the above–mentioned ion–atom systems play a key role in this respect and are routinely used for calibration purposes. More details can be found in the original papers.

b) H^-/D^- collisions

An extensive study has been performed for the $H^- + H_2/D_2$ collision system. The scheme of the various competing processes for this system can be illustrated as follows:

$$H^- + D_2 \longrightarrow H^- + D_2(v',j') \qquad (1)$$

$$\longrightarrow HD(v',j') + D^- \qquad (2)$$

$$\longrightarrow H + D_2 + e \qquad (3)$$

$$\longrightarrow HD + D + e \qquad (4)$$

The measurements have been concentrated on the collision energy range $E_{cm} = 0.3 - 3$ eV, because the competition between the various processes becomes most evident at these low energies. At higher energies, electron detachment becomes the dominant channel and the H^- ion is readily destroyed in collisions with the target gas.

It should be mentioned at this point that it has yet to be ascertained if negative ions play a significant role in the edge plasma. The presence of H^-/D^- ions (binding energy 0.75 eV) is certainly restricted to the low temperature regions of the edge plasma, but they may be relatively abundant in these regions. This suggests that low energy H^-/D^- collisions with the main neutral constituents of the edge plasma (i.e. H, H_2, He and their isotopes) deserve consideration in the present context. Incidentally, we mention that collision processes involving H^-/D^- ions, in particular formation and destruction processes of these ions in hydrogen discharges, are of crucial importance in the development of H^-/D^- volume sources designed for neutral beam heating in fusion reactors.

Out of the above reaction scheme, the most detailed study has been performed for the rearrangement reaction $H^- + D_2(v = 0) \rightarrow HD(v') + D^-$. From the vibrationally state–resolved energy and angular spectra of the D^- product ions, we derive state–specific differential cross sections in the centre–of–mass system. Absolute units are obtained by using elastic $H^- +$ He scattering as a reference system. The state–resolved differential measurements of the present work allow detailed conclusions concerning the reaction mechanism, e.g. the results indicate that the reaction occurs preferentially for a collinear configuration of the reactants. By integrating over angles and summing over partial cross sections (for individual v′), we determine the absolute total cross section of the reaction. The reaction has a threshold at $E_{cm} = 0.42 \pm 0.12$ eV. The cross section rises to a maximum of 2×10^{-16} cm^2 near 1.5 eV and then rapidly decreases again. The present results resolve a gross discrepancy between two previous measurements of the total cross section.

A first report on this work has been published recently [2]. More results, including state–resolved measurements of rotationally inelastic scattering of H^- from H_2, will be presented in forthcoming papers [3–5].

In previous work on H^-/D^- collisions, we have studied vibrationally inelastic scattering of H^- ions from various molecules [6] as well as electron detachment in H^-/D^- collisions with rare gas atoms [7–9]. In the latter case, we have measured angular distributions of the neutral H/D atoms and energy spectra of the detached electrons for collision energies ranging from 2 eV to 250 eV. More recently, we have performed a very detailed study of the detachment process by measuring electron–neutral coincidences including time–of–flight analysis of the products [10].

c) He^+ collisions

In the above–mentioned review [1], a rather confusing situation was found for charge transfer in $He^+ + H_2$ collisions at centre–of–mass energies below 1000 eV. There is general agreement that dissociative charge transfer $He^+ + H_2 \rightarrow He + H + H^+$ is the dominant process. However, the data are in a very unsatisfactory state. The disagreement between different data sets amounts up to more than a factor of 100 in certain energy regions.

This motivated us to perform additional measurements on this system using our crossed beam technique. One should note that in the experimental methods, which are typically used for total cross section measurements, considerable uncertainties can arise from insufficient and inaccurately known collection efficiencies. The energy and angular distributions of the product ions, which are a priori unknown, play an important role in this respect. It was our aim, therefore, to measure exactly these kinetic energy distributions of the H^+ product ions in order to help clarifying the situation.

The measurements have been performed for centre–of–mass collision energies $E_{cm} = 4 - 300$ eV. The product ions are detected for angles from $\Theta = 0^0$ to $\Theta = 100^0$ with respect to the primary He^+ beam. The system $He^+ + He$ is used to calibrate the transmission properties of the detector system and to determine absolute units of the measured cross sections.

The results show kinetic energy distributions of the H^+ product ions reaching up to 15 eV and more. The shape of the energy distribution varies with the angle, but on the whole the intensity is about equally strong under all angles. It becomes immediately clear that under these conditions the total cross section measurements are likely to suffer from collection efficiency problems. On the other hand, it is not surprising that the H^+ product ions have large kinetic energies, since they are expected to be formed from H_2^{+*} intermediates in strongly repulsive states.

The H^+ kinetic energy distribution shows a strong dependence on the He^+ collision energy. At the higher collision energies, one observes clear evidence of a structure which is tentatively explained by a two–step model:

$$He^+ + H_2 \longrightarrow He + H_2^{+*} \qquad (1)$$

$$H_2^{+*} \longrightarrow H^+ + H(n\ell) \qquad (2)$$

Measurements of optical emissions resulting from $He^+ + H_2$ collisions [1] are in agreement with this interpretation. At lower He^+ collision energies, the reaction mechanism becomes more complex and the H^+ kinetic energy distribution is completely different in shape.

The evaluation of the measurements is currently in progress, and we hope to report on the results shortly [11].

In previous work on low energy ion–molecule charge transfer reactions, we have performed a detailed study of the $He^+ + O_2$ system in the collision energy range 0.5 – 200 eV [12,13]. Similar measurements have been performed for the systems $He^+ + N_2$,NO,CO. These results will be reported in forthcoming papers [14].

3. Future work

The author has agreed to prepare two data–oriented reviews on "Ion–molecule reactive collisions" and "Collision processes involving H^-/D^- ions", respectively. These articles will be part of a book which is intended to represent the final CRP document.

Concerning the continuation of our experimental studies for the time period 1992/93, we will mainly concentrate on completing the work described above. In the case of H^-/D^- collisions, we plan to include other isotopic variants of the $H^- + H_2$ system. Another interesting aspect is to study in more detail the competition between the various processes including the electron detachment channel. The work on He^+ collisions will continue with studies of the reactions $He^+ + H_2 \longrightarrow He + H_2^+$ and $He^+ + H_2 \longrightarrow HeH^+ + H$ which are competing processes to the dissociative charge transfer channel $He^+ + H_2 \longrightarrow He + H + H^+$ discussed above. It may also be of interest to include other isotopic variants of this collision system. Some measurements of total cross sections for these processes exist in the literature, but the present differential scattering experiments will provide additional information (product distributions, partial cross sections, reaction mechanisms, etc.). A a further step, we plan to study reactive collisions of He^{++} at low energies. However, this work will probably not start before the end of 1993 and will therefore not be included in the present CRP.

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This report should not be finished without giving credit to the students of my group who carried out the experiments and contributed in various other ways. Their names are found in the references of this report. I wish to thank all of them for their dedicated work.

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