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Second Research Coordination Meeting on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Institute of Plasma Physics, Nagoya University, Nagoya, Japan

31 August-2 September 1983

SUMMARY REPORT

K. Katsonis and A. Lorenz

March 1984

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

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Abstract

Proceedings of the second meeting of the participants in the IAEA Coordinated Research Programme F4.30.02 on atomic collision data for diagnostics of magnetically confined fusion plasmas, convened by the IAEA Nuclear Data Section on 31 August - 2 September 1983, at the Institute of Plasma Physics, Nagoya University, Nagoya, Japan.

The meeting participants reviewed the work in progress and the current status of data on electron impact excitation, ionization and recombination and on charge transfer for selected fusion relevant elements, made specific recommendations on the use of these existing data, and identified those data which needed to be measured or calculated.

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I. Summary of the Meeting

Introduction

The second meeting of the participants in the IAEA Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas was convened by the IAEA Nuclear Data Section on 30 August - 2 September 1983 at the Institute of Plasma Physics, Nagoya University, Nagoya. This Research Coordination Meeting (RCM) was run by the Scientific Secretary K. Katsonis with the assistance of three co-chairpersons, T. Kato, H. B. Gilbody and G. Dunn. A. Lorenz participated in the meeting as Head of the Atomic and Molecular Data Unit.

In connection with the RCM, a Symposium on Atomic Collision Data for Diagnostics and Modelling of Fusion Plasmas was held on 29-30 August 1983. The Symposium was organized by the staff of the Research Information Center, Institute of Plasma Physics, Nagoya University under the auspices of the grant-in-aid of scientific research, the Special Research Program on Nuclear Fusion by the Ministry of Education, Science and Culture. It aimed at bringing together scientists working in the fields of atomic data, plasma diagnostics and plasma modelling to discuss problems of common interest and increase mutual understanding. About twenty papers were presented on modelling, diagnostics and the activities of the present RCM. It is to be mentioned that some of the papers discussed how atomic data could be obtained by making use of plasmas. The proceedings of the Symposium are available as report IPPJ-AM-33.

The participants in the second RCM are listed in Appendix 1, and the Adopted Agenda is given in Appendix 2. The meeting began with an Opening Speech given by H. H. Kakihana, Director of the hosting Institute. The text of the speech is given in Appendix 3.

Objectives

The goal of the Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas is to generate evaluated sets of atomic collision data in accordance with requirement priorities determined by the fusion community. The necessary work to achieve this goal will be performed by the atomic collision physicists participating in this CRP under the coordinating guidance of the A+M Data Unit.

The objectives of this second meeting of the CRP were:

- to review the status of the data for those processes and reactants identified by the fusion community to have high priority;

- to assess the accuracy and validity of those data;

- to decide which of the required data can now be considered to be in a satisfactory state; and

- to identify those data which can be generated experimentally, calculated theoretically, or represented by empirical formulae.

The results of this annual survey summarized in this report should thus give overall guidelines for the work to be performed by the CRP participants during their further participation in this international project, as well as for the use of the existing data by the fusion community.

Conclusion and Recommendations

The conclusions and recommendations of the meeting were formulated during its last day in plenary session, on the basis of the working group reports (WGR).

In the area of electron impact excitation of ions (WGR I), the evaluated data on C and O ions of the US-Japanese collaboration (WGR I, Ref. 5) could be recommended as 'best' values for use. The rate coefficient for Li-like ions excitation evaluated in Rutherford Appleton Laboratory (WGR I, Ref. 6) are also recommendable.

In the area of electron impact ionization, (WGR II) the data of Bell et al. as modified last year (WGR II, Ref. 4) can be recommended without reservation. The formulae by Burgess and Chidichimo (WGR II, Ref. 2) can be recommended for plasma modeling. The parametric formulae of Shevelko et al. (WGR II, Ref. 3) constitute an improvement on the Lotz formula for isoelectronic series from H to Ca.

In the area of dielectronic recombination (WGR III) it was felt that because of substantial on-going activity in this area it was too soon to make any specific recommendation.

Finally, in the area of charge exchange processes (WGR IV) attention was drawn to a number of precise experiments and to compilations (WGR IV, Ref. 1) and parametric formulas (WGR IV, Ref. 4) mostly related with collisions involving H.

A draft version of the WGR was included in the issue no. 24 of the International Bulletin on Atomic and Molecular Data for Fusion.

Next Meeting

Vienna was choosen as the place of the next meeting of this CRP and the preferred time was the third week of June. This will give to the CRP participants the possibility to meet the members of the IFRC Sub-committee on A+M Data for Fusion whose third meeting is scheduled for this time, and discuss with them any problem arising from the evaluation and dissemination of A+M data for fusion.

II. Meeting Programme

1. Opening speech by Prof. H. H. Kakihana, Director of the Institute of Plasma Physics, Nagoya University, Nagoya.

2. Progress reports from CRP Participants

   The following reports were presented at the meeting by scientists participating in the CRP. Dr. Janev was unable to attend and send his report by mail.

2.1. S. Bliman (Centre d'Etudes Nucleaires de Grenoble, France)

   Progress report.

2.2. G. Dunn (JILA, Boulder Co, USA)

   Progress report on the fusion related work.

2.3. H. B. Gilbody (Queen's University, Belfast, UK)

   Progress report.

2.4. P. Hvelplund (Institute of Physics, University of Aarhus, Denmark)

   Progress report on the work at the Institute of Physics of the University of Aarhus.

2.5. Y. Itikawa (Institute of Space and Astronautical Science, Tokyo, Japan)

   Progress report.

2.6. R. K. Janev (Institute of Physics, Belgrade, Yugoslavia)

   Progress report.

2.7. E. Salzborn (Institut fuer Kernphysik, Universitaet Giessen, FRG)

   Progress report.

2.8. H. Winter (Institut fuer Allgemeine Physik, Vienna, Austria)

   Progress report.

3. Progress reports from invited observers

3.1. V. A. Abramov (Kurchatov Institute, Moscow, USSR)

   Progress report.

3.2. Y. Kaneko (IPP, Nagoya University, Japan)

Report on the Present Status of the Naked Ion Collision Experiment (NICE).

3.3. T. Kato

Progress report on the work at the Nagoya University Institute of Plasma Physics.

3.4. Y. Nakai (JAERI, Ibaraki-Ken, Japan)

Progress report on the work at the JAERI Division of Physics.

3.5. T. Watanabe (RIKEN, Wako, Saitama, Japan)

Progress report on the Work at the Atomic Processes Laboratory of the Institute of Physical and Chemical Research (RIKEN).

Individual reports are available on request from the IAEA Nuclear Data Section.

4. Review of the Data Status and of the Data Requirements

Review of the status of the required data was performed by four separate groups, each one addressing one of the priority collision process categories:

Electron Impact Excitation: reviewed by Y. Itikawa, T. Kato (Chairperson), K. Katsonis and M. R. C. McDowell.

Electron Impact Ionization: reviewed by V. A. Abramov, G. H. Dunn (Chairman) and E. Salzborn.

Dielectronic Recombination: reviewed by V. A. Abramov, G. H. Dunn (Chairman) and E. Salzborn.

Charge Exchange and Related Processes: reviewed by V. A. Belyaev, S. Bliman, H. B. Gilbody (Chairman), P. Hvelplund, R. K. Janev, Y. Nakai, H. Tawara, T. Watanabe and H. Winter.

The reports of the working groups constitute the major product of this meeting, and are given below in their entirety. In their reports, the groups also assessed the accuracy and validity of the data, and identified those sets of data which could be considered to be in a satisfactory state and could be proposed to be recommended to the fusion community.

Working Group Report on Electron Impact Excitation of Ions

Y. Itikawa, T. Kato (Chairperson), K. Katsonis[+]

I. Introduction

The work on electron impact excitation of ions published since the first CRP meeting is not extensive. Although the data presented here are of general interest to fusion research, emphasis is given to species and reactions currently used for diagnostics of magnetically confined plasmas.

Bibliographic sources used for the present report consist mainly of the bibliography on electron collisions with atomic positive ions (1) as updated for the period 1978-1982 (2) and 1982-1983 (3) and of a more general bibliographic bulletin (4).

A major evaluation of carbon and oxygen ion data has been lately accomplished in the frame of a collaborative program of the U.S. and Japanese atomic data centers for fusion research, the Controlled Fusion Atomic Data Center of Oak Ridge National Laboratory and the Research Information Center of Institute of Plasma Physics, Nagoya University (5). This evaluation constitutes a part of the present CRP. A selection of the compiled electron impact excitation cross sections of carbon and oxygen ions has been made, in order to recommend 'best' values for use. The resulting recommended values are fitted to an analytical formula and the fitting coefficients are given in a table. The cross sections (in the form of collision strengths) and the rate coefficients calculated therefrom are shown graphically. The reliability of the recommended data is roughly estimated.

[+]The members of the electron impact excitation Working Group gratefully aknowledge the contribution of Prof. McDowell, unable to attend the meeting for technical reasons, in writing the final version of this report. Thanks are also due to Dr. G. Dunn for critically reading the manuscript.

Another important evaluation of Li-like ion rate coefficients was published by the Rutherford Appleton Laboratory (6). It includes all the available good quality quantal calculations of excitation cross sections by electron collision for Li-like ions. A comparison was also made with the small amount of experimental data of $2s\ ^2S - 2p\ ^2P$ cross sections. The cross sections chosen on the basis of these data were integrated over maxwellian distributions of the electron energies to give excitation rate coefficients. The results are presented graphically and as simple formulae.

General isoelectronic sequence studies were done for H-like ions. Scaled collision strengths were given with an empirical formula based on the Coulomb-Born (CB) approximation with time dependant perturbation of the electrostatic interaction between the electrons (7). In this work levels up to n=5 were considered. Also, an empirical formula based on Close Coupling (CC) results was obtained for collision strengths corresponding to excitation of the level n=2 (8). This formula summarises the computed collision strengths for H, He^{+}, C^{5+}, O^{8+}, Ar^{17+} and Fe^{25+} within about 5% accuracy, and enable the rapid computation of rate coefficients for all hydrogenic systems with $Z < 26$.

The work given in Ref. 7 was extented by the same group to derive empirical formulae for He-like ions, for transitions among $2s^2$, 2s2p, $2p^2$ levels (9, 10) and for inner-shell excitation among 1s2s, 1s2p, 2s2p, $2p^2$ levels (11); also for inner-shell excitation of Li-like ions from the levels $1s^22p$, $1s^22s$ to all fine structure levels of the $1s2\ell2\ell'$ configurations (12, 13).

2. Calculations

Data of interest to fusion published after June 1982 (through August 1983) are tabulated in Table I. The corresponding energy range is given in eV or Ry when the calculations are resulting to cross sections and in ^{o}K when rate coefficients are calculated. Three theoretical methods were mostly used in obtaining these data: Close Coupling (CC) approximation (Refs. 15, 17, 18, 19, 21, 25, 31), R-Matrix (RM) method (Refs. 14, 16, 20, 23, 24, 26, 27, 28, 29, 30, 32, 34, 35) and Distorted Wave (DW) approximation (Refs. 22, 33 and 36 to 43).

a. Lighter elements ($Z \leq 18$)

In principle we do not refer here to calculations based on Born (B) or Coulomb-Born (CB) approximations. These calculations, though giving rough estimates of missing data, are only considered as preliminary estimations, and not sufficient for the accuracy needed in plasma diagnostics.

For He^{+} excitation, the angular distribution of scattered electrons has been calculated (14). This calculation can be used for comparison with experiment. Also, several calculations were done for oxygen ions (Refs. 15 to 24) and the results were used in determining the electron density and temperature of hot plasmas (e.g. in the solar corona, Ref. 19). Active solar regions and plasmas with electron densities higher than 10^{11} cm^{-3} could also be diagnosed by Mg-like (e.g. Si^{2+}) and Al-like (Si^{+}, S^{3+}) ions (Ref. 28).

b. Heavier elements ($Z > 18$)

Calculations for ions heavier than Ar are very scarce. They pertain to Ca^{14+} (34), Ca^{16+} (35), Ti^{3+}, Zr^{3+}, Hf^{3+} (36), Mn^{16+} - Mn^{22+} (37), Fe^{6+} (38), Fe^{9+}, Fe^{14+} - Fe^{25+} (39), Fe^{24+}, Se^{32+}, Mo^{40+} (40), Ni^{+} (41), Kr^{26+} (42) and Kr^{27+} - Kr^{33+} (43) ions. The DW approximation was used for all cases except for Ca ions. RM calculations of (34) are implying that DW results are sometimes overestimated, in confirmation of the collision strengths comparison of (30) for transitions in Si^{8+}. Data presented in (35) extend the previous calculations for Be-like ions by the Belfast group to the more highly ionised Ca^{16+} ion. Ref. includes data also useful for calculation of energies and electron collision strengths for other (Li to F) isoelectronic series ions where atomic data are not available and for density diagnostic purposes. The calculations of (42) are extending the Ne-like data with vacuum-uv laser applications in mind. Finally, calculations of excitation - autoionization of (36) assess the importance of the indirect mechanism of inner-shell excitation followed by autoionization up to energies of many times the first ionization potential.

3. Experimental Data

There are very few new experimental results on electron impact excitation published recently. Recent experimental results on He^{+} excitation rates (44) suggest that no large discrepancies of the type found for H^{o} and He^{o} excitation exist between theory and experiment in the case of a plasma hot enough to consist largely of He^{+}.

The measurement of excitation rate coefficients of Fe^{9+} with a theta pinch device should be mentioned (45). A gun-injection method was used in order to improve on previous measurements of Fe^{7+}, Fe^{8+} and F^{9+} excitation rate coefficients with the same experimental device. Measurements of rate coefficients for Fe^{8+} and Fe^{9+} are under way.

Differential cross sections for Zn^{+} excitation were obtained at a small scattering angle (46) using crossed beam technique and subsequently compared with CC calculations (47). Crossed beam technique measurements constitute (see also Refs. 48 and 49) a rigorous test of theories and models of electron-ion scattering. A series of such measurements should be made in order to extend previous measurements of Na-like Al^{2+} and Mg^{+} ions from JILA Laboratory mentioned in the report of the first meeting of this CRP. There are also measurements of Cd^{+} excitation (50, 51), though of limited interest for fusion.

4. Data Requirements

The data on ions of the working gases (H, D, T, He) and the common impurities (C, O, Al, Ti, Cr, Fe, Ni) encountered in devices confining high temperature plasmas are the most required. Nevertheless other intrinsic impurities (N, S, Cl, Cu, Zr, Mo, W, Au) are used for diagnostics as well as the common impurities mentioned above and the corresponding excitation data are to be known with an accuracy better than 10%. Equally needed are data for elements which are introduced for diagnostic purposes by blow off injection (Be, Si, Sc, V, Co, Zn, Ge, Se), injected with the working gas (e.g. Ne, Ar, Kr) or added in compound gas form (e.g. GeH_4 in Doublet III). The injection of impurities by blow off techniques currently used in PLT allows systematic study of the He-, Li-, Ne- and P-like ions.

Elements expected as intrinsic plasma impurities are often added for diagnostics and atomic physics studies (e.g. O in ISX, Al, Ar in TEXT and Alcator C, Ti in Doublet III and in the NBS theta pinch, Cr and Ni in TFR 600, Ti and Mo in PLT and Alcator C) and the corresponding data need to be known accurately. Also data on elements used in diagnostic beams (e.g. He, Li, Be, B, Tl) are of special importance.

Attention is further to be drawn to the excitation cross sections of metastable states possessing a longer lifetime in the plasma.

The need for data on a number of elements to be used as diagnostic tools or being now used in the development of special diagnostic methods (e.g. Rare gases, Au for inertially confined plasmas, K, Rb, Cs, Ba for beam diagnostics) should also be stressed (see Proceedings of Nagoya Symposium on Atomic Collision Data for Diagnostics and Modelling of Fusion Plasmas, 29-30 August 1983, in Report IPPJ-AM-33). It has to be mentioned that data used for diagnostics of astrophysical plasmas are also important for their potential use in diagnostics of high temperature laboratory plasmas.

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Table I

Theoretical data on electron impact excitation of ions

ION	Ref. No.	Method	Energy range, observations
He^{+}	14	RM	3-3.3 Ry, angular distribution
C^{3+}	21	CC	near threshold
N^{2+}	25	CC	$(0.4-6) \times 10^4$ °K
O^{+}	15	CC	less than 10^6 °K
O^{2+}	16	RM	0 - 7.36 eV
O^{2+}	15	CC	less than 10^6 °K
O^{3+}	17	CC	$(1-4) \times 10^4$ °K
O^{3+}	18	CC	3 - 5.6 Ry
O^{3+}	19	CC	$(0.1 - 40) \times 10^3$ °K
O^{4+}	20	RM	$10^{4.9} - 10^{5.7}$ °K
O^{5+}	21	CC	near threshold
O^{5+}	22	DW (CC)	resonance
O^{6+}	23	RM	$10^4 - 10^7$ °K
O^{6+}	24	RM	$10^4 - 10^7$ °K
Ne^{4+}	26	RM	5 - 40 Ry
Ne^{4+}	27	RM	less than 10^6 °K
Ne^{7+}	21	CC	near threshold
Si^{+}	28	RM	0.1 - 10 eV
Si^{8+}	29	RM	$(0.3-25) \times 10^6$ °K
Si^{8+}	30	RM	$(0.5-25) \times 10^4$ °K
Si^{8+}	27	RM	less than 2.5×10^6 °K
S^{+}	31	CC	less than 10^6 °K

ION	Ref. No.	Method	Energy range, observations
S^{3+}	32	RM	$10^4 - 10^{5.6}$ °K
S^{3+}	22	DW (CC)	resonance
S^{11+}	33	DW	9 - 70 Ry
Ar^{15+}	21	CC	near threshold
Ca^{14+}	34	RM	(0.5-50) x 10^4 °K
Ca^{16+}	35	RM	$10^{6.4} - 10^{7.2}$ °K
Ti^{3+}	36	DW	30 - 55 eV
Mn^{16+} -Mn^{22+}	37	DW	5 - 60 Ry
Fe^{6+}	38	DW	0.7 - 2.8 Ry
Fe^{9+}, Fe^{14+} -Fe^{25+}	39	DW	1 - 100 times threshold
Fe^{24+}	40	DW	580 - 5000 Ry
Ni^{+}	41	DW	at threshold
Se^{32+}	40	DW	1010 - 10000 Ry
Kr^{26+}	42	DW	140 Ry
Kr^{27+} -Kr^{33+}	43	DW	10 - 150 Ry
Zr^{3+}	36	DW	25 - 55 Ry
Mo^{40+}	40	DW	1570 - 15000 Ry
Hf^{3+}	36	DW	25 - 55 Ry

Working Group Report on Electron Impact-Ionization of Ions

V. A. Abramov, G. H. Dunn (Chairman) and E. Salzborn

General

This group stands on the report and recommendations made last year (1). There has been substantial activity during the past year, and new data are indicated below. The tables and recommendations of last year are not reproduced here. New semi-empirical formulae have been put forth by Burgess and Chidichimo (2), to try to account for cases where indirect processes contribute heavily. These formulae are commended to those who need formulae in computer models of plasmas. Shevelko et al. (3) have made fitting formulae based on the Coulomb-Born approximation with exchange to account for both direct and indirect processes for isoelectronic series H to Ca. For cases where indirect processes contribute substantially to ionization, formulae introduced in these papers should be an improvement over the usually applied Lotz formula.

Greatest needs for further study are:

a. Further measurements and theory determining the magnitudes and trends of cross sections for excitation-autoionization (EA) and of resonant excitation - double autoionization (REDA).

b. More measurements and theory for multiple ionization of all relevant fusion species.

c. Measurements and theory for ionization from all charge states (with exceptions noted in parentheses) of iron (except +1, +2), titanium (except +2, +3), chromium, aluminum (except +1, +2), and possibly copper, nickel, molybdenum, and tungsten.

1. Single ionization cross sections for ions

1.1 Z=1-8, H - O

The data of Bell et al. were previously recommended with two reservations. The report of these authors in a manuscript to be published (4) has been changed to include recent data (Be^{+}) but retains a recommendation for C^{3+} which is substantially higher than given by experiment. This group commends the data and formulae of Bell et al. for general use except for C^{3+} (5) and B^{2+} (6). Added experimental data for ions in this Z range have recently been pbulished, for Be^{+} (7), B^{+}, C^{2+}, N^{3+}, and O^{4+} (8), and will be submitted shortly (6) for B^{2+}.

1.2 Z=9-18, F - Ar

In our previous report (1) crossed beam measurements were recommended for Na^{+}, Mg^{+}, Mg^{2+}, Al^{+}, Al^{2+}, Si^{3+}, Ar^{+}, Ar^{2+}, Ar^{3+}, Ar^{4+}, Ne^{+} and Ne^{3+}. New data and some re-evaluation would alter last year's table to include F^{2+} (9), Ne^{3+} (10), Al^{+} (11), Cl^{2+} (9), Ar^{2+} (9, 12), and Ar^{3+} (10).

Note that in last year's report (1), two references for Ar^{+} were cited on page 18. On page 5, one reference is cited in Table 11, and is cited as "recommended." In fact, in the experiments of P. R. Woodruff, M. C. Hublet, and M. F. A. Harrison, J. Phys. B 11, 2305 (1978), form factors were measured during the actual experiment as opposed to "pre-set-up" measurements of Mueller et al. cited in Table 11 of Ref. 1. Thus, the data of Woodruff et al. are instead recommended.

1.3 Z=19-102

Most notable in this range are the first measurments on some iron ions. This is a high priority system for fusion and one for which no measurements previously existed. The table for last year should be amended to include:

Ti^{2+} (9), Ti^{3+} (13), Fe^{+} (14), Fe^{2+} (9), Kr^{2+} (12), Kr^{3+} (10), Zr^{3+} (13), Xe^{+} (15), Xe^{2+} (15), Xe^{3+} (10, 15), Xe^{4+} (15), Xe^{6+} (16), Cs^{+} (17), Hf^{3+} (13), Ta^{3+} (13), W^{+} (14).

2. Multiple Ionization Cross Sections for Ions

The availability of cross sections for multiple ionization of ions, $\sigma_{q,q+k}$ with $k > 1$, is still very limited. The only data published so far are the following:

σ_{13}	σ_{14}	σ_{15}	σ_{24}	σ_{25}	σ_{35}	σ_{46}	
Li							Ref. 18
Na							Ref. 19
Ar	Ar	Ar	Ar	Ar	Ar		Ref. 20
Rb	Rb	Rb	Rb				Ref. 21
I							Ref. 22
Xe			Xe		Xe	Xe	Ref. 22
Cs	Cs	Cs					Ref. 23

Further measurments have been taken and will be published soon on:

σ_{13}	σ_{14}	σ_{15}	σ_{24}	σ_{25}	σ_{35}	σ_{46}	
					Ar		Ref. 25
					Kr		Ref. 25
Xe	Xe	Xe	Xe	Xe	Xe	Xe	Ref. 24,25

The measurements for Xe σ_{14} to σ_{36} were submitted for publication in the J. Phys. B in September 1983 (Ref. 24); the measurements for Ar, Kr and Xe σ_{46} and σ_{69} were communicated privately (25).

Cross sections for multiple ionization have so far been neglected in plasma modelling codes. However, the recent data for high Z elements show that this is not justified. The multiple ionization cross sections may be quite large, e.g. σ_{13} reaches values of up to 5×10^{-17} cm^2 for I^+ and Xe^+ ions. Furthermore, the ratio of cross sections σ_{24}/σ_{23} for Xe ions increases strongly with electron energy and reaches the value 0.7 at E_e=700 eV.

We again emphasize to the fusion community that these multiple ionization processes should be considered in diagnostics and modelling - particularly for Z > 20. In view of the small data base available, there is a strong need for further measurements, especially since theoretical models for multiple ionization are at best qualitative.

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Working Group Report on Charge Exchange and Related Processes

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1. Collisions involving hydrogen atoms

Experimental and theoretical data on the process

$$X^{q+} + H \rightarrow X^{(q-1)+} + H^+ \qquad (1)$$

are now available for many ion species of fusion interest over a wide energy range. A compilation of such cross sections is available [1]. In a review [2], Gilbody has considered the experimental data in relation to current theoretical predictions while a critical review of the theoretical methods and predictions has been carried out by Janev and Bransden [3]. For multiply charged ions, cross sections are dependent on q rather than ion species and, at high velocities, can often be adequately described by simple scaling relations.

At velocities $V < 1$ a.u. (corresponding to 2.2×10^8 cm/s or 25 keV/amu) process (1) is the main mechanism for electron removal from H atoms. At higher velocities the ionisation process

$$X^{q+} + H \rightarrow X^{q+} + H^+ + e^- \qquad (2)$$

becomes dominant and there is a need to consider the total cross section for electron removal from H through the combined processes (1) and (2).

At velocities $V > 1$ a.u., cross sections for (1) decrease with increasing velocity and, for a given velocity, increase with q. Cross sections $\sigma_{q,q-1}$ for different ions with the same initial charge q are not greatly different and can be described by simple relations of the form

$$\sigma = \sigma_o q^n \qquad (3)$$

where σ_o and n are empirical scaling parameters which depend on velocity. Values of n between 2 and 3 are typical. A more general discussion of scaling laws for charge transfer with an indication of the likely accuracy has been given by Janev and Hvelplund [4].

At velocities $V < 1$ a.u., charge transfer may occur very effectively through one or more pseudo-crossings of the adiabatic potential energy curves of the molecular system formed during the collision. This involves capture into one or a limited number of excited states. In general no simple scaling laws apply and cross sections $\sigma_{q,q-1}$ for $q \geq 4$ generally exhibit only a weak dependence on velocity between 0.2 and 1 a.u. [5,6]. For systems with high initial charge $q \geq 10$, $\sigma_{q,q-1}$ is approximately linearly dependent on q. Experimental data for ions of high q are still very limited, especially at low energies less than about 1 keV/amu. Measurements of $\sigma_{q,q-1}$ of the type carried out recently at ORNL by Phaneuf et al. [7, 8, 9] for multiply charged ions of C, O, Al and Fe, need to be extended to other species. For low charge states, the experimental cross sections may be strongly influenced by the presence of metastable ions in the primary beam. This problem requires further attention.

Experimental data of high precision are now available [10, 11, 12, 13, 14] for the ionisation process (2) for H^+, He^{2+}, Li^+-Li^{3+}, C^{2+}-C^{6+}, O^{2+}-O^{6+} and Ar^{3+}-Ar^{9+}. Results for C, N and O ions show that cross sections for different ions with the same q agree closely, both in magnitude and in velocity dependence. At high velocities where the cross sections have decreased below the peak value cross sections can be described by the simple scaling relation (3). A more general scaling relation has recently been given by Gillespie [15] in which the ionisation cross section σ_i is given by

$$\sigma_i = q^2 f(q^{1/2}\, \alpha/\beta)\, \sigma_B(\beta) \qquad (4)$$

where $f\,(q^{1/2}\, \alpha/\beta)$ is a universal function with a simple analytic form, α is the fine structure constant, $\beta = v/c$ and $\alpha_B\,(\beta)$ is the Bethe cross section for ionisation of H by fast protons. The experimental data are correctly described to within 15% when $f(q^{1/2}\ \alpha/\beta) = \exp[-\lambda(q^{1/2}\ \alpha/\beta)]$ and $\lambda = 0.76$, [14, 15]. For the bare nuclei, H^+, He^{2+}, Li^{3+} and C^{6+} experimental data [13] show that the ionisation cross sections scale according to Z^2 (as predicted by the Born approximation) only at very high velocities. The velocity at which the Born approximation becomes valid progressively increases with Z. A general scaling relation for ionisation based on a model due to Bohr (see Knudsen [16]) has a more restricted range of validity [14].

Olson et al. [17] have used the classical trajectory Monte-Carlo (CTMC) method to calculate total cross sections σ_e for electron removal (i.e. the sum of the cross sections for (1) and (2)) from H for ions with $1 \leq q \leq 50$ in the range 50 - 5000 keV/amu. An analytical fit to the theoretical cross sections provides a general scaling relation for σ_e. Calculated reduced cross sections σ_e/q plotted against the reduced energy E/q lie on the universal curve given by

$$\sigma_e/q = 4.6\ \ (32\ q/E)\ [1-\exp\ (-E/32q)]\ \ 10^{-16}\ cm^2 \qquad (5)$$

where E is the energy in keV/amu. An expression little different from (5) has recently been derived by Janev [18] using a classical approach. Although there are departures from this universal curve at both low and high velocities, experimental data [14] indicate agreement to within a factor of 2 in the E/q range 20-150 keV/amu. Hardie and Olson [19] have recently modified (5) to allow for a better distribution of the H(1s) electronic radial distribution. The modified expression which predicts cross sections up to 40% larger, provides better agreement with experiment for E/q values less than 20 keV/amu (see [14]).

Cross sections for the process

$$X^{q+} + H \rightarrow X^{(q-1)+}\ (n, \ell\ ) + H^+ \qquad (6)$$

involving capture into specific excited states (n, ℓ) of the product ion are of particular importance particularly at velocities $V < 1$ a.u. Theoretical predictions have recently been reviewed by Janev [20, 21]. Until recently, experimental data were available only for H^+ and He^{2+} impact. In Belfast [22], the first measurements of state selective capture have been carried out for N^{2+}, C^{2+} and C^{3+} impact at keV energies using translational energy spectroscopy in a furnace-target configuration. Cross sections are accurate to within 10% and the measurements provide a final state energy resolution about 0.3 eV. The method requires only low primary ion beam fluxes and provides an unambiguous indication of the presence of any metastable species. Measurements are being extended to a wide range of ionic species. In Grenoble [23] intense beams of fully stripped C, N, O and Ne ions are being used with a furnace target to carry out measurements of state-selective capture by photon emission spectroscopy in the VUV. The method is limited to emission wavelengths beyond the background radiation of the furnace but, in principle, a higher energy resolution than methods based on translational spectroscopy is possible. The accuracy of such measurements is limited mainly by the VUV calibration accuracy of $\pm$ 40%. Photon emission studies are also being carried out in Dubna [24, 25]. The availability of a number of new high intensity sources of multiply charged ions, e.g. EBIS, ECR and recoil type (see Ref. 26) has increased the prospect of further measurements.

2. Collisions involving multi-electron targets

A number of fusion diagnostic schemes in use or under consideration require accurate cross sections in targets other than in atomic hydrogen.

Critical reviews of theoretical data are new available for charge transfer involving all ionic and target species [27, 28, 29]. Extensive experimental data are now available for total electron capture cross sections by multiply charged ions in H_2 and He. A compilation of data for H_2 targets is available [30]. Some data are also available for the ionisation of H_2 and He by multiply charged ions. Many of the data have been compared with theoretical predictions and general scaling rules in a review by Janev and Presnyakov [31]. The case of one- and two-electron capture by O^{8+} in He has also recently been considered by Bliman et al. [32].

For H_2 it is important to note that cross sections for both charge transfer and ionisation may be significantly different from twice the corresponding cross sections in atomic hydrogen even at high velocities. At low velocities the corresponding transfer ionisation process

$$X^{q+} + H_2 \rightarrow X^{(q-1)+} + H^+ + H^+ + e^- \qquad (7)$$

has an important role [33]. For many electron targets, transfer ionisation processes of the type

$$X^{q+} + Y \rightarrow X^{m+} + Y^{n+} + (m+n-q)e^- \qquad (8)$$

involving capture of one or more electrons with the simultaneous multiple ionisation of the target have large cross sections even at low velocities [34]. A statistical interpretation of such processes at $V < 1$ a.u. is very successful [35].

For a lithium target, cross sections for the two-electron capture process

$$He^{2+} + Li \rightarrow He + Li^{2+} \qquad (9)$$

are available over a wide energy range [36, 37]. Cross sections for one-electron capture into particular states of He^+ which may involve simultaneous excitation of the Li atom are also available [38]. Cross sections for state selective capture by C^{4+} from Li have also been measured recently [39].

For H_2 and He targets experimental cross sections for state selective capture by C^{4+} [39, 40] and by O^{6+} ions have been measured [40].

Measurements on helium carried out in Nagoya and other laboratories for a wide variety of projectiles have been presented by Ohtani [41]. There is evidence [40] that electron capture occurs primarily into states with the same principal quantum number for projectiles with the same initial charge.

Cross sections for the emission of Balmer H radiation in the passage of H, H^+, H_2^+ and H_3^+ through H_2 have been determined [42] in the range 1-100 keV from studies of the 3s-2p, 3p-2s and 3d-2p decay modes following the collisional formation of excited H atoms. Measurements have recently been extended to H_2-H_2 collisions [43]. Data are available for the separate contributions from both target and projectile. Cross sections for the collisional destruction of H_2^+ and H_3^+ in H_2 are also available. All these data are relevant to the diagnostics of energetic neutral hydrogen beams used for plasma heating.

3. Collisions between positive ions

A limited amount of experimental data on collisions between positive ions is now available. These have been considered in relation to current theory in a review by Gilbody [44]. Theoretical studies [45, 46] of a few selected cases have shown the effectiveness of ion-ion collisions as well as electron-ion collisions in describing the ratio of concentration of impurity ions to electrons in present Tokamak plasmas. Theoretical ion-ion charge exchange data have been recently reviewed and evaluated [29] and a bibliography on all the available data is available [47].

Cross sections for the charge transfer process

$$H^+ + X^{q+} \rightarrow H + X^{(q+1)+} \qquad (10)$$

and the ionisation process

$$H^+ + X^{q+} \rightarrow H^+ + X^{(q+1)+} + e^- \qquad (11)$$

involving impurity ions are relevant to particle escape and enhanced energy loss in fusion devices. For low values of q, cross sections may be very large. A knowledge of cross sections for (10) and (11) is also relevant to plasma diagnostics using heavy ion beam probes. The corresponding cross sections for He^{2+} impact are also of considerable importance in the context of alpha particle heating.

Experimentally determined (absolute) cross sections at keV energies for X^{2+} production from the combined processes (10) and (11) are available for targets of He^+, Li^+, C^+, N^+, Mg^+, Ti^+ and Fe^+ (see Ref. 44). Recent measurements for Al^+ and Tl^+ are also available [48]. For He^+ and Li^+, separate measurements of the cross sections for the charge transfer process have been carried out. Provided that ground state collidant and product ions are dominant in these reactions, there is evidence [44] that cross sections for the reverse reaction

$$X^{2+} + H \rightarrow X^+ + H^+$$

can provide reliable estimates of charge transfer in H^+ - X^+ collisions. At energies where measured cross sections for X^{2+} production are dominated by ionisation, the data can be described by a classical scaling relation [44] which permits cross sections to be predicted to within about a factor of two.

At energies below 100 eV, calculations and preliminiary measurements [49] have been carried out for the production of protons in H_2^+ - H_2^+ collisions. Cross sections estimated to be about 10^{-16} cm^2 indicate that further investigations are desirable.

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Working Group Report on Dielectronic Recombination

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During 1982-83 very substantial changes have occured in the picture for dielectronic recombination (DR). After 20 years where the only touch with experiment was through relatively recent rate measurements (1-4), direct cross section measurements were made in four different laboratories (5-8) on C^{+}, Mg^{+}, Ca^{+}, B^{2+}, and C^{3+}. In all but one case (B^{2+}), the experimental cross section is substantially (five times for C^{+} and for Mg^{+}, three times for Ca^{+}, and one and half for C^{3+}) larger than theoretical predictions of Hahn et al. (9-12) (for Ca^{+} there were no DW calculations and the comparison is made with the Burgess general formula (13)). Also, work on what appears to be a related process, resonant-transfer and excitation (RTE) for S^{13+} + Ar indicates (14) dielectronic recombination cross sections for S^{13+} which are two to three times those predicted theoretically. All this has generated a substantial amount of theoretical work.

One tentative explanation of the discrepancies lies in the hypothesis that extrinsic fields mix in more ℓ levels and substantially enhance the cross section. For the cases of Mg^{+} and C^{3+}, theoretical estimates of LaGattuta and Hahn (15) show that most of the discrepancy can be removed. However, more completed calculations are needed, and the effect on the other ions needs to be looked at before conclusions are drawn. The effect of extrinsic fields has been previously considered (16-18).

Rate measurements have been made in a Tokamak plasma during 1982-83 using a new technique which involves measuring dielectronic statellite lines compared to the resonance line. For Fe^{24+} the measured rates are in good agreement with theory (3). This is encouraging, though one must be cautious, since only two satellite lines were resolved (the other are subsumed by the resonance lines) and theory was used to extrapolate to the effect of higher n levels. High n levels are, of course, the ones affected by extrinsic fields.

Also during this period M. J. Seaton (19) has recast the entire theory of DR into a more comprehensive form. This is yet to be used and tested widely.

Thus, for DR we are in a period of substantial agitation and re-examining. The bringing together for the first time of theory and experiment should lead eventually to cross sections and rates which can be used with confidence. For the time being, however, it appears that one should use the theoretical data with caution, incorporating external effects as best as currently estimated (15-18).

At the 1982 IFRC Subcommittee meeting, it was recommended that a review be commissioned by experts on recombination to recommend data to the fusion community. In view of the present high level of theoretical and experimental activity in this field, we recommend that such a commissioned review be deferred for one to two years so that impact of present advances in the field can be consolidated and incorporated.

It is recommended that in the meanwhile the IAEA and other concerned agencies support and encourage the activities the DR measurement, DR theory and the related work in RTE.

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Appendix 1

Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Second Research Coordination Meeting
Nagoya, 31 August - 2 September 1983

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Appendix 2

Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Second Research Coordination Meeting
Nagoya, 31 August - 2 September 1983

ADOPTED AGENDA

1. Opening Statements and Announcements

   1.1. Opening of meeting (9:30 hrs)
   1.2. Appointment of chairmen of working groups
   1.3. Adoption of Agenda
   1.4. Announcements

2. Short Progress Reports by CRP participants on their work

3. Reports on related work in progress in laboratories not included in CRP

4. Report on last IFRC Subcommittee Meeting

5. Review of the status of the existing required A+M Data, their accuracy and completeness

   5.1. Electron Impact Excitation
   5.2. Electron Impact Ionization
   5.3. Electron capture and charge exchange
   5.4. Recombination

6. Writing of working group reports

7. Reports of the working groups on the conclusions on the current status and availability of the required data

8. Distribution of responsibilities among the participants in the CRP

9. Summary of Conclusions

10. Next Meeting

Opening Speech on the second Research Coordination Meeting on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Prof. H. H. Kakihana
Director
Institute for Plasma Physics
Nagoya University
Nagoya 464, Japan

My colleagues, excellent scientists from the field of atomic and molecular collisions!

First of all I would like to express my heartful thanks on behalf of the host institute, the Institute of Plasma Physics at Nagoya, for coming from all corners of the world to this hot city of Nagoya. As the former Deputy Director General of IAEA in Vienna, I especially welcome my friends Drs. Lorenz and Katsonis, who have organized this meeting and have decided to come to Nagoya.

I believe that the meeting on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas is of special importance for three reasons. First, atomic and molecular data are essentially important for promoting plasma physics experiments, especially of high temperature plasma confined by any kind of magnetic system: Tokamak, Stellarator, Mirror and further advanced systems. Second, atomic and molecular collisions themselfs are full of scientific meaning and future. The field might not be sensational of the kind reported by journalists, as in the case of other fields like cancer science, accelerator science and fusion science. Nevertheless, the scientific results from atomic and molecular collision experiments, carefully and presicely obtained by well-designed machines and well-organized groups, will give countless contribution to our scientific knowledge. In this respect our Nagoya group, the NICE group, has done really a nice job to present new and trustworthy results, especially on multi-valent Kr ions. Third, but not of least importance, this meeting offers the opportunity for the mixing and mutual understanding between atomic and molecular scientists and plasma scientists. This kind of mixing is extremely important not only to promote the use of up-to-date atomic and molecular data for the ever-advancing demands from the field of plasma physics, especially because of the interaction between the first wall and the plasma, but also, in promoting mutual understanding which stimulate the scientists working in the atomic and molecular data field to explore new areas and challenge new fields connected directly or indirectly with future possible demands from nuclear fusion research. In this sense, my Institute has supported Japanese atomic and molecular scientists especially the NICE group for the last ten years. This kind of effort to support and to understand the challenging scientists of atomic and molecular field will be continued and be even more promoted by my Institute.

It is my pleasure to have the second Research Coordination Meeting (RCM) on Atomic Collision Data for Diagnostics of Magnetic fusion plasmas here at the Institute of Plasma Physics of the Nagoya University, especially because this Coordinated Research Programme (CRP) was initiated during my stay with the IAEA. I strongly supported the idea to have this meeting hosted by the Japanese Government because of the simultaneous presence in Japan of numerous well known atomic physics specialists from abroad who contribute to the development of a tight international cooperation in the measurement, calculation, and evaluation of atomic data of interest to fusion. On this occasion we organized a Symposium on Atomic Collision Data for Diagnostics and Modelling of Fusion Plasmas. During the two days of this Symposium the Japanese specialists had the occasion to present their current results on the topic. Some of them will stay the next three days to contribute also to the RCM starting today.

The CRP comprises now a dozen laboratories located in many parts of the world. Its goal is to generate atomic collision data in accordance with requirement priorities determined by the fusion community. In accordance with the recommendations of the Atomic and Molecular Data Subcommittee of the International Fusion Research Council (IFRC), the processes currently emphasised in calculating and evaluating required data in the frame of this project, are: electron impact excitation and ionisation, charge transfer and ionisation in atom-ion and ion-ion collisions, and electronic and dielectronic recombination.

The species of interest are those covered by the International Bulletin on Atomic Data for Fusion, the bibliographic quarterly issued by the IAEA, and are reviewed periodically by the IFRC subcommittee.

I wish you good success in your difficult task and declare the meeting open.