International Atomic Energy Agency

INDC(NDS)-136/GA

INDC

INTERNATIONAL NUCLEAR DATA COMMITTEE

First Research Coordination Meeting on

Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Vienna, 21-25 June 1982

IAEA, Vienna

SUMMARY REPORT

K. Katsonis and A. Lorenz

October 1982

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

Reproduced by the IAEA in Austria
October 1982
82-06904

INDC(NDS)-136/GA

First Research Coordination Meeting on

Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas

Vienna, 21-25 June 1982

IAEA, Vienna

SUMMARY REPORT

K. Katsonis and A. Lorenz

October 1982

Abstract

Proceedings of the first meeting of the participants in the IAEA Coordinated Research Programme on atomic collision data for diagnostics of magnetically confined fusion plasmas, convened by the IAEA Nuclear Data Section on 21 - 25 June 1982, at IAEA Headquarters in Vienna.

The meeting participants reviewed the status of electron excitation, electron ionization and charge transfer data 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.

Foreword

Following the review of the Agency's A+M Data Programme by the IFRC Subcommittee on A+M Data for Fusion in January 1981, the objectives of the proposed Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas were reoriented so as to comply with the recommendations of the Subcommittee, namely "that the effort in this CRP concentrate on the calculation and evaluation of the required data". The collision processes which were to be emphasized by the CRP were those which the Subcommittee identified to have the highest priority (INDC(SEC)-77/GA), namely

- electron impact ionization
- electron excitation, and
- electron capture.

With the view to determine more specifically the data types which the CRP should cover and to establish an order of priority among the needed data, the A+M Data Unit, using the recommendations of the May 1980 IAEA Technical Committee Meeting on A+M Data for Fusion (reference: Physica Scripta 23 69 (1981) 206-209), formulated a questionnaire and conducted a survey among the fusion research community. The emphasis of the CRP is thus based on the initial IFRC subcommittee recommendation and on the results of the Data Priority Questionnaire.

Table of Content

List of Appendixes

Definition of Terms

(Terminology recommended by the IFRC Subcommittee on A+M Data for Fusion)

Tabulation: systematic collection and transcription of numerical information without critical selection or manipulation.

Compilation: systematic collection and transcription of information on a given subject with collation and re-organization for optimal presentation to the users.

Evaluation: critical appraisal by one or more evaluators of all available data on a given topic (e.g., specific reaction for a given element), supplemented by theory or semi-empirical models, and the deriviation of a consistent set of best or preferred values, possibly with their uncertainties.

Bibliographic Data: information related to the documentation of numerical data, consisting of the reference citation, publication status and indexation.

Numerical Data: numerical values which fall into one of the following categories:

- Experimental data: numerical values resulting from a physics experiment (i.e., measurement)

- Calculated data: numerical values resulting from computation (e.g., calculated from theory)

- Derived data: numerical values calculated from data obtained in the analysis of experimental data (e.g., reaction rates calculated from reaction cross sections)

- Evaluated data: set of numerical values which have resulted from an evaluation (see above)

- Recommended data: set of numerical data, chosen by a recognized body to be recommended as the best set among a set of evaluated data.

- Standard data: set of numerical data established by general agreement as a basis for the measurement of other physical quantities, or set of accurately known data relative to which other data are determined (normalized)

- Provisionally recommended data: set of numerical data, which, because of its uniqueness, is recommended as the best set.

I. Summary of the Meeting

Introduction

The first 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 21-25 June 1982 at IAEA Headquarters in Vienna. The meeting was chaired by A. Lorenz with the assistance of three co-chairmen: M.R.C. McDowell, H.B. Gilbody and G. Dunn. The Scientific Secretary of the meeting was K. Katsonis.

The participants in this meeting are listed in Appendix I, and the Adopted Agenda is given in Appendix 2. The papers submitted to the meeting are listed 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 first 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 initial 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.

Conclusions and Recommendations

The CRP reviewed the overall status of electron collision and electron capture data of importance to the diagnostics of magnetic fusion plasmas; the summary of this review is given in Table I.

In reviewing the existing electron collision data, from the point of view of reliability and presently accepted accuracies, the CRP could identify only certain electron impact ionization data which could be proposed to be recommended to be used by the fusion community at this time. The accuracy of these data could be taken to be ± 10%. The list of the proposed recommended electron impact ionization data is given in Table II. All of the proposed recommended data and associated references are available from the A+M Data Unit.

Next Meeting

The preferred time for the next meeting of this CRP is the first week of September 1983. The exact time and place will depend to some extent on the schedule of other meetings of interest to the CRP participants.

Table I: Status of atomic collision data for diagnostics of magnetic fusion plasmas.*

Required Data	Experiment	Theory	Principal Source	Estimates (if necessary)	Comments
Electron Capture (H)					
Total σ $v > v_0$ (also ionization)	Considerable experiment (~ 20%) H - ovens	UDW[(a)] CTMC Eik-BK (20% to X2)[(b)]	Janev and Bransden Review (1) Nagoya - IPPJ AM-15 (2) Gilbody Review (3)	Scaling rules e.g., $\sigma = \sigma_0\, q^p$ where σ_0 and p depend on v. Also Hvelplund and Janev (4)	Scaling rules usually better than ±50%
			Total electron removal (5) $\sigma = 4.6q \times 10^{-16}\ \mathrm{cm}^2 \{\frac{32q}{E}\ [T-\exp(-E/32q)]\}$		
Total σ $v < v_0$	Some experiment (~ 20%) H - ovens	CC M-LZ Tunneling (20% to X2)	Janev and Bransden (1) Phaneuf et al. (6) (C & O ions)	Scaling rules $\sigma = \sigma_0\, q^{1.0}$ independent of v	Scaling rule fails seriously for low v and few electron systems
$\sigma(n,\ell)$ $v > v_0$	Only a little experiment - not H	UDW CTMC Eik-BK (X2 or so)	Janev and Bransden (1) and current research papers - mostly theory Janev - Stockholm (7)	Scaling rules $\frac{\sigma(n)}{\sigma(n_0)} = \left(\frac{n_0}{n}\right)^3$	A fair number of calculations are available for fully stripped ions
$\sigma(n,\ell)$ $v < v_0$	Only a little experiment - not H NICE-1 (Ref. 7) and Gilbody (Ref. 8)	CC (MO & AO) M-LZ Tunneling (20% to X2)	Refs. (1) and (7) and Green et al. (8)	Scaling rules n = q/2 Crossings at $(2q)^{1/2} < R_c < 2q$	Often only one n dominates; most cal- culations are for fully stripped ions
Electron Impact Excitation					
Ions Z < 30 q < Z/2	Crossed beams Be^+, C^{3+}, N^{4+} (9,10) Mg^+, Al^{2+} (11) Li^+ (12) other singly ionized - very few experiments - (~ 20%)	CC DWX (20% to X2)	Henry Review (13) Crandall Reviews (14) LA-8267 MS (15) ORNL/TM-7957 (16)	Gaunt factor (not better than X3)	Resonances are often significant. Lowest q may require CC and correlation. Gaunt factor not very reliable.
Ions Z < 30 q > Z/2	No experiment	DWX (usually 20-50% may be much worse for forbidden transitions)	Henry Review (13) Crandall Reviews (14) LA-8267 MS (15) ORNL/TM-7957 (16)	Gaunt factor (not better than X3)	Relativistic effects may begin at Z=20 — intermediate coupling?
Ions Z > 30	No experiment except singly ionized with strong lines (e.g., Ba^+ - see 13, 14)	CC, DWX Relativistic needed for high q. Effect of resonances reduces due to recombination	None	Gaunt factor (not better than X3)	No tests. Reliability unknown due to impor- tance of intermediate coupling, resonances.
Atoms H	Experiment (17) 1s-2p and 1s-2s at 11 eV agree with best theory	CC 1s-2ℓ,3ℓ (20%)	Callaway and McDowell (18)	n→n', n, n'≥5	Not as well known as one would expect
He	Experiment (19)	CC - doesn't agree well with exp. at several times threshold DWX	Scott and McDowell (20)	Don't use estimates	Critical Review in progress in UK (Belfast, London)
Electron Impact Ionization of Ions					
Z < 8 all q	Crossed beams (~ 10%)	DWX, CBX (20-30%)	Review of Bell et al. (21) except C^{3+} and Be^+ - use experiment	0.9 x Lotz	Fairly complete and reliable
8 < Z < 20	Crossed beams experiment for a few low q (10%) EBIS trap (22) - (X2)	DWX, CBX (20-30% except indirect effects)	Younger - DWX (23) + estimate exc.-autoion.	Lotz + estimate exc.-autoion.	Indirect effects like exc.-autoion. are important and are not well represented
Z > 20 q < Z/2	Crossed beams experiment for a few low q (10%) EBIS trap (22) - (X2)	Not generally available or reliable	None	Lotz uncertain	Only experiment will be generally reliable even to and order of magnitude
Z > 20 q > Z/2	Only EBIS trap (22) experiments - (X3 uncertain)	DWX CBX	Lotz	Lotz + estimate indirect effects	Relativistic as well as indirect effects may be important. Uncertainty always at least X2.
Recombination					
all ions	Only plasma observa- tions (Fe +24, for example) (Ref. 24)	Various - all approximate sums of resonances	Burgess-Merts (25) Dubau and Volonte (26)	Burgess-Merts	No useful tests. Reliability unassessed.

* Prepared by D..H. Crandall

Footnotes for Table I:

[a]UDW = Unitarized Distorted Wave
CTMC = Classical Trajectory Monte Carlo
Eik-BK = Eikonal Brinkman-Kramers
CC = Close Coupling
DWX = Distorted Wave with Exchange
CBX = Coulomb-Born with Exchange

[b]Values in parentheses represent rough estimate of reliability of the data — "X2" means uncertain by a factor of 2.

References for Table I:

1. R. K. Janev and B. H. Bransden, "Charge Exchange Between Highly Charged Ions and Atomic Hydrogen: A Critical Review of Theoretical Data," prepared at JILA, to be published 1982.

2. Y. Kaneko et al., "Cross Sections for Charge Transfer Collisions Involving Hydrogen Atoms," Report IPPJ-AM-15, Institute of Plasma Physics, Nagoya, Japan (1980).

3. H. B. Gilbody, Phys. Scr. 23, 143 (1981), also 24, 716 (1981), and report prepared for the Stockholm Symposium — to be in Physica Scripta.

4. R. K. Janev and P. Hvelplund, Comm. At. Molec. Phys. 11, 75 (1981).

5. R. E. Olson, K. H. Berkner, W. G. Graham, R. V. Pyle, A. S. Schlacter, and J. W. Stearns, Phys. Rev. Lett. 41, 163 (1978).

6. R. A. Phaneuf, I. Alvarez, F. W. Meyer, and D. H. Crandall, "Electron-Capture in Low-Energy Collisions of C^{q+} and O^{q+} with H and H_2" (accepted for Physical Review A).

7. R. K. Janev, "Excited States Created in Charge Transfer Collisions between Atoms and Highly Charged Ions," prepared for the Stockholm Symposium and to be published in Physica Scripta.

8. T. A. Green, E. J. Shipsey, and J. C. Browne, Phys. Rev. A 25, 1364 (1982).

9. P. O. Taylor, R. A. Phaneuf, and G. H. Dunn, Phys. Rev. A 22, 435 (1980).

10. D. Gregory, G. H. Dunn, R. A. Phaneuf, and D. H. Crandall, Phys. Rev. A 20, 410 (1979).

11. G. H. Dunn, R. A. Falk, D. S. Belić, D. H. Crandall, C. Cisneros, and D. C. Gregory, experiments on excitation of Al^{2+} at ORNL and Mg^{+} at JILA during 1981-82, private communication.

12. W. T. Rogers, J. O. Olsen, and G. H. Dunn, Phys. Rev. A 18, 1353 (1978).

13. R.J.W. Henry, "Excitation of Atomic Positive Ions by Electron Impact," Phys. Rep. 68, 1-91 (1981).

14. D. H. Crandall, "Electron Impact Excitation of Ions" in The Physics of Ion-Ion and Electron-Ion Collisions, 1981 NATO summer school organized by F. Brouillard and J. W. McGowan, to be published by Plenum Press, N.Y. and London, 1982. Also, "Electron-Ion Collisions" in Atomic Physics of Highly Ionzied Atoms, 1982 NATO summer school organized by R. Marrus and J. P. Briand, to be published by Plenum Press, 1983.

15. A. L. Merts, J. B. Mann, W. D. Robb, and N. H. Magee, Jr., "Electron Excitation Collision Strengths for Positive Atomic Ions: A Collection of Theoretical Data," Report LA-8267-MS of Los Alamos Scientific Laboratory, March 1980.

16. M. S. Pindzola and D. H. Crandall, "A Compilation of Theoretical Electron-Impact Excitation Cross Sections for Fe Atomic Ions," Report ORNL/TM-7957, Oak Ridge National Laboratory, Nov. 1981.

17. J. F. Williams, J. Phys. B 9, 1539 (1976).

18. J. Callaway and M.R.C. McDowell, "What We Do and Do Not Know About Electron Impact Excitation of Atomic Hydrogen," Comments Atom. Mol. Phys. (in press)

19. B. Van Zyl, G. H. Dunn, G. Chamberlain, and D.W.O. Heddle, Phys. Rev. A 22, 1916 (1980).

20. T. Scott and M.R.C. McDowell, J. Phys. B 8, 2369 (1975), also T. Scott, Ph.D. Thesis, London (1976).

21. K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, and F. J. Smith, "Recommended Data on the Electron Ionization of Light Atoms and Ions," to be published in Journal of Physical and Chemical Reference Data (1982).

22. E. D. Donets and V. P. Ovsyannikov, Report P7-80-404 of Joint Institute for Nuclear Research, Dubna, USSR (ORNL-tr-4702), and E. D. Donets, "Electron-Beam Method of Production fo Highly Charged Ions and Its Applications," report at Stockholm Symposium and to be published in Physica Scripta (1982).

23. S. M. Younger, Phys. Rev. A 22, 111 (1981); Phys. Rev. A 22, 425 (1980); Phys. Rev. A 23, 1138 (1981); Phys. Rev. A 24, 1278 (1981); J. Quant. Spect. Rad. Trans. 26, 1329 (1981). [This work summarized in "Atomic Data for Fusion," Vol. 7, No. 6 (1981) - printed June 1982.]

24. M. Bitter et al., Phys. Rev. Lett. 47, 921 (1981).

25. A. L. Merts, R. D. Cowan, and N. H. Magee, Jr., "The Calculated Power Output from a Thin Iron-Seeded Plasma," Report LA-6220-MS, Los Alamos Scientific Laboratory (March 1976).

26. J. Dubau and S. Volonté, Rep. Prog. Phys. 43, 199 (1980).

Table II

Recommended Electron Impact Ionization Data

Z = 1 - 8

Evaluated cross sections of all species, from hydrogen to oxygen, with the exception of Be^+ and C^{3+}, including all stages of ionization, published by Bell et al., (Culham report CLM-R216 (1982)), are proposed to be recommended.

Z = 9 - 18

In this Z range reasonable sets of cross sections could be generated based on prediction formulae and more accurate calculations. At present, the following cross-beam measurement results (with an uncertainty of about 10%) are proposed to be recommended:

Na^+	Peart and Dolder, J. Phys. B2 1 (1968)
Mg^+	Martin, et al., J. Phys. B2 1 (1968) 537
Mg^+	Crandall et al., Phys. Rev. A 25 (1982) 143
Mg^{2+}	Peart, et al., J. Phys. B 2 (1969) 1176
Al^+	Belic, et al., Priv. Comm. (1982)
Al^{2+} Si^{3+}	Crandall, et al., Phys. Rev. A 25 (1982) 143
Ar^+ Ar^{2+} Ar^{3+} Ar^{4+}	Mueller, et al., J. Phys. B 13 (1980) 1877
Ne^+	Dolder, et al., Proc.Roy.Soc. A 274 (1963) 546
Ne^{3+}	Gregory, Dittner and Crandall, Priv. Comm. (1982)

Z = 19 - 102

For Z > 19, with the exception of a few good cross-beam measurements, no recommended cross sections can be proposed. Those proposed to be recommended, having a 10% uncertainty, are

K^+	Peart and Dolder, J.Phys. B2 1 (1968) 240
Ca^+	Peart and Dolder, J.Phys. B 8 (1975) 56
Ti^{3+}	Falk, et al., Phys.Rev.Lett. 47 (1981) 494
Zn^+ Ga^+	Rogers, et al., Phys.Rev. A 25 (1982) 737
Kr^{3+}	Gregory, Dittner and Crandall, Private Comm. (1982)
Rb^+ Sr^+ Cs^+	Peart and Dolder, J.Phys. B 8 (1975) 56
Zr^{3+} Hf^{3+} Ta^{3+}	Falk, et al., Phys.Rev.Lett. 47 (1981) 494
Cd^+ Hg^+	Belic, et al., Priv. Comm. (1982)
Xe^+	Mueller, et al., J.Phys. B 13 (1980) 1877
Xe^{3+}	Gregory, Dittner and Crandall, Priv. Comm. (1982)
Ba^+	Peart, et al., J. Phys. B 6 (1973) 146
Tl^+	Divine, et al., Phys.Rev. A 13 (1976) 54

II. Meeting Programme

1. Progress reports from CRP Participants

1.1. Y. Itikawa (IPP/Nagoya)

Progress report on the work at the Nagoya University Institute of Plasma Physics is given in Appendix 4.

Progress report on the work at the JAERI Division of Physics is given in Appendix 5.

1.2. H. Winter (Institut fuer Allgemeine Physik, Vienna)

Progress report is given in Appendix 6.

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

Progress report is given in Appendix 7.

1.4. V.A. Abramov (Kurchatov Institute, Moscow)

Translated progress report is given in Appendix 8.

1.5. M.R.C. McDowell (Royal Holloway College, London)

Progress report is given in Appendix 10.

1.6. R.K. Janev (Institute of Physics, Belgrade, Yugoslavia)
Progress report is given in Appendix 11.

1.7. D.H. Crandall, et al. (Oak Ridge National Laboratory, USA)
Progress report is given in Appendix 12.

1.8. E. Salzborn (Institut fuer Kernphysik, Universitaet Giessen)
Progress report is given in Appendix 13.

1.9. P. Hvelplund (Institute of Physics, University of Aarhus, Denmark)
Progress report is given in Appendix 14.

1.10. S. Bliman (Centre d'Etudes Nucléaires de Grenoble, France)
Progress report is given in Appendix 15.

2. Review of Data Requirements

In their discussion of the data requirements by the fusion community, based on the IAEA data requirements survey (see Appendix 13), the participants agreed to use the survey results as a general guideline, but felt on the other hand that emphasis should also be given to species pertinent to specific diagnostics techniques, or other processes of importance.

3. Review of the Data Status

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 Excitation: reviewed by D.H. Crandall, Y. Itikawa, and M.R.C. McDowell (Chairman).

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

Charge Exchange: reviewed by S. Bliman, H.B. Gilbody (Chairman), P. Hvelplund, R.V. Janev and H. Winter

Dielectronic Recombination: reviewed by V.A. Abramov, D.H. Crandall and G.H. Dunn

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. A summary list of the data which were proposed to be recommended is included in the recommendations given in Table II above.

4. Standardization of Measurement Energies

In an effort to encourage a certain degree of standardization among measurers of electron capture data, so as to facilitate intercomparison of experimental and theoretical results, the CRP endorsed the following suggested recommendation:

> In order to allow for a more effective and efficient comparison of experimental data with theory and other experimental results, it is proposed that measurements of electron capture from H(1s) leading to excited ion states be made at the following standard collision energies:
>
> | | |
> |---|---|
> | 25 keV/amu | 1 keV/amu |
> | 10 keV/amu | 0.25 keV/amu |
> | 2.5 keV/amu | 0.1 keV/amu |

Working Group Report on Electron impact excitation of neutral atoms and positive atomic ions of interest in magnetically confined fusion plasmas

D.H. Crandall, Y. Itikawa, M.R.C. McDowell (Chairman)

1. Introduction

The theory of electron impact excitation processes has been reviewed recently by e.g. Bransden and McDowell [1,2] and more specifically for positive ions by Henry [3]. A bibliography from 1978 covering both theory and experiment has been prepared by Itikawa [4]. Recent reviews have been given at NATO Summer Schools, by Crandall [5,6] and more recently by McDowell [7].

It is all too often current practice to obtain excitation rate coefficients for plasma interpretation from Gaunt factor formulas and oscillator strengths. It is now clear that such results are not reliable and that significantly improved reliability is obtained from detailed calculations of collision strengths for individual transitions using close coupling or distorted wave approximations. The number of calculations required is very large (at least hundreds of thousands) but a beginning has been made and the techniques are being refined which will allow the production of the extensive data desired for fusion plasma applications.

Lorenz [8] in consultation with active members of the fusion community has suggested that the three highest priority groups of targets are

Priority 1 C,O,Ti,Fe

Priority 2 Al,Cr,Ni

Priority 3 H (and D,T), He

though other targets, especially Li and the rare gases (Priority 4) may be important for diagnostics. In each case, all stages of ionization need to be considered. As Priority class 5 we take all the other species given in Table 2 of Lorenz's paper.

2. Experiment

The role of experiment in electron impact excitation is foreseen to be principally in testing theory. All experiments to date have relied on measurements of the radiation emitted by the excited system. Such measurements become progressively more difficult as the charge state of the ion increases, both because the cross sections decrease rapidly with increasing q, and because the photon wavelengths become shorter. The crossed beams technique has produced a few accurate tests of collision theoretical models, notably for the resonance line 2s-2p $^2P_{1/2,3/2}$ of Li-like ions from Be^+ [9] to N^{4+} [10]. More recently Dunn et al. [11] have obtained results on the resonance lines of Na-like systems Al^{2+} and Mg^+ which add to the previous measurements of Zapesochnyi [12] for Mg^+. Apart from resonance transitions there are a few measurements on e.g. intercombination lines of Li^+ [13] and on several transitions in systems of less interest to fusion. There are of course two classic measurements on the 1s-2s transition in He^+ [3], but unfortunately no measurement of the 1s-2p transition which extends to high energies. (See however the results of Zapesochnyi [3]). An absolute measurement of the total n=1 to n=2 excitation cross section in He^+ is of high priority, particularly near threshold.

3. Theory

Theoretical calculations of excitation cross sections of positive ions are generally carried out in few state close-coupling (CC), or a simplification of that known as distorted wave exchange (DWX). The results are often unitarized (DWXII). For low q and neutral (q=0) atoms it is essential to include short range correlations, and also to ensure that the leading non-Coulomb term of the long-range interaction in each open channel considered is correctly represented, if accurate results are to be obtained. Unfortunately there are no published calculations fully satisfying these criteria.

For all species (other than hydrogen-like) accurate results require the use of accurate target wave functions. These should reproduce the observed energy levels, though all matrix diagonalization methods have difficulty obtaining this accuracy for the ground state. In addition it is desirable to obtain accurate oscillator strengths, in the sense that the dipole length and velocity results should be in agreement to better than 10%. These properties do not suffice to ensure accuracy, and, as we have mentioned, it is also important to obtain accurate static dipole polarizabilities of each level. These can be systematically improved variationally.

Further, for high Z ions, ($Z \gtrsim 20$) relativistic structure effects should be included, at least to the level of the Breit interaction, and full account taken of intermediate and j-j coupling.

Few, if any, published calculations meet these criteria fully, so it would be dangerous to suppose that the accuracy achieved so far is better than 20% except for hydrogenic systems. Readers are invited to consider the comparison of theory with experiment for the benchmark case of Be^+ 2s-2p. (Ref. [3], Fig. 5.7).

Users of atomic collision data generally require it in the form of the collision strength Ω_{if} which is related to the cross section σ_{if} (πa_0^2 units) by

$$\Omega_{if} = w_i \, k_i^2 \, \sigma_{if} \, (\pi a_0^2)$$

where w_i is the statistical weight of the initial state, and k_i^2 is the energy (in Rydbergs) of the incident electron relative to the lower lying of the two states. For evaluation of diagnostic observations of radiation from complex ions, these are required for all J to J' transitions. The use of a rate coefficient or rate parameter presupposes a Maxwellian distribution of electron energies.

4. Targets of Priority Class 1

4.1 Carbon and Oxygen

There do not appear to be any reliable calculations or measurements on the neutral or singly ionized species. The available data on the neutrals are summarized by Bransden and McDowell [2]. For C^+ there are five-state close coupling (5-CC) and unitarized Coulomb-Born with exchange (CBXII) calculations by Robb and Mann [14], but it is difficult to assess their reliability, for such open shell systems. Further accurate calculations are required for C^o and C^+ especially, in view of their special interest in Tokamaks with carbon inner liners.

The Japanese and US data centers are currently preparing a compilation and selection of data on ions of C and O, which will be published in association with this CRP. There are a significant number of detailed calculations for excitation from the ground states of each of these ions, which in most cases should allow a recommendation to be made, but not necessarily an assessment of reliability.

4.2 Ti and Fe

There is a substantial amount of data (theoretical) for ions of Fe [15,16]. The current situation for excitation of Fe ions illustrates both what can be accomplished by detailed calculations and that significant work remains to be done before a complete set of reasonably reliable rate coefficients is obtained. A recent compilation [15] selects calculated cross sections for about 1150 transitions of $\Delta n=0$ type for Fe^{8+} - Fe^{25+} and $\Delta n=1$ type for Fe^{16+} - Fe^{25+} from low lying states. All of the selected data are from DWXII or few state CC calculations. It is desirable to represent collision strengths and rate coefficients for each transition by a four parameter fit in a standard form involving powers of transition energies such as is given in Ref. [16], p. 206. For the 1150 transitions mentioned about half of the calculations provide a cross section at only one energy, whereas about seven values, well spread in energy, are needed to allow a reasonably accurate fit. Thus the work is far from finished for the 1150 transitions considered so far. Sufficient detail has been provided primarily for Be-like through H-like cases but refinements may significantly change these results. It seems clear that many of these calculations needed to be carried out in intermediate rather than L-S coupling [17] and further that the effects of resonances are not yet correctly accounted for in these highly charged ions [18].

From the perspective of plasma fusion diagnostics, it is a matter of highest priority to improve and complete the detailed calculations for specific J to J' transitions for all $\Delta n=0$ and most $\Delta n=1$ transitions from low lying states of Fe ions. Some of this work is currently in progress at Los Alamos Scientific Lab. (J.B. Mann and A.L. Merts).

There are as yet few data of any sort for Ti ions. Bhatia et al. [19] have reported DWX values for various transitions among $2s^m\ 2p^n$ configurations for Ti^{q+} ($q=13,\ldots,19$). In view of the general considerations discussed above, their reliability must be open to question.

4.3 Al, Cr, Ni

There are DWXII calculations available for some transitions in Al^{+} to Al^{5+}. Mann [10] gives coefficients from which cross sections and rate coefficients may be obtained for a few transitions. It is again difficult in general to assess the reliability of these calculations at this stage, especially for the lower stages of ionization. Various approximations for H-like and He-like ions of both Al and Ni are discussed by Henry [3]. There have been no calculations on Cr ions since 1970 [20]. In view of the priority attached to these species a major research programme needs to be initiated.

4.4 H (including D,T) and He

Callaway and McDowell [21] have analysed the available theoretical and experimental data on excitation of atomic hydrogen. They give recommended values, in the form of four parameter fits for the $1s \rightarrow 2s$, $1s \rightarrow 2p$, $1s \rightarrow 3s$, $1s \rightarrow 3p$, which they believe accurate to better than 20%, and a less certain fit for $1s \rightarrow 3d$. The $1s \rightarrow 2s$ transition in hydrogenic ions of low q remains a significant problem, at impact energies up to a few times threshold. In particular the well known factor of two discrepancy for He^{+} between theory and experiment remains unresolved and must cast doubt on the situation for all low q ions.

Except in the region of validity of the first Born approximation there are no reliable results for excitation to states of hydrogenic systems with $n > 3$, though work is in progress. The theoretical CC calculations for neutral He are in poor agreement with experiment below 200 eV, except close to threshold. The experimental values for the $1^1S \rightarrow n^1S$ and $1^1S \rightarrow n^1P$ $(n \leq 5)$ are consistent with the DW calculations of Scott and McDowell [22] (cf the benchmark experiment of Van Zyl et al. [23] on 3^1S) and the tables given by Scott [24] may be used as a guide. The UK groups (Belfast and London) intend to provide a critical assessment of the data for He.

There are very extensive DWX calculations for He-like ions by Pradhan et al. [25] which include resonances effects by a backwards Gailitis extrapolation, and these authors also provide collision strengths and rate parameters [26]. However, it recently became apparent that the accuracy of these results decreases with increasing atomic number beyond Z=6 and for Z=26 may be in error by more than an order of magnitude [17,18] (see the discussion of Fe ions above).

5. Lower priority systems

There are reasonably accurate results available for H-like and He-like ions of B,N,F,Si,Ne,Ar and Kr. Again many charge states of N,Ne and Ar have been considered. Readers are referred to the attached bibliography for details. No attempt can yet be made to asses the reliability of the calculations, but the uncertainties will increase with increasing Z and decreasing q.

References

1. B. H. Bransden and M. R. C. McDowell, Phys. Rept. 30 207 (1977)

2. B. H. Bransden and M. R. C. McDowell, Phys. Rept. 46 249 (1978)

3. R. J. W. Henry, Phys. Rept. 68 1 (1981)

4. Y. Itikawa, IPPJ-AM-24, Institute of Plasma Physics, Nagoya University, Japan (1982)

5. D. H. Crandall, in "Proc. NATO Summer School, The Physics of Ion - Ion and Electron - Ion Collisions", by F. Brouillard and J. Wm. McGowan Edts., Plenum Press (to be published)

6. D. H. Crandall, in "Proc. NATO Summer School, Atomic Physics of Highly Ionized Atoms", R. Marrus and J. P. Briand Edts., Cargese 1982, Plenum Press (to be published) and report ORNL/TM-8453

7. M .R. C. McDowell, in Proceedings of the NATO Advanced Study Institute on Atomic and Molecular Processes in Controlled Fusion Plasmas, edited by C.J. Joachain and D. Post, Plenum Press, New York, 1983

8. A. Lorenz: See Appendix 17 of this report

9. P. O. Taylor, R. A. Phaneuf and G. H. Dunn, Phys. Rev. A 22 435 (1980)

10. D. C. Gregory, G. H. Dunn, R. A. Phaneuf and D. H. Crandall, Phys. Rev. A 20 410 (1979)

11. G. H. Dunn, R. A. Falk, D. S. Belic, D. H. Crandall, D. C. Gregory and C. Cisneros, Private communication

12. I. P. Zapesochnyi, V. A. Kel'man, A. I. Imre, A. I. Daschenko and F. F. Danch, Sov. Phys. JETP 42 989 (1976)

13. W. T. Rogers, J. O. Olsen and G. H. Dunn, Phys. Rev. A 18 1353 (1978)

14. N. H. Magee, Jr., J. B. Mann, A. L. Merts and W. D. Robb, Report LA-6691-MS (1977)

15. M. S. Pindzola and D. H. Crandall, Report ORNL/TM-7957 (1981)

16. A. L. Merts, J. B. Mann, W. D. Robb and N. H. Magee, Jr., Report LA-8267-MS (1980)

17. R. E. H. Clark, N. H. Magee, Jr., J. B. Mann and A. L. Merts, Astrophys. J. 254 412 (1982)

18. A. K. Pradhan, Phys. Rev. Lett. 47 79 (1981)

19. A. K. Bhatia, U. Feldman and G. A. Doschek, J. Appl. Phys. 51 1464 (1980)

20. T.K. Krueger and S.J. Czyzak, Proc. Roy. Soc. A 318 531 (1970), S.J. Czyzak, T.K. Krueger, P. de A.P. Martins, H.E. Saraph and M.J. Seaton, Mon. Not. Roy. Astr. Soc. 148 361 (1970)

21. J. Callaway and M. R. C. McDowell, Comments Atom. Mol. Phys. (in press)

22. T. Scott and M. R. C. McDowell, J. Phys. B 8 2369 (1975)

23. B. Van Zyl, G. H. Dunn, G. Chamberlain and D. W. O. Heddle, Phys. Rev. A 22 1916 (1980)

24. T. Scott, PhD Thesis, London (1976)

25. A. K. Pradhan, D. W. Norcross and D. G. Hummer, Phys. Rev. A 23 619 (1981)

26. A. K. Pradhan, D. W. Norcross and D. G. Hummer, Astrophys. J. 246 1031 (1981)

Working Group Report on Electron Impact Ionization of Ions

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

1. Single Ionization Cross Sections for Ions

1.1. Z = 1 - 10, H - Ne

A "recommended" set of cross sections has been assembled by Bell et al. [1] and distributed. This CRP recognizes the care that has gone into this compilation and recommends the use of these cross sections by the fusion community with the following exceptions:

a) For Be^+, experimental measurements [2] now exist which differ substantially (30-60%) from the Bell et al. recommendations, and - in fact - are in quite good (about 5%) agreement with the Lotz formula [3] predictions. The committee recommends use of these experimental values.

b) For C^{3+}, Bell et al. chose to be guided in their recommendations by the theoretical work of Jakubowitz et al. [4] rather than the experimental work of Crandall et al. [5]. In fact, the experiments - when scaled - don't "fit" the common pattern of other ions in the Li isoelectronic sequence and there may be reason to be concerned. However, in view of the fact that the experiment was done twice and was done the same way [5] as N^{4+} and O^{5+}, this committee recommends that, for the present, the experimental values be used by the fusion community.

Good experiments exist for all species and ionization stages except for Li^{2+}, Be^{3+}, B^{2+}, B^{4+}, C^{5+}, N^{6+}, O^{6+} and O^{7+}.

Strong excitation-autoionization effects are evidenced in the Li isoelectronic sequence, and the effect increases rapidly with Z. This needs further work, e.g. in O^{+5}. Thus, in Be^{+} it is a 5% effect and in O^{+5} the effect increases the cross section by about 30%. Extrapolating to higher charged states of the sequence, the effect could become even more important than in O^{+5}.

No data exist for any ionization stage of F, even though it is a priority species. It is recommended that work should be done to improve the situation. Predictor formulae (particularly Lotz') should give reasonable values for F ions if excitation-autoionization is estimated for F^{6+}.

Good beam measurements exist for Ne^{+} [6,7], Ne^{3+} [8]. Trap measurements exist [9] for all ionization stages of Ne. The beam measurements can be recommended to the fusion community, with an accuracy of the order of 10%. The trap measurements, which have been done only at energies above 2 keV cannot be considered to be more reliable than a factor of two, with the exception of Ne ions for which the accuracy may be $\pm$ 70%.

1.2. Z = 11 - 18, Na - Ar

Good beam measurements have been made on Na^{+} [10], Mg^{+} [11,12], Mg^{2+} [13], Al^{+} [14], Al^{2+} [12], Si^{3+} [12], Ar^{+} [7,15], Ar^{2+} [7], Ar^{3+} [7], Ar^{4+} [7], Ar^{5+} [7] and are recommended to the fusion community for use with the stated accuracies, usually of the order of 10%. Trap measurements exist [9] on all Ar ionization stages above 3. The analysis of these data is complex and involves many assumptions; also these data have probably a factor of 3 uncertainty. The Na isoelectronic sequence shows excitation-autoionization effects [12] which increase rapidly with Z. No theories nor scaling formulae seem to do well to represent the direct process: the Lotz formula for example, gives values which are 50 % or more too high. Resonant inner-shell dielectronic capture followed by double autoionization also seems important [16]. Branching ratios for autoionization may not agree with theory. Experimental work on a more highly ionized member of the Na isoelectronic sequence is needed, and theoretical work should continue in order to understand why there is disagreement and to understand how to extrapolate to higher Z members of the sequence.

There is insufficient work on Al ions, considering the priority nature of this species.

There is no work on Cl, a priority species, and this committee recommends both experimental and theoretical effort on Cl ions. Pending further studies the Lotz formula may provide a reasonable prediction if some effort is made to include scaled effects of excitation-autoionization for members of the Na and Li isoelectronic sequences.

1.3. Z = 19 - 36, K - Kr

There exist good beam measurements for K^+ [10], Ca^+ [17], Ti^{3+} [18], Zn^+ [19], Ga^+ [19], Kr^{3+} [8], and these are recommended to the stated accuracies - usually of the order of 10 %. The main points are that:

a) Excitation-autoionization can (and often does) dominate the ionization cross section by more than an order of magnitude .

b) There is experimental evidence that d subshells contribute about half as much to the direct process as would be expected from s and p subshells. Thus, simple Lotz-type methods can't be used without inventing new coefficients.

c) There are no data for Fe ions, and data on only one Ti ion (Ti^{3+}), despite the fact that these are two of the highest priority metals. Work should be done as soon as possible on these species. Work should also be done on ions of Cr, Cu and Ni. There are currently no measurements nor calculations.

d) Multiple ionization may be very important, as discussed in more detail later.

1.4. Z = 37 - 102, Rb - No

Good beam measurements exist for Rb^+ [17], Sr^+ [17], Zr^{3+} [18], Cd^+ [20], Xe^+ [7], Xe^{3+} [8], Cs^+ [17], Ba^+ [21], Hf^{3+} [18], Ta^{3+} [18], Hg^+ [20], Tl^+ [22] and these are recommended to the stated accuracies of the order of 10%. Trap measurements exist on many ionization stages of Xe, Cs, Ba, Hg.

In addition to the specific data, the main points are much the same as for Z = 19 - 36:

a) Excitation-autoionization can (and often does) totally (by up to more than an order of magnitude) dominate the ionization cross section.

b) Electrons in the d and f subshells probably contribute less than those in s and p subshells as noted earlier, and their contribution may vary substantially with species. Simple formulae such as Lotz's may not be readily applicable without significantly altered coefficients for these subshells.

c) There are no data for Mo and W, and data on only one ionization stage of Zr. Work on these species should be done, though one should do it methodically including other species, recognizing points a) and b) above.

2. Multiple Ionization Cross Sections for Ions

Cross sections for multiple ionization of ions $\sigma_{q,q+k}$ with $k > 1$, have generally been considered to be small compared to single step ionization cross sections $\sigma_{q,q+1}$. As a consequence, these ionization processes are neglected in plasma modelling codes. This is not entirely justified by the very few data presently available. These are:

$\sigma_{1,3}$	Li [23]	Na [24]	Ar [25]	Rb [26]
$\sigma_{1,4}$			Ar	Rb
$\sigma_{1,5}$			Ar	Rb
$\sigma_{2,4}$ 2,5 3,5			Ar	

Recent data for Xe^{q+} ions (Ref. [27] to be published), comprising $\sigma_{1,3}$ $\sigma_{1,4}$ $\sigma_{1,5}$ $\sigma_{2,4}$ $\sigma_{2,5}$ $\sigma_{2,6}$ $\sigma_{3,5}$ $\sigma_{3,6}$ and $\sigma_{4,6}$ show that for this heavy (Z = 54) ion multiple ionization cross sections are quite large, e.g. $\sigma_{1,3}$ reaches values of up to 5.10^{-17} cm^2. The ratio of cross sections $\sigma_{1,3}/\sigma_{1,2}$, taken at electron energies $E > 400$ eV, rapidly increases with Z and approaches the value 0.3 for Xe. This shows that for high Z elements multiple ionization processes should not be neglected. Clearly more data are needed. It is very important to have reliable and extensive experimental data to guide development of models for multiple ionization cross sections. Available classical models are at best qualitative.

We emphasize to the fusion community that these multiple ionization processes should probably be considered in diagnostics and modelling - particularly for $Z > 20$.

3. Sources

Very good recent sources on ionization of ions are:

a) "Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions" by K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith [1]. This gives recommended cross sections for all stages of ionization for hydrogen through oxygen, and compares with experimental data, frequently used formulae, and "quality" theory.

b) "Empirical Formulas for Ionization Cross Sections of Atomic Ions for Electron Collisions: Critical Review with Compilation of Experimental Data" by Y. Itikawa and T. Kato [28]. Gives compilation of experimental data available to authors for Z = 2 - 19 and compares with Lotz [3] and scaled Coulomb - Born [29].

c) "Bibliography on Electron Collisions with Atomic Positive Ions, 1978 through 1982" by Y. Itikawa [30]. This supplements and updates the earlier version IPPJ-AM-7 by K. Takayanagi and T. Iwai [31].

d) "Calculations of Electron Impact Ionization Cross Sections at NBS, Washington, D.C." by S.M. Younger. Atomic Data For Fusion 7 6 (1981) 143-201. This summarizes earlier work referred to under Ref. 33 of this Working Group Report.

4. Conclusions and Recommendations (See also Table II, p.5)

4.1. With exceptions noted (for Be^+ and C^{3+}), the cross sections "recommended" by Bell et al. should be adopted for the fusion community for hydrogen through oxygen (Z = 1 - 8) at all ionization stages. Those using the Lotz formula for plasma calculations should recognize that the differences between the cross sections recommended by Bell et al. [1] and the Lotz formula [3], average about 20-30% up to a maximum of about 50% different for B^{2+}.

4.2. In all cases for which there are beam measurements, this working group recommends these data to the fusion community to an accuracy within the stated uncertainties, usually about 10%.

4.3. For Z = 9 - 18, a reasonable set of cross sections could be generated based on estimator formulae (Lotz [3], scaled Coulomb Born [29], scaled plane-wave Born [32], and more accurate [4,33] calculations (for example, distorted wave, Coulomb-distorted wave with exchange, etc.) where available and taking care to scale excitation-autoionization for the sequences where it has been seen to be important (Li, Na,...). This should be done, especially for Al ions. However, more work will be needed to experimentally establish the validity of the predicted cross sections.

4.4. For $Z > 19$ it is very dangerous at this time to generate recommended cross sections except for species on which measurements have been made. More work, both theoretical and experimental, needs to be done to establish systematics of subshell contributions and contributions from excitation-autoionization (also resonant excitation/capture followed by double autoionization). Some cross sections for high ionization stages corresponding to low Z atom isoelectronic sequences may be reasonably predicted with care as in comment 3 above.

4.5. Relativistic effects which may become important for $Z > 20$, have not been included in the theory nor in semi-empirical formulae.

References

1. K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, and F.J. Smith, Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions, Culham Laboratory Report CLM-R216 (submitted to Journal of Chemical and Physical Reference Data)

2. R.A. Falk and G.H. Dunn, Private Communication (submitted to Phys. Rev. A)

3. W. Lotz, Z. Physik 206 205 (1967), Z. Physik 220 446 (1969), Z. Physik 216 241 (1968), Astroph. J. Suppl. 14 207 (1967)

4. H. Jakubowitz and D.L. Moores, J. Phys. B. 14 3733 (1981), Comm. Atom. Mol. Phys. 9 55 (1980)

5. D.J. Crandall, R.A. Phaneuf and P.O. Taylor, Phys. Rev. A 18 1911 (1978), D.H. Crandall, R.A. Phaneuf, B.E. Hasselquist and D.C. Gregory, J. Phys. B 12 L249 (1979)

6. K.T. Dolder, M.F.A. Harrison and P.C. Thonemann, Proc. Roy. Soc. A 274 546 (1963)

7. A. Mueller, E. Salzborn, R. Frodl, R. Becker, H. Klein and H. Winter, J. Phys. B 13 1877 (1980)

8. D. Gregory, P.F. Dittner and D.H. Crandall, Private Communication, (1982)

9. E. Donets and V.P. Ovsyannikov, Sov. Phys. JETP 53 466 (1981)

10. B. Peart and K.T. Dolder, J. Phys. B 1 240 (1968), J.W. Hooper, W.C. Lineberger and F.M. Bacon, Phys. Rev. 141 165 (1966)

11. S.O. Martin, B. Peart and K.T. Dolder, J. Phys. B 1 537 (1968)

12. D.H. Crandall, R.A. Phaneuf, R.A. Falk, D.S. Belic and G.H. Dunn, Phys. Rev. A 25 143 (1982)

13. B. Peart, S.O. Martin and K. T. Dolder, J. Phys. B 2 1176 (2969)

14. D.S. Belic, K. Timmer and G.H. Dunn, Private Communication (1982)

15. P.R. Woodruff, M.C. Hublet and M.F.A. Harrison, J. Phys. B 11 2305 (1978)

16. K. J. LaGattuta and Y. Hahn, Phys. Rev. A 24 2273 (1981)

17. B. Peart and K.T. Dolder, J. Phys. B 8 56 (1975)

18. R.A. Falk, G.H. Dunn, D.C. Griffin, C. Bottcher, D.C. Gregory, D.H. Crandall and M.S. Pindzola, Phys. Rev. Lett. 47 494 (1981)

19. W.T. Rogers, G. Stefani, R. Camilloni, G.H. Dunn, A. Z. Msezane and R.J.W. Henry, Phys. Rev. A 25 737 (1982)

20. D. Belic, R.A. Falk and G.H. Dunn, Private Communication (1982)

21. B. Peart, J.G. Stevenson and K.T. Dolder, J. Phys. B 6 146 (1973)

22. T.F. Divine, R.F. Feeney, W.E. Sayle and J.W. Hooper, Phys. Rev. A 13 54 (1976)

23. B. Peart and K.T. Dolder, J. Phys. B 2 1169 (1969)

24. W.E. Sayle and R.K. Feeney, 10th ICPEAC (1977) 1084

25. A. Mueller and R. Frodl, Phys. Rev. Lett. 44 29 (1980)

26. D.W. Hughes and R.K. Feeney, Phys. Rev. A 23 2241 (1981)

27. Ch. Achenbach, A. Mueller, R. Becker, H. Klein and E. Salzborn, Private Communication (1982)

28. Y. Itikawa and T. Kato, Empirical Formulas for Ionization Cross Section of Atomic Ions for Electron Collisions, Report IPPJ-AM-17, Institute of Plasma Physics, Nagoya, Japan (June 1981)

29. D.H. Sampson and L.B. Golden, J. Phys. B 11 541 (1978), J. Phys. B 12 L 785 (1979)

30. Y. Itikawa, Bibliography on Electron Collisions with Atomic Positive Ions, 1978 through 1982. IPPJ-AM-24, Institute of Plasmas Physics, Nagoya, Japan (1982).

31. K. Takayanagi and T. Iwai, Bibliography on Electron Collisions with Atomic Positive Ions, 1940 through 1977. Report IPPJ-AM-7, Institute of Plasma Physics, Nagoya, Japan (June 1978).

32. E.J. Mc Guire, Phys. Rev. A 16 73 (1977)

33. S.M. Younger, J. Quant. Spectrosc. Rad. Transfer, 26 329 (1981), Phys. Rev. A 24 1278 (1981), Phys. Rev. A 24 1272 (1981), Phys. Rev. A 23 1138 (1981), Phys. Rev. A 22 1425 (1980), Phys. Rev. A 22 111 (1980).

Working Group Report on Charge Exchange and Related Processes

S. Bliman, H.B. Gilbody (Chairman), P. Hvelplund, R.K. Janev, H. Winter

1. Collisions involving hydrogen atoms

During the past few years experimental and theoretical data on the process

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

have become available for a variety of ion species of fusion interest over a wide energy range. A recent review by Gilbody [1] of the experimental data in relation to current theoretical prediction is available, while a critical review of the theoretical methods and predictions has been carried out by Janev and Bransden [2] in context of this CRP. For multiply charged ions, since cross sections are dependent on q rather than on the ion species and can often be described by scaling relations, no specific reference is made to those ions designated by Lorenz [3] to be of priority interest to the fusion community.

At velocities $v < 1$ au (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 ionization 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 $v > 1$ au, 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 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. 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 $v < 1$ au, 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 rules apply, but for systems with high initial charge states ($q \geq 10$), $\sigma_{q,q-1}$ is approximately linearly dependent on q. Experimental data on (1) for ions of high q at energies less than about 1 keV/amu are still very limited and additional measurements of the type recently carried out by Phaneuf et al. [5] for C and O ions are required to check the validity of theoretical predictions.

Experimental data of high precision are now available [4,5,6] for the ionization process (2) for H^+, He^{2+} and multiply charged ions of lithium, carbon, nitrogen and oxygen. Results for C, N and O ions show that cross sections for different ions with the same q agree closely both in magnitude and velocity dependence. At high velocities where the cross sections have decreased below the peak value, cross sections can be described by a simple scaling relation. A more general discussion has been given by Janev and Hvelplund [4]. For the bare nuclei H^+, He^{2+} and Li^{3+}, there is evidence that ionization cross sections scale according to Z^2 (as predicted by the Born approximation) only at very high velocities. The velocity at which the Born prediction becomes valid progressively increases with Z.

Olson et al. [9] 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. The calculated reduced cross sections σ_e/q plotted against the reduced energy E/q lie on the universal curve given by

$$\sigma_e/q = 4.6\left\{(32q/E)\ [1 - \exp(-E/32q)]\right\} 10^{-16}\ \mathrm{cm}^2 \qquad (4)$$

where E is the energy in keV/amu. Although there are departures from this universal curve at both low and high velocities, the available data [7,8] indicate agreement to within a factor of 2 within the range 20 - 150 keV/amu.

Cross sections for the electron capture process

$$X^{q+} + H \longrightarrow (X^{(q-1)+})^{*} + H^{+} \qquad (5)$$

involving capture into specific excited states (n,l) of the product ion are now urgently required particularly at velocities $v < 1$ au. Measurements are now proceeding in a number of laboratories using techniques based on both optical spectroscopy of the excited collision products and from precise studies of the change in kinetic energy of the incident ions (translational energy spectroscopy). Future experimental work in this area will be facilitated by the availability of sources for the production of intense beams of highly charged ions [10]. While there are some theoretical predictions [2,11], limited experimental data are available [1] only for H^{+} and He^{2+} impact.

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 atomic hydrogen.

Quite extensive experimental data are now available for total electron capture cross sections by multiply charged ions in H_2 and He. Some data are also available for ionization of H_2 and He by multiply charged ions. These data are considered in relation to theoretical predictions and general scaling rules in a recent review by Janev and Presnyakov [12].

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

$$X^{q+} + H_2 \longrightarrow X^{(q-1)+} + H^{+} + H^{+} + e^{-} \qquad (6)$$

has an important role [13]. For many-electron targets tranfer ionization processes of the type

$$X^{q+} + Y \rightarrow X^{m+} + Y^{n+} + (m + n - q)\ e^{-} \qquad (7)$$

involving capture of one or more electrons with the simultaneous multiple ionization of the target have large cross sections even at low velocities [14].

Cross sections for the two electron capture process

$$He^{2+} + Li \rightarrow He + Li^{2+} \qquad (8)$$

have recently been determined [15,16]. Some data are also available [17] for one-electron capture into particular states of He^{+}. These processes are relevant to possible schemes for alpha particle diagnostics.

Cross sections for the emission of Balmer Hα radiation in the passage of H, H^{+}, H_2^{+}nd H_3^{+} through H_2 have recently been determined [18] 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. Data for the separate contributions from both target and projectile are available. These results are relevant to the diagnostics of energetic neutral hydrogen beams which are used for plasma heating. There is a need for further data on the total collisional destruction of fast H_2, H_2^{+} and H_3^{+} in H_2.

Some experimental cross sections for the emission of radiation from excited hydrogen-like ions formed in the passage of fully stripped C, N, O and Ne through H_2 are now available [19,20].

3. Collisions between positive ions

A limited amount of experimental data on collisions between positive ions are now available. These have been considered in relation to current theory in a recent review by Gilbody [21].

Cross sections for the charge transfer process:

$$H^+ + X^{q+} \rightarrow H + X^{(q+1)+} \qquad (9)$$

and the ionization process

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

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 the cross sections for (9) and (10) is also relevant to plasma diagnostics using heavy ion beam probes. The corresponding processes involving He^{2+} ions are of interest in the context of alpha particle heating.

Experimentally determined cross sections for X^{2+} production from the combined processes (9) and (10) are available for targets of He^+, Li^+, C^+, N^+, Mg^+, Ti^+ and Fe^+. For He^+ and Li^+, separate measurements of the cross section for the charge transfer process (9) are available. Provided that ground state collidants and product ions are dominant in these reactions, there is evidence that cross sections for the reverse reaction

$$X^{2+} + H \rightarrow X^+ + H^+ \qquad (11)$$

can provide reliable estimates for charge transfer in $H^+ - X^+$ collisions.

At energies where measured cross sections for X^{2+} production are dominated by ionization there is evidence [21] that the data can be described by a simple classical scaling relation which permits cross sections to be predicted to within about a factor of two.

References

1. H.B. Gilbody, Physica Scripta 24 712 (1981)

2. R.K. Janev and B.H. Bransden, IAEA report INDC(NDS)-135/GA

3. A. Lorenz, see Appendix 17 to this report

4. R.K. Janev and P. Hvelplund, Comments on Atomic and Molecular Physics 11 75 (1981)

5. R.A. Phaneuf, I. Alvarez, F.W. Meyer and D.H. Crandall, Phys. Rev. A (to be published in 1982)

6. M.B. Shah and H.B. Gilbody, J. Phys.B 14 2361 (1981)

7. M.B. Shah and H.B. Gilbody, J. Phys.B 14 2831 (1981)

8. M.B. Shah and H.B. Gilbody, J. Phys.B 15 415 (1982)

9. R.E. Olson, K.H. Berkner, W.G. Graham, R.V. Pyle, A.S. Schlachter and J.W. Stearns, Phys. Rev. Lett. 41 163 (1978)

10. J. Arianer and R. Geller, Ann. Rev. Nucl. Part. Sci. 31 19 (1981)

11. R.K. Janev, Proc. Symp. on Production and Physics of Highly Charged Ions, Stockholm 1982 (to be published in Physica Scripta)

12. R.K. Janev and L.P. Presnyakov, Phys.Rep. 70 1 (1981)

13. M.B. Shah and H.B. Gilbody, J.Phys.B (to be published in 1982)

14. W. Groh, A. Mueller, Ch. Achenbach, A.S. Schlachter and E. Salzborn, Phys.Lett. 85A 77 (1981)

15. R.W. McCullough, T.V. Goffe, M.B. Shah, M. Lennon and H.B. Gilbody, J.Phys.B. 15 111 (1982)

16. G.A. Murray, J. Stone, M. Mayo and T.J. Morgan, Phys.Rev. A25 1805 (1982)

17. K. Kadota, D. Dijkkamp, R. Van der Woude, Pan Guang Yan and F.J. de Heer, Phys.Lett. 88A 135 (1982)

18. I.D. Williams, J. Geddes and H.B. Gilbody, J.Phys.B 15 1377 (1982)

19. V.V. Afrosimov, A.A. Basalaev, Yu.S. Gordeev, E.D. Donets, A.N. Zinov'ev, S.Yu. Ovchinnikov and M.N. Panov, Sov. Phys.-JETP Lett. 34 316 (1981)

20. S. Bliman, M. Bonnefoy, J.J. Bonnet, A. Fleury, D. Hitz and B. Jacquot, Proc. Symp. on Production and Physics of Highly Charged Ions, Stockholm 1982 (to be published in Physica Scripta).

21. H.B. Gilbody, in "Physics of Electronic and Atomic Collisions" S. Datz Edt., N. Holland, pp.223-34 (1982)

Working Group Report on Dielectronic Recombination

V.A. Abramov, D.H. Crandall and G. Dunn

This process has been recognized to be important in hot plasmas for at least two decades, and the associated satellite lines are observed in the spectroscopy of fusion [1] and astrophysical plasmas [2]. Currently one relies totally on theory to take this process into account. There are no experimental measurements of cross sections for this process, though there are at least two rate measurements [3, 4] (factor of two accuracy). There are several efforts worldwide to make measurements of cross sections, and these should be encouraged in order to verify and gain confidence in the theory being used.

When the process occurs, one is left with an excited core of the parent ion and a high Rydberg state of the daughter. The core must radiate before autoionization occurs, and the Rydberg state must then relax before a net recombination results. Clearly, in a plasma environment, ionization of the Rydberg state may result from field ionization or collisional effects (electrons or ions). These must be accounted for separately (from any measurement of cross section for dielectronic recombination) in order to obtain recombination rates appropriate to particular plasma environments. The current, most widely used source for dielectronic recombination rates is the Burgess [5] - Merts [6] formula which is likely to remain the best overall source for the immediate future. Detailed calculations for specific cases [7] and including estimates of collisional (density) effects [8] can be usefully compared to the general formula but no reliability should be inferred.

References

1. M. Bitter, K.W. Hill, N.R. Sauthoff, P.C. Efthimion, E. Meservey, W. Roney, S. von Goeler, R. Horton, M. Goldman and W. Stodiek, Phys. Rev. Lett. 43 129 (1979), M. Bitter, S. von Goeler, K.W. Hill, R. Horton, D. Johnson, W. Roney, N. Sauthoff, E. Silver, and W. Stodiek, Phys. Rev. Lett. 47, 921 (1981)

2. J. Dubau, and S. Volonte, Dielectronic Recombination and Its Applications in Astronomy, Rep. Prog. Phys. 43, 199-251 (1980)

3. R.L. Brooks, R.U. Datla, and H.R. Griem, Phys. Rev. Lett. 41, 107 (1978)

4. C. Breton, C. De Michelis, M. Finkenthal, and M. Mattioli, Phys. Rev. Lett. 41, 110 (1978)

5. A. Burgess, Astrophys. J. 141, 1588 (1965)

6. A.L. Merts, R.D. Cowan, and N.H. Magee Jr., The Calculated Power Output from a Thin Iron-Seeded Plasma, Report LA 6220-MS, Los Alamos Scientific Lab., Los Alamos, N.M. (March 1976)

7. Hahn, Y., Phys. Rev. A 22, 2896 (1980)

8. V.L. Jacobs, and J. Davis, Phys. Rev. A 18, 697 (1978)

Appendix 1

LIST OF PARTICIPANTS

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

Vienna, 21-25 June 1982

ABRAMOV, Prof. V.A.	Institut Atomnoi Energii I.V. Kurchatova Plochchad I.V. Kurchatova Moscow, D-182, 123182, USSR
BLIMAN, Prof. S.	C.E.N. Grenoble 85X Ave. des Martyrs F-38041 Grenoble Cedex
CRANDALL, Dr. D.H.	Oak Ridge National Lab. Physics Division Oak Ridge, Tenn. 37830, USA
DUNN, Dr. G. H.	University of Colorado J.I.L.A., Campus Box 440 Boulder, Colorado 80303, USA
GILBODY, Prof. H.B.	The Queen's University of Belfast Pure & Applied Physics Belfast BT7 1NN, Northern Ireland, U.K.
HVELPLUND, Prof. P.	University of Aarhus Institute of Physics DK-8000 Aarhus C
ITIKAWA, Prof. Y.	Research Information Center Institute of Plasma Physics Nagoya University Nagoya 464, Japan
JANEV, Prof. R.K.	Institute of Physics Studentski trg 12/V P.O.B. 57 YU-11001 Belgrade
KATSONIS, Dr. K.	IAEA Atomic & Molecular Data Unit Scientific Secretary P.O.B. 100 A-1400 Vienna
LORENZ, Dr. A.	IAEA Head, Atomic & Molecular Data Unit P.O.B. 100 A-1400 Vienna

MCDOWELL, Prof. M.R.C.	Royal Holloway College University of London Dept. of Mathematics Egham Hill, Egham Surrey TW20 OEX, U.K.
SALZBORN, Prof. E.	Justus Liebig-Universität Institut f. Kernphysik Leihgesterner Weg 217 D-6300 Giessen
SCHMIDT, Dr. J.J.	IAEA Head, Nuclear Data Section P.O.B. 100 A-1400 Vienna
WINTER, Prof. H.	Technische Universität Institut f. Allgemeine Physik Karlsplatz 13 1040 Wien

Appendix 2

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

First Research Coordination Meeting
Vienna, 21 - 25 June 1982
VIC, Room A2346

ADOPTED AGENDA

1. Opening Statements and Announcements

    1.1. Opening of meeting (9:30) by J.J. Schmidt
    1.2. Appointment of chairmen (J.J. Schmidt)
    1.3. Introduction to CRP (A. Lorenz)

    - Objectives
    - Procedures and organization
    - Assignment of responsibilities
    - Questions and answers

    1.4. Adoption of Agenda (A. Lorenz)
    1.5. Announcements (K. Katsonis)

2. Short Progress Reports by participants on their work

3. Brief Review of the data requirements and their priorities (A. Lorenz)

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

    4.1. Electron excitation
    4.2. Electron ionization
    4.3. Electron capture and charge exchange
    4.4. Recombination

5. Writing of working group reports

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

7. Identification of data which can be calculated or measured, or be represented by empirical formulae, and methods to generate the required data

8. Distribution of responsibilities among the participants in the CRP

9. Summary of Conclusions

10. Next meeting

Appendix 3

List of Papers Submitted to the Meeting

1. "Review of Data Requirements and their Priorities", A. Lorenz, IAEA, Vienna. (Included in this report as Appendix 13).

2. "What we do and do not know about electron impact excitation of atomic hydrogen", J. Callaway and M.R.C. McDowell, Royal Holloway College, England. (To be issued in IAEA report INDC(NDS)-137/GA).

3. "Current theoretical techniques for electron-atom and electron-ion scattering", M.R.C. McDowell, Royal Holloway College, England. (To be published in Proceedings of the NATO Advanced Study Institute on Atomic and Molecular Processes in Controlled Fusion Plasmas, edited by C.J. Joachain and D. Post, Plenum Press, New York, 1983).

4. "Ion-atom and ion-ion collision processes relevant to fusion", H.B. Gilbody, et al., The Queen's University of Belfast, UK. (Included in this report as Appendix 7).

5. "Comments on electron-impact ionization of ions", Gordon Dunn, JILA, Boulder, Colorado, USA. (Included in this report as Appendix 16).

6. "Evaluation of electron-impact excitation cross sections of carbon and oxygen ions", Y. Itikawa, Institute of Plasma Physics, Nagoya University, Japan. (Included in this report as Appendix 4).

7. "Data compilation and evaluation on atomic collision and structure data in JAERI", JAERI, Japan. (Included in this report as Appendix 5).

8. "Charge exchange between highly charged ions and atomic hydrogen: A critical review of theoretical data", R.K. Janev and B.H. Bransden, JILA, Boulder, Colorado, USA (to be published in IAEA report INDC(NDS)-135/GA).

9. "Atomic and Molecular Data for Fusion, Part 1. Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions", K.L. Bell et al., Culham Laboratory report CLM-R216. (Not included in these proceedings).

10. "Influences of Charge Exchange and Fast Ions on Impurity Radiation in a Hot Plasma", V.A. Abramov, V.G. Gontis and V.S. Lisitsa, I.V. Kurchatov Institute of Atomic Energy, Moscow, 1982. (Translated by IAEA, included in this report as Appendix 9).

Evaluation of electron-impact excitation cross sections of carbon and oxygen ions

Y. Itikawa
Research Information Center
Institute of Plasma Physics
Nagoya University

This program has started in April, 1981. As a joint research project of data compilation and evaluation at the Research Information Center, Institute of Plasma Physics, a small group of atomic physicists has been organized. The carbon and oxygen ions have been chosen as a first target because of its importance in fusion plasmas and availability of a rather large number of data. This program is also a part of the U.S.-Japan collaboration program of atomic data for fusion.

The actual procedure of data evaluation has been taken as follows:
(1) Prepare a list of relevant literature
(2) Review the literature and fill the worksheet
(3) Select reliable set of data
(4) Compare graphically the selected data with each other
(5) Determine the recommended values and estimate their accuracy, if possible

The literature list was made based on the bibliography (IPPJ-AM-7) compiled by Takayanagi and Iwai, supplemented by our own survey of recent literature. Each member of the group is assigned to specific ions (say, H-like) and reviews the relevant papers. To make it easy to summarize the content of the papers, a common worksheet (Appendices A and B) has been distributed to be filled by the evaluators.It includes a check list for the calculation or experiment. The Research Information Center has developed a computer system (called AMDIS) for the storage, retrieval and display of electron-ion collision data. The most of the relevant data are already stored in the system. The system, therefore, can be fully utilized to make graphs for comparison of the data. In some cases, an inquiry to the original author was made to get more detailed information about his method of data production.

The first stage of data evaluation has been completed and recommended cross sections have been determined for the processes listed in the Appendix C. The results are planned to be compared with those determined by the Oak Ridge Data Center. When a conclusion will be reached, a set of recommended cross sections will be published as a joint report of IPP/Nagoya and ORNL.

The next step of our plan is to extend the evaluation along isoelectronic sequence. That is, the task of data evaluation has started this year on all the ions of H-like through N-like sequences. This program will be incorporated into the Coordinated Research Program on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas coordinated by IAEA.

(May 21, 1982)

Appendix A

ELECTRON-ION COLLISIONS: EXCITATION-THEORETICAL

Data set

Date ________ Reviewer's name ____________

Author(s)

Reference

Title

Processes

Energy range

Excitation energy (experimental or theoretical?)

Method of calculation	abbreviated form
	additional explanation

Wavefunctions used

Critical factors considered:

About the wavefunctions used

[ ] configuration mixing

[ ] reproducibility of the relevant energy levels/oscillator strengths

[ ] Coupling among the states

[ ] Electron-exchange effects

[ ] Resonance effects

Accuracy estimated by the author (if any)

Comments

Appendix B

Electron-ion collision cross section (data form)

Reference:

Author(s) _____ Laboratory _____ Title __________

Data set: _____ Table __________ Graph __________

Process: Excitation { Transition __________ / Excitation energy __________

Ion species _____ Ionization ___

Recombination ___

Collision-energy range _____

Method of measurement:

___crossed beam
___merging beam
___others: _____

___absolute
___normalization

___radiation(light emission) : wave length __________
___change of charge state
___others: _____

Ion source: _______

Critical factors considered:

_____ _____ Beam purity

_____ _____ Collision volume accuracy

_____ _____ Space charge effect

_____ _____ Form factor

_____ _____ Background gas effect

_____ _____ Detector efficiency

_____ _____ Beam collection

_____ _____ Detector calibration

_____ _____ Anisotropy correction

_____ _____ Life-time correction

_____ _____ Cascade correction

_____ _____ Linearity on I_e, I_i

Comments: __________

Accuracy estimated by the author _____

Accuracy estimated by the reviewer _____

December 8, 1981
IPP/Nagoya

Excitation processes evaluated

H-like:	C^{5+}	O^{7+}
1s - 2s	x	x
2p	x	x
3s	x	
3p	x	
3d	x	
4s	x	
4p	x	
5p	x	

He-like:	C^{4+}	O^{6+}
$1s^2$ - 1s2s ^3S	x	x
1s2s ^1S	x	x
1s2p ^3P	x	x
1s2p ^1P	x	x
1s3s ^3S		x
1s3s ^1S		x
1s3p ^3P		x
1s3p ^1P	x	x
1s3d ^3D		x
1s3d ^1D		x

Li-like:	C^{3+}	O^{5+}
2s - 2p	x	x
3s	x	x
3p	x	x
3d	x	x

Be-like:	C^{2+}	O^{4+}
$2s^2\ ^1S$ - 2s2p ^3P	x	x
2s2p ^1P	x	x
$2p^2\ ^3P$	x	
$2p^2\ ^1D$	x	
$2p^2\ ^1S$	x	

B-like:	C^{+}	O^{3+}
$2s^22p\ ^2P$ - $2s2p^2\ ^4P$	x	x
$2s2p^2\ ^2D$	x	x
$2s2p^2\ ^2S$	x	x
$2s2p^2\ ^2P$	x	x

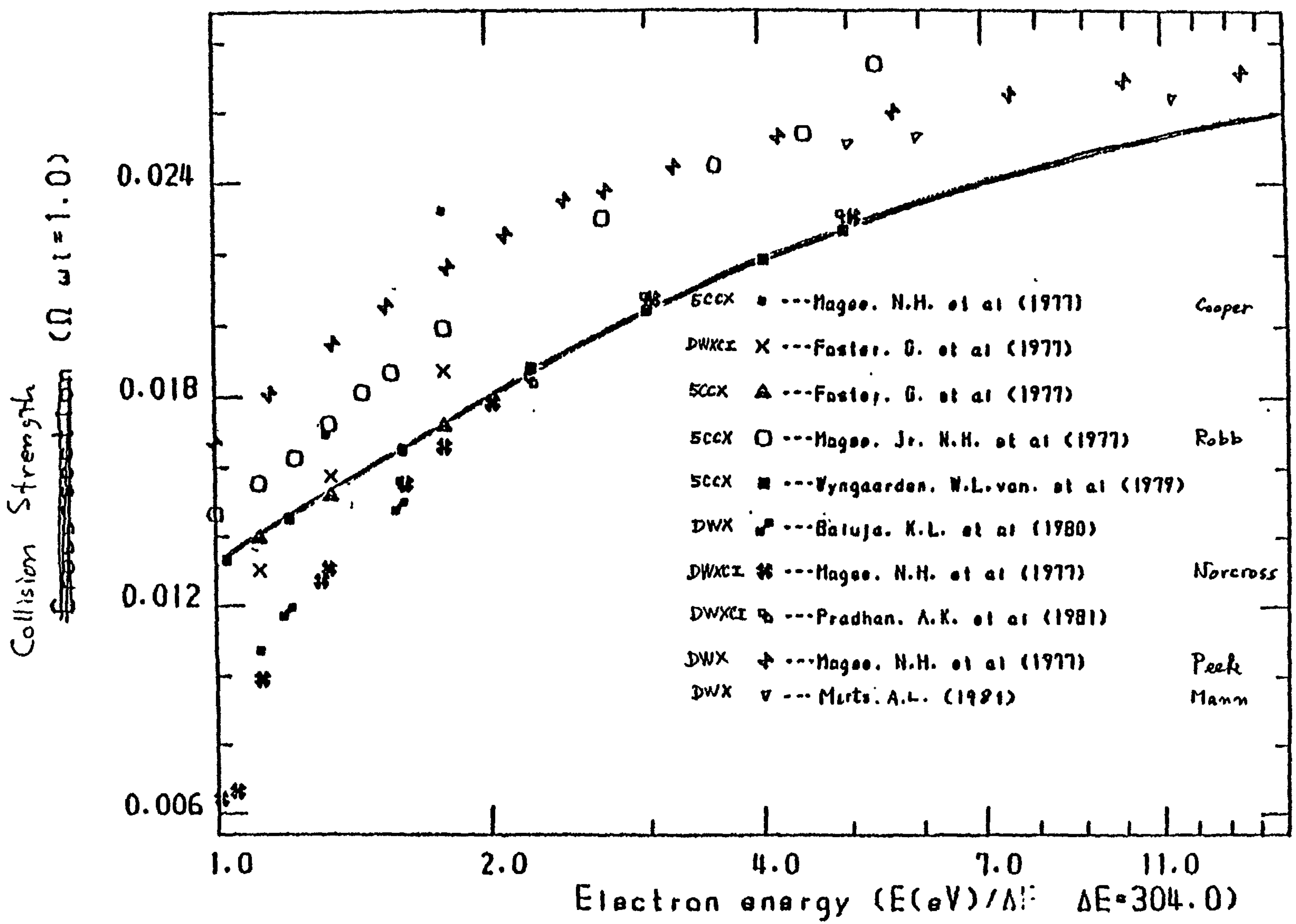
C-like:	O^{2+}
$2s^22p^2\ ^3P$ - $2s^22p^2\ ^1D$	x
$2s^22p^2\ ^1S$	x
$2s2p^3\ ^5S$	x
$2s2p^3\ ^3D$	x
$2s2p^3\ ^3P$	x
$2s2p^3\ ^1D$	x
$2s2p^3\ ^3S$	x
$2s2p^3\ ^1P$	x

N-like:	O^{+}
$2s^22p^3\ ^4S$ - $2s^22p^3\ ^2D$	x
$2s^22p^3\ ^2P$	x
$2s2p^4\ ^4P$	x
$2s^22p^23s\ ^4P$	x

Appendix C

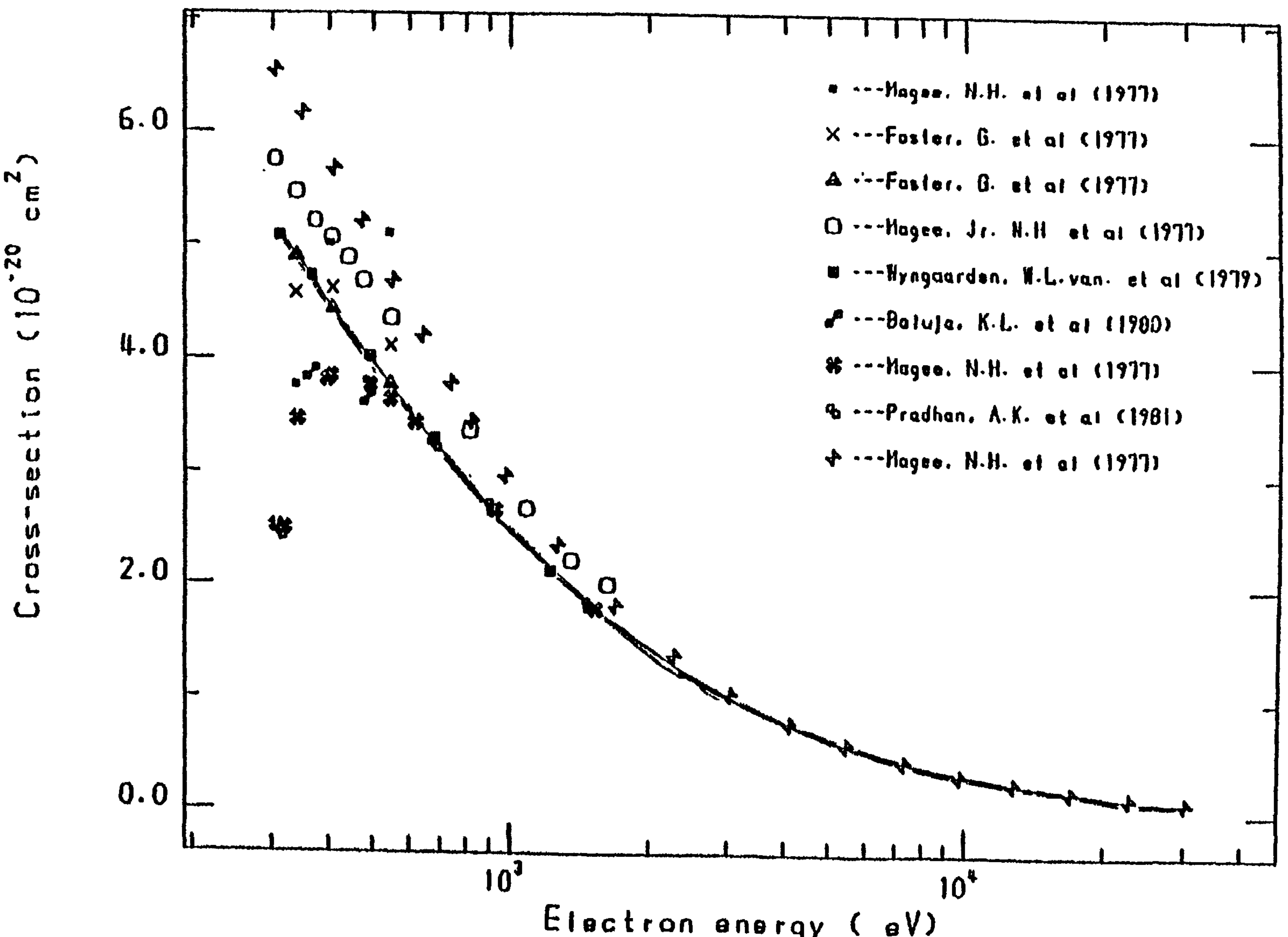
C^{+4} | $1s^2\ ^1S$ ---> $1s2s\ ^1S$| ...

81-11-24 14: 33



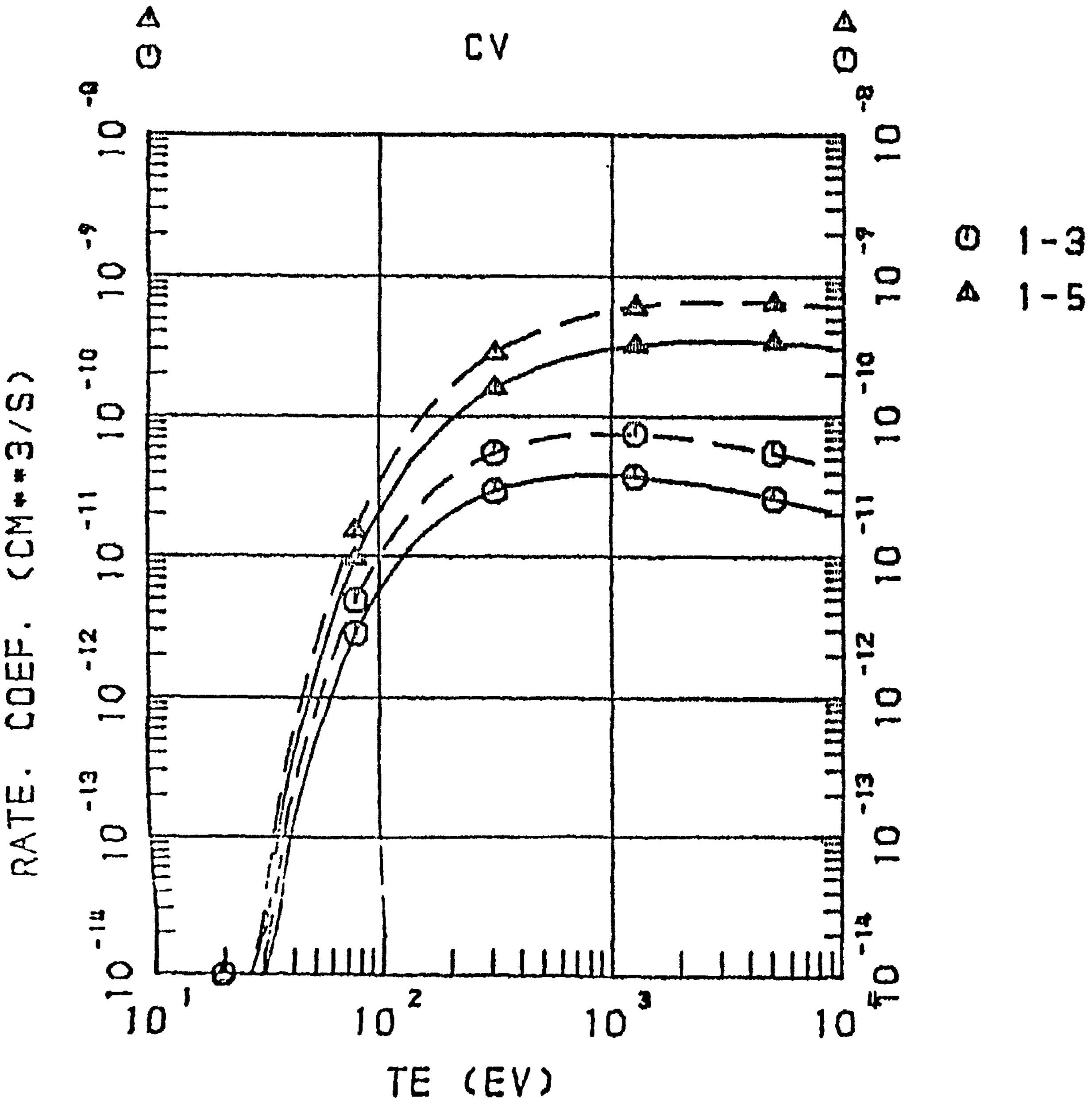
key in I..I=1(END),2(DISPLAY),3(KOSEI),4(COPY)(I1)= ?

C^{+4} ($1s^2\ {}^1S$ ---> $1s2s\ {}^1S$) ...   81-11-24 14: 33



key in I..I=1<END>,2<DISPLAY>,3<KOSEI>,4<COPY>(I1)= ?

82-06-04 23: 30 NO-1



1s2s ¹S

<ERASE> AND <RETURN>

Data Compilation and Evaluation
on Atomic Collision and Structure Data in JAERI

1. Atomic Collision

1.1. Charge Transfer Cross Section: H^+, H + (Target)
(σ_{10}, σ_{1-1}, σ_{0-1}, σ_{01}, σ_{-10}, σ_{-11})
(a) Target: H_2, N_2, O_2, CO, CO_2, H_2O, C, CH_4 etc (100%)
(b) Target: He, Ne, Ar, Kr, Xe (90%)
(c) Target: Alkali and Alkali-earth vapors (80%)

1.2. Charge Transfer Cross Section: He ion and atom + (Target)
Target: same as 1.1.(a),(b) and (c) (60%)

1.3. Ionization Cross Section: H, He + H, H_2, He (100%)

1.4. Charge Transfer Cross Section: C^{q+}, O^{q+} + H, H_2
(U.S.-Japan joint research on A+M data for fusion)
Formulation of empirical formula for A^{q+} + H, H_2
$\rightarrow A^{(q-1)+}$ (90%)

1.5. Charge Transfer Cross Section: A^{q+} + He (80%)

2. Atomic Structure (Energy levels and transition probabilities)

2.1. Ti-V - Ti-XXII (1980-1981)
wavelength tables and Grotorian diagrams (in press)

2.2. Ni, Mo data (1981-1982: compilation)

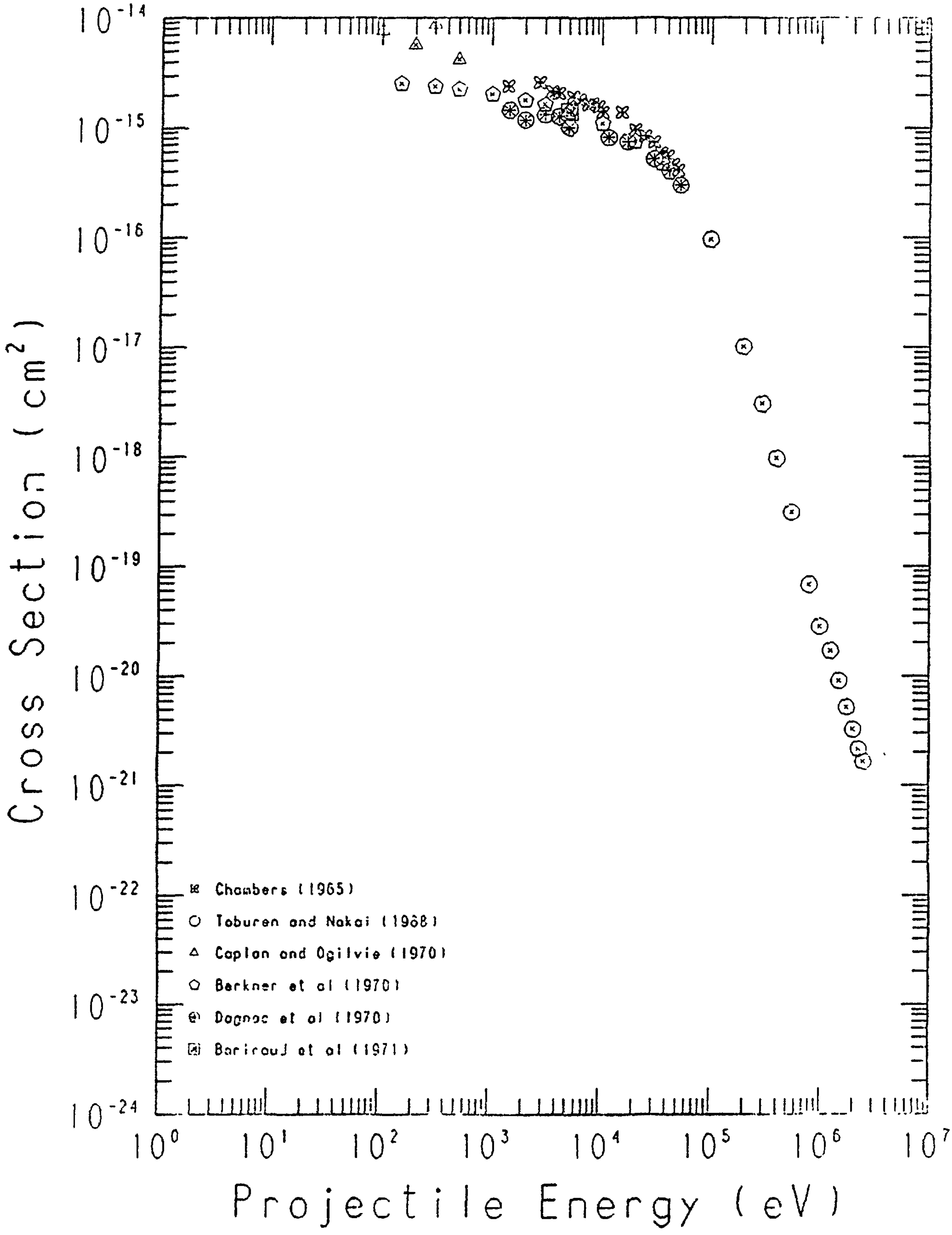
2.3. Computer programs
(a) wavelength tables: completed, also for input data of Grotorian diagrams
(b) Grotorian diagrams: (1982-1983)
(expected preliminary diagram by Data Centre Network Meeting of Nov.)

Above all compiled data are stored in JAERI-Computer FACOM M-200.

An example of 1.1. (a)

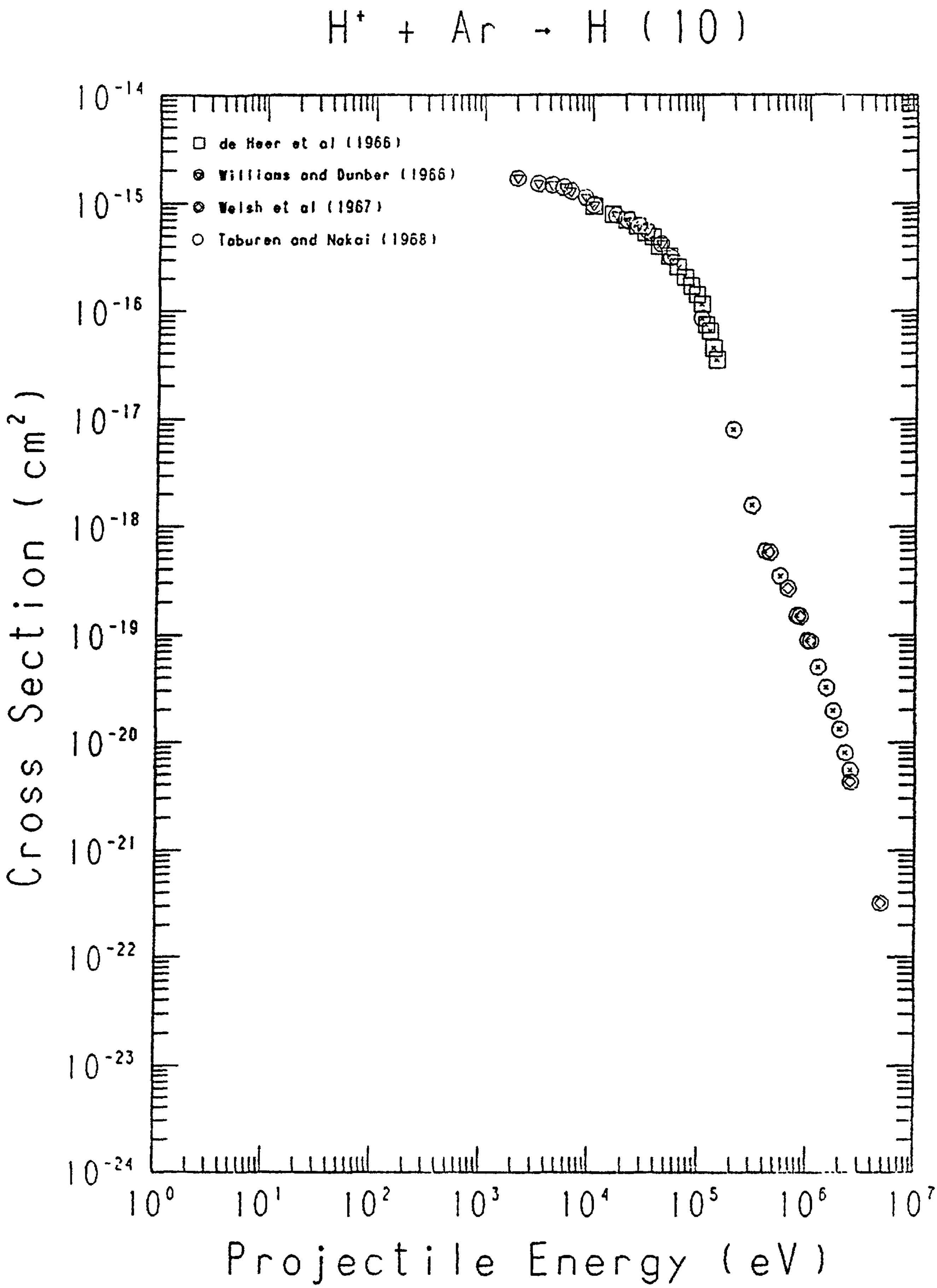
Graph No. 6

$H^+ + H_2O \rightarrow H(10)$



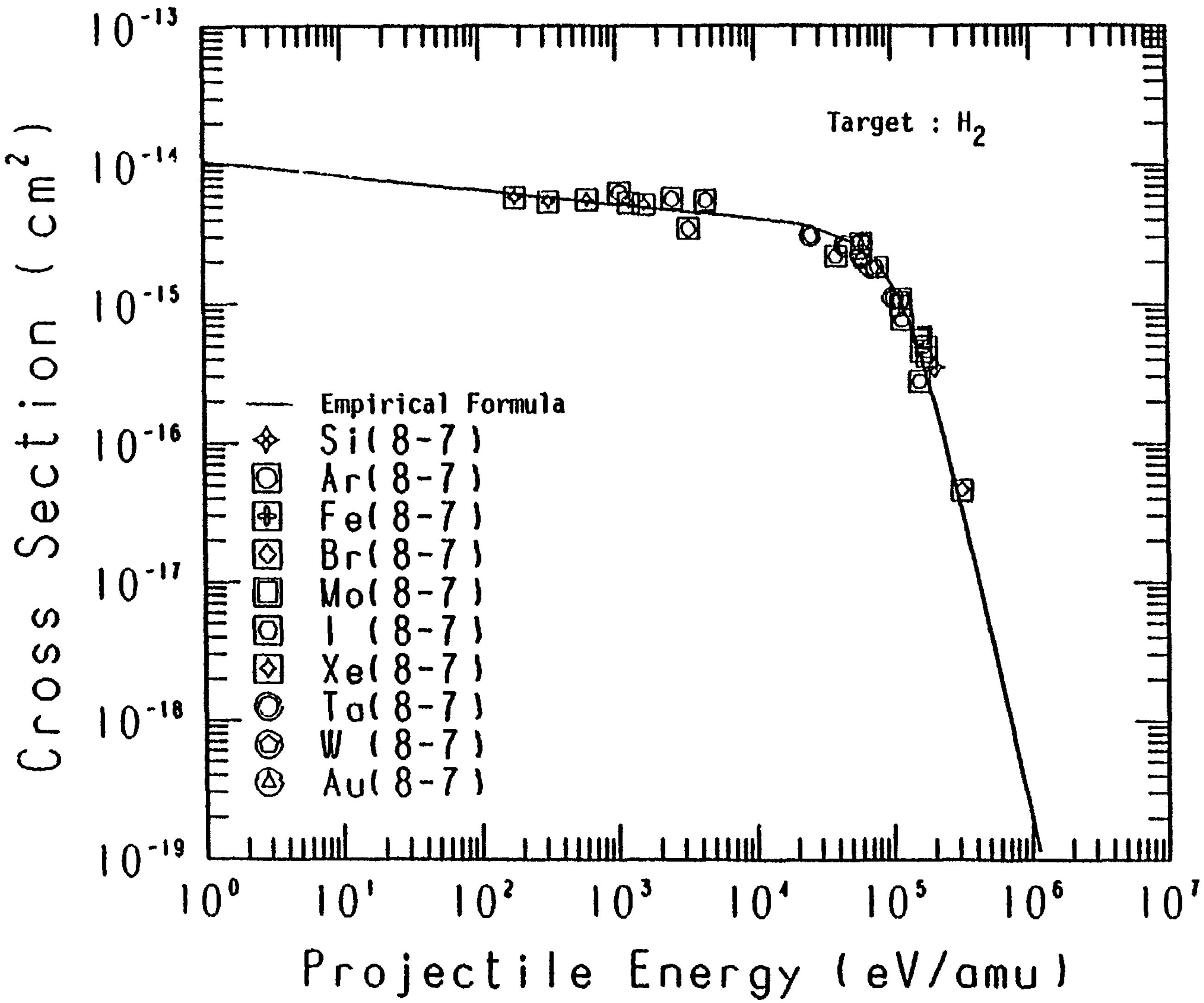
An example of 1.1. (b)

Graph No. 14



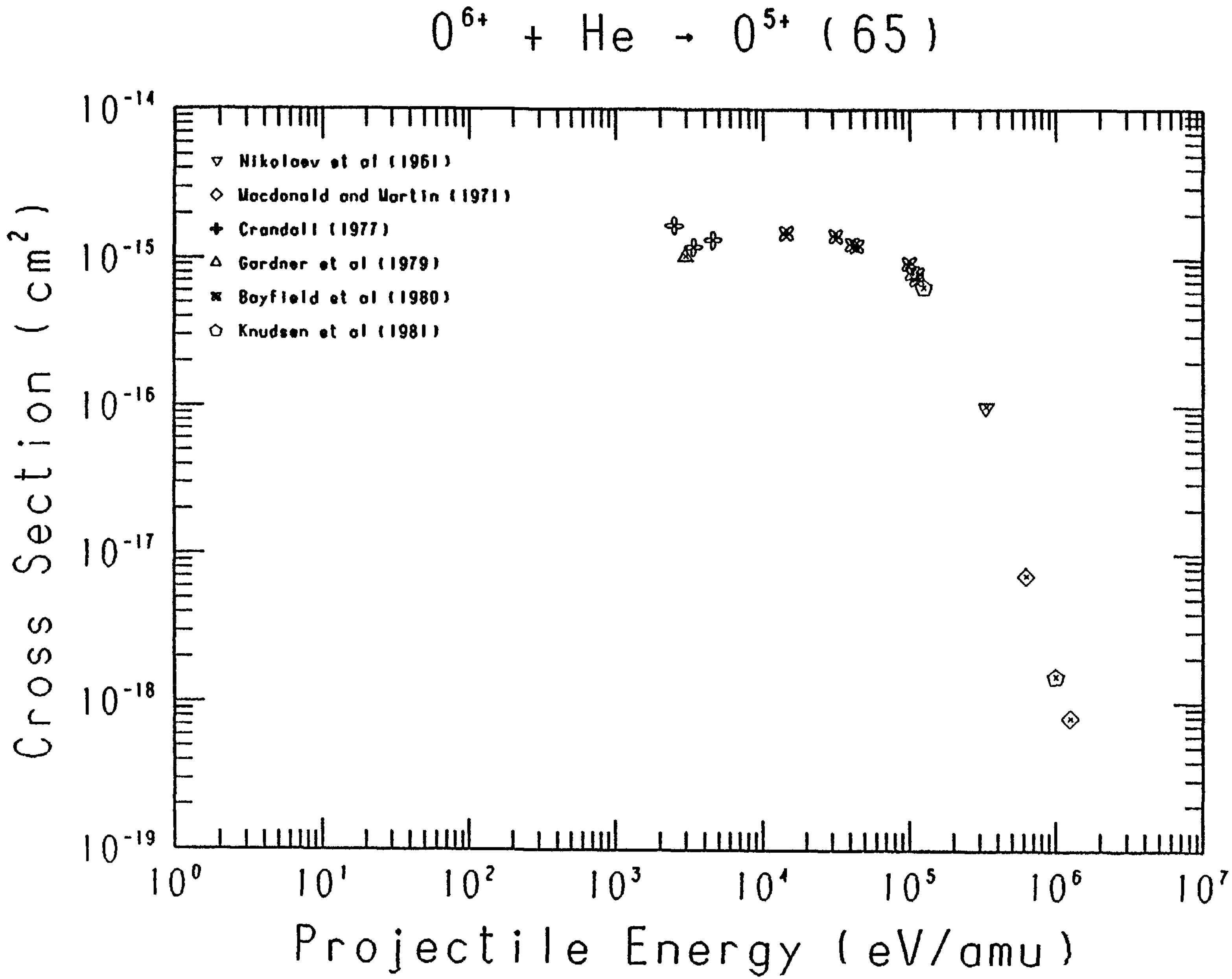
An example of 1.4. Graph No. 8

Sigma(8-7)



An example of 1.5.

Graph No. 7



Examples of 2.1.

Ti XV (O-Sequence) IP = 7597000 cm^{-1} (941·9 eV)

λ (A)	Configuration		Energy level (cm^{-1})		Int	f/Type	A (s^{-1})	Acc	Reference
148·588	$2s^2 2p^4\ ^3P_1$	$2s2p^5\ ^3P^o_2$	39292	712285	500	4·52−2	8·2+9	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 91, 104, 123○
142·750	0	1	42345	742882	250	1·08−1	1·18+10	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 104, 123○
142·130	1	1	39292	742882	200	2·82−2	9·3+9	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 104, 123○
140·395	2	2	0	712285	800	8·3−2	2·81+10	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 104, 123○
138·357	1	0	39292	762060	300	3·92−2	4·10+10	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 104, 123○
134·609	2	1	0	742882	400	3·11−2	1·91+10	C	14*, 38, 81Δ, 86, 104, 123○
189·62[C]	$2s^2 2p^4\ ^1S_0$	$2s2p^5\ ^3P^o_1$	215521	742882		4·3−3	2·7+8	D	86*
131·146	$2s^2 2p^4\ ^1S_0$	$2s2p^5\ ^1P^o_1$	215521	978030	60	6·5−2	8·4+9	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 91, 104, 123○
165·690	$2s^2 2p^4\ ^1D_2$	$2s2p^5\ ^3P^o_2$	108720	712285		3·5−3	8·5+8	D	86*, 123○
115·031	$2s^2 2p^4\ ^1D_2$	$2s2p^5\ ^1P^o_1$	108720	978030	350	1·37−1	1·15+11	C	14*, 24, 38, 50, 53, 56, 81Δ, 82, 86, 104, 123○

Ti XV (O-Sequence) IP=7597000 cm^{-1} (941·9eV)

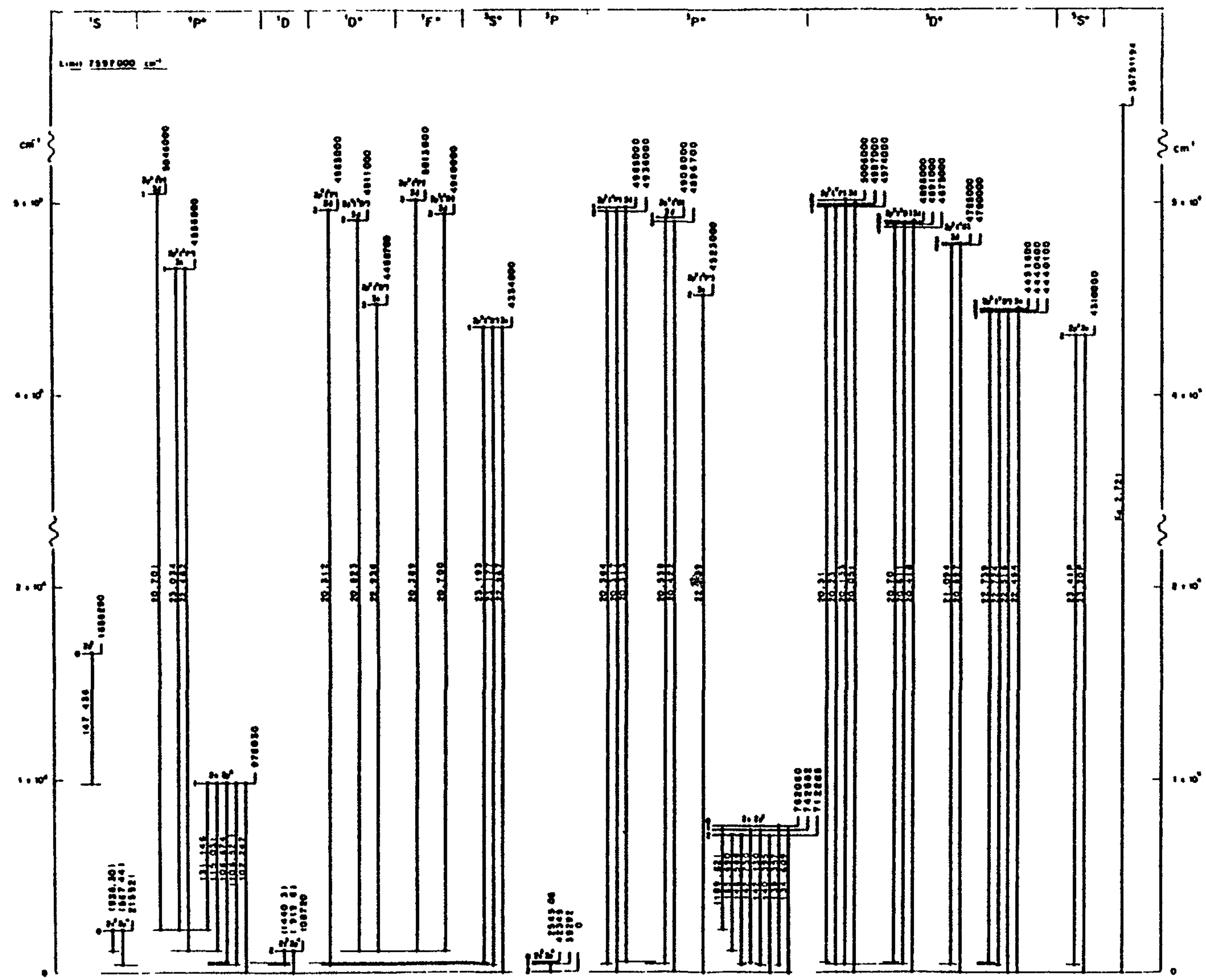
λ (Å)	Configuration		Energy level (cm^{-1})		Int	f/Type	A (s^{-1})	Acc	Reference
106·874	$2s^22p^4\ ^3P_0$	$2s2p^5\ ^1P^o_1$	42345	978030		2·6 3	5·1+8	D	14^{*}, 56 123^{U}
$106·52^{C}$	1	1	39292	978030		3·8-4	2·2+8	E	14^{U*}, 56, 82
102·247	2	1	0	978030		4·8−3	5·1+9	D	14^{*}, 38, 56, 86, 123^{U}
147·436	$2s2p^5\ ^1P^o_1$	$2p^6\ ^1S_0$	978030	1656290	50	1·30−1	1·20+11	C	14^{*}, 26, 38, 52, 53, 56, $81^{\wedge}$, 91, 123^{U}
23·193	$2s^22p^4\ ^3P_0$	$2p^3(^4S^o)3s\ ^3S^o_1$	42345	4354000					23
23·177	1	1	39292	4354000	200				23^{O}, 68 82^{Δ}
22·967	2	1	0	4354000	200				23^{O}, 68, 82^{Δ}
22·109	$2s^22p^4\ ^3P_2$	$2p^3(^2P^o)3s\ ^3P^o_2$	0	4523000	100				68^{O}, 82^{Δ}
22·739	$2s^22p^4\ ^3P_0$	$2p^3(^2D^o)3s\ ^3D^o_1$	42345	4440100					23
22·724	1	2	39292	4440400	200				23^{O}, 82^{Δ}
22·518	2	2	0	4440400					23
22·464	2	3	0	4451600	350				23^{O}, 82^{Δ}
23·034	$2s^22p^4\ ^1S_0$	$2p^3(^2P^o)3s\ ^1P^o_1$	215521	4556800	150				23^{O}, 68, 82^{Δ}
22·482	$2s^22p^4\ ^1D_2$	$2p^3(^2P^o)3s\ ^1P^o_1$	108720	4556800					23
22·936	$2s^22p^4\ ^1D_2$	$2p^3(^2D^o)3s\ ^1D^o_2$	108720	4468700	300				23^{O}, 68, 82^{Δ}
$23·41^{P}$	$2s^22p^4\ ^3P_1$	$2p^33s\ ^5S^o_2$	39292	4310000		8·6−5	6·3+8		78^{*}
$23·20^{P}$	2	2	0	4310000		3·9−4	4·8+9		78^{*}
20·364	$2s^22p^4\ ^3P_1$	$2p^3(^2P)3d\ ^3P^o_2$	39292	4936000					54
20·317	2	2	0	4936000	300				68^{O}, 82^{Δ}
20·313	0	1	42345	4965000					10

Ti XV (O-Sequence) IP = 7597000 cm^{-1} (941·9 eV)

λ (A)	Configuration		Energy level (cm^{-1})		Int	f/Type	A (s^{-1})	Acc	Reference
20·538	$2s^22p^4\ ^3P_1$	$2p^3(^2D)3d\ ^3P^\circ_1$	39292	4908000					10
20·422	$_2$	$_2$	0	4896700	450				10, 68°, 82$^\Delta$
21·094	$2s^22p^4\ ^3P_1$	$2p^3(^4S)3d\ ^3D^\circ_2$	39292	4780000	50				68°, 82$^\Delta$
20·897	$_2$	$_3$	0	4785000	150				54°, 68, 82$^\Delta$
20·31	$2s^22p^4\ ^3P_0$	$2p^3(^2P)3d\ ^3D^\circ_1$	42345	4974000					50, 54°
20·23	$_1$	$_1$	39292	4974000					10°, 91
20·133	$_1$	$_2$	39292	5006000					50, 54°
20·051	$_2$	$_3$	0	4987000	100				50, 54°, 68, 82$^\Delta$
20·70	$2s^22p^4\ ^3P_0$	$2p^3(^2D)3d\ ^3D^\circ_1$	42345	4873000					54
20·611	$_1$	$_2$	39292	4891000					54
20·418	$_2$	$_3$	0	4898000					50, 54°
20·701	$2s^22p^4\ ^1S_0$	$2p^3(^2P)3d\ ^1P^\circ_1$	215521	5046000					10
20·823	$2s^22p^4\ ^1D_2$	$2p^3(^2D^\circ)3d\ ^1D^\circ_2$	108720	4911000	300				54°, 68, 82$^\Delta$
20·389	$2s^22p^4\ ^1D_2$	$2p^3(^2P)3d\ ^1F^\circ_3$	108720	5013000					10, 54°
20·700	$2s^22p^4\ ^1D_2$	$2p^3(^2D)3d\ ^1F^\circ_3$	108720	4940000	200				54°, 68, 82$^\Delta$
20·312	$2s^22p^4\ ^3P_1$	$2p^3(^2P)3d\ ^1D^\circ_2$	39292	4963000					10
2545·08	$2s^22p^4\ ^3P_2$	$2s^22p^4\ ^3P_1$	0	39292		M1	1·27+3	C	14*, 78°, 86
936·30^C	$2s^22p^4\ ^1D_2$	$2s^22p^4\ ^1S_0$	108720	215521		E2	1·4+1	D	14*

Ti XV (O-Sequence) IP=7597000 cm^{-1} (941·9 eV)

λ (A)	Configuration		Energy level (cm^{-1})		Int	f/Type	A (s^{-1})	Acc	Reference
1440·3^{C}	$2s^2 2p^4\ {}^3P_1$	$2s^2 2p^4\ {}^1D_2$	39292	108720		M1	2·44+2	C	14*, 78°, 86
919·8^{C}	$_2$	$_2$	0	108720		M1	2·55+3	C	14*, 78°, 86
567·44^{C}	$2s^2 2p^4\ {}^3P_1$	$2s^2 2p^4\ {}^1S_0$	39292	215521		M1	2·41+4	C	14*, 78*, 86
2·721	K_α								



Ti XV (O- Sequence)

ELECTRON CAPTURE IN LOW ENERGY COLLISIONS OF MULTIPLY CHARGED IONS WITH Li ATOMS

Institut für Allgemeine Physik, Technische Universität Wien

A-1040 Wien, Karlsplatz 13, Austria

Staff involved in the Research Programme (as per July 1, 1982)

H. Winter, F. Aumayr, A. Brazuk, G. Hertenberger, W. Vanek, P. Varga

Aim of Work

Electron capture from Li(2s) into multiply charged ions involves practically only one "active" electron and therefore can be expected to follow similar rules as electron capture from H(1s). Its investigation is therefore of general interest for elucidation of pertinent physical processes.
Additionally, electron capture from Li into multiply charged ions is of interest for several diagnostic schemes for magnetically confined fusion plasmas. Specifically, we have proposed active neutral Li beam probing of the Tokamak plasma edge to measure low-Z and medium-Z ion densities for impurity transport studies /1/.

Experimental Methods

The investigations involve quantitative photon emission spectroscopy (vuv, near-uv and visible spectral region). To account for the influence of long-lived excited (metastable) ion species in initial and final collision products, we have developed several techniques /2/, /3/, /4/, which are applied for the measurements. In the near future a simple translational spectrometer will be incorporated into the experimental setup. Total one-electron capture cross sections are determined by means of the parallel plate condenser technique.

Research Activities

At present, the primary interest is devoted to total and state-selective one-electron capture from Li into low-Z ions. Respective cross section data are compared with empirical calculations and available theory. First results on vuv emission in Ne^{+}/Ne^{2+} collisions with Li(2s) have been obtained /5/. The collision systems C^{q+}/O^{q+} - Li (q = 1, 2, 3,- ion impact energies between 0.5 and 5 keV/amu) are presently studied. For the same species with higher ion charges similar work is planned in cooperation with KVI, University of Groningen, and FOM Institute for Atomic and Molecular Physics (F.J. de Heer and coworkers). This will involve the use of a novel multiply charged ion source of the ECRIS type.

References

1 H. Winter, Comments on Atomic and Molecular Physics (1982, in print)
2 P. Varga and H. Winter, Phys. Rev. A 18, 2453 (1978)
3 A. Brazuk and H. Winter, J.Phys.B:At.Mol.Phys. 15 (1982, in print)
4 H. Winter, Rev. Sci. Instr. 53 (1982, in print)
5 E. Rille and H. Winter, J.Phys.B:At.Mol.Phys. 15 (1982, acc. f. publ.)

The work as described above is supported by Kommission zur Förderung der Kernfusionsforschung in Österreich, Austrian Academy of Sciences, by Austrian Fonds zur Förderung der Wissenschaftlichen Forschung, Projekte Nr. 3593 and 4376, and by International Atomic Energy Agency, Research Contract No. 2497 RB.

ION-ATOM AND ION-ION COLLISION PROCESSES RELEVANT TO FUSION RESEARCH

Department of Pure and Applied Physics
The Queen's University of Belfast

1. STAFF INVOLVED IN ONE OR MORE ASPECTS OF THE PROGRAMME

H B Gilbody, J Geddes, K F Dunn, G C Angel, M B Shah and R W McCullough.

2. SUMMARY OF CURRENT WORK

Ion-atom and ion-ion collision processes directly relevant to supplementary heating, particle escape and energy loss in magnetically confined fusion plasmas are being studied experimentally at energies ranging from ∿ 100 eV to 2500 keV. Collisions between positive ions relevant to schemes to promote heavy-ion fusion are also being investigated.

The programme includes the following measurements.

(a) Charge transfer in collisions with hydrogen atoms

Cross sections for processes of the type

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

are being determined from measurements employing a tungsten tube furnace to provide a target of highly dissociated hydrogen. At velocities $V > 1$ a.u. the results obtained for different ionic species can be described by simple scaling rules according to the charge state q.[1] Measurements are continuing at the lower velocities where simple scaling rules do not apply.

Measurements based on energy loss spectroscopy are being used to study processes of the type

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

involving electron capture into particular excited states. Cross sections for capture into particular states n will be determined in measurements within the range ∿ 100 eV - 30 keV. Measurements with targets other than atomic hydrogen are also being investigated.

(b) Ionisation of hydrogen atoms

Cross sections for the ionisation process

$$X^{q+} + H \rightarrow X^{q+} + H^{+} + e$$

are being determined with high precision using a new technique. A beam of multiply charged ions is arranged to intersect a thermal energy beam of highly dissociated hydrogen. The collision products are selectively recorded by a coincidence counting in conjunction with time-of-flight spectroscopy. Data obtained for H^+, He^{2+} and multiply charged ions of carbon, nitrogen, oxygen[2,3] and lithium[4], is being extended to other species over a wide velocity range and to measurements in H_2 where data on the dissociation and in non-dissociative channels are being separately determined.

(c) Ion-ion collisions

An intersecting beam technique is being used to determine cross sections for processes of the type

$$H^{+} + X^{+} \rightarrow H + X^{2+} \quad \text{charge transfer}$$

$$H^{+} + X^{+} \rightarrow H^{+} + X^{2+} + e \quad \text{ionisation.}$$

Cross sections $\sigma(X^{2+})$ for the production of X^{2+} ions are being determined in the c.m. range 40 - 500 keV. In some cases it is possible to use a coincidence technique to obtain a separate measurement of the charge transfer cross section. Measurements will be extended to processes involving He^{2+} ions which are relevant to alpha particle heating.

Studies are also being carried out of the processes

$$X^{+} + X^{+} \rightarrow X + X^{2+} \quad \text{charge transfer}$$

$$X^{+} + X^{+} \rightarrow X^{+} + X^{2+} + e \quad \text{ionisation}$$

involving species of relevance to heavy ion fusion.

Our measurements are summarised in a recent review[6]. A recent re-measurement of Cs^+ - Cs^+ collisions shows the importance of large angle scattering in the interpretation of experiments involving collisions between heavy ions[7].

(d) Processes relevant to alpha particle diagnostics

Cross sections for the two-electron capture process

$$He^{2+} + Li \rightarrow He + Li^{2+}$$

has recently been determined[8] in the range 5 - 500 keV. The efficiency of neutral Li beam production by the process

$$Li^{-} + X \rightarrow Li + X(\Sigma) + e$$

has also been determined[9] for a variety of targets within the range 100 - 2500 keV.

(e) Processes relevant to neutral H beam diagnostics

Cross sections for the emission of H_α radiation in the passage of H, H^+, H_2^+ and H_3^+ through H_2 are being determined in the range 1 - 100 keV from studies of the 3s - 2p, 3p - 2s, 3d - 2p decay modes following collisional excitation. The separate contributions from the projectile and target have been determined in a recent series of measurements[10].

Total cross sections for collisional destruction of fast H_2, H_2^+ and H_3^+ are also being determined.

PUBLICATIONS

1. Charge transfer and ionisation in collisions with hydrogen atoms. H B Gilbody, Physica Scripta 24, 712-24, 1981.
2. Experimental study of the ionisation of atomic hydrogen by fast H^+ and He^{2+} ions. M B Shah and H B Gilbody, J Phys B 14, 2361-77, 1981.
3. Experimental study of the ionisation of atomic hydrogen by fast multiply charged ions of carbon, nitrogen and oxygen. M B Shah and H B Gilbody, J Phys B 14, 2831-41, 1981.
4. Experimental study of the ionisation of atomic hydrogen by fast lithium ions. M B Shah and H B Gilbody, J Phys B 15, 413-21, 1982.

5. Ionisation of H_2 by fast protons and multiply charged ions of He, Li, C, N and O. M B Shah and H B Gilbody, J Phys B - in course of publication.

6. Collisions between positive ions. H B Gilbody. Invited papers 12th ICPEAC, pp 223-34, North Holland, 1982.

7. Collisions between Cs^+ ions - a further experimental study. P A Neill, G A Angel, K F Dunn and H B Gilbody. J Phys B - submitted for publication.

8. Electron capture by He^{2+} and He^+ ions in lithium vapour. R W McCullough T V Goffe, M B Shah, M Lennon and H B Gilbody. J Phys B, 15, 111-7, 1982.

9. Electron loss by fast Li^- ions. R W McCullough, M B Shah, M Lennon and H B Gilbody. J Phys B 15, 791-5, 1982.

10. Balmer alpha emission in collisions of H, H^+, H_2^+ and H_3^+ with H_2. I D Williams, J Geddes and H B Gilbody. J Phys B 15, 1377-89, 1982.

L82-22930 Appendix 8
Translated from Russian

PROGRESS REPORT ON IAEA RESEARCH CONTRACT 2936/RB

Contract No.: 2936/RB

Title of project: Collision Research in the eV-keV Region (Part of a Co-ordinated Programme on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas)

Institution where the research is carried out: I.V. Kurchatov Institute of Atomic Energy

Chief Scientific Investigator: Professor N.N. Semasko, Doctor of Physico-Mathematical Sciences

Collaborators: V.A. Belyaev, Candidate of Physico-Mathematical Sciences, M.M. Dubrovin, Scientific Officer, and A.N. Khlopkin Scientific Officer

Period covered: Nine months from 1 November 1981

In accordance with the plan of work for the first year of a research contract with the IAEA, starting from 1 November 1981, a number of activities were carried out in the ATOS device [1] to improve the measurement accuracy in determining the effective charge-exchange cross-sections in collisions of hydrogen atoms with multi-charge impurity ions in tokamaks with an energy ranging from a few eV to a few keV per nucleon.

As was shown in Ref. [2], to determine the cross-section, we have to know the values of the parameters entering into the expression

$$\sigma = \frac{\dot{i}_p}{\dot{i}_1 \dot{i}_2} \cdot \frac{s}{L} \cdot \frac{v_1 v_2}{v} = K \frac{\dot{i}_p}{\dot{i}_1 \dot{i}_2} \cdot \frac{s}{L} \cdot \frac{\sqrt{E_1 E_2}}{\sqrt{T}} \quad . \tag{1}$$

Here i_1, i_2 and i_p are the beam intensities of atoms, ions and newly formed particles (current created by the newly formed particles) in particles per second, s is the cross-section of the atom beam (fully enclosing the ion beam) in cm^2, L the length of the beam interaction region in cm, $v_1(E_1)$ and $v_2(E_2)$ are the velocities (energies) of atoms and ions in cm/s (eV/nucleon), v(T) is the relative velocity (collision energy) of atoms and ions in cm/s (eV/nucleon).

The error in the value of the cross-section measured is associated with the uncertainty of all the quantities contained in the expression given above:

$$\frac{\Delta\sigma}{\sigma} = \frac{\Delta i_p}{i_p} + \frac{\Delta i_1}{i_1} + \frac{\Delta i_2}{i_2} + \frac{\Delta S}{S} + \frac{\Delta L}{L} + \frac{1}{2}\cdot\frac{\Delta E_1}{E_1} + \frac{1}{2}\cdot\frac{\Delta E_2}{E_2} + \frac{1}{2}\frac{\Delta T}{T} \qquad (2)$$

Analysis shows that the most substantial contribution to $\Delta\sigma/\sigma$ is made by two terms in this expression: the first and the last.

In order to evaluate the last term, we will consider that the collision energies lie in the range [2]:

$$(\sqrt{E_1} - \sqrt{E_2})^2 \leqslant T \leqslant (\sqrt{E_1} - \sqrt{E_2})^2 + \varphi^2\sqrt{E_1 E_2} ,$$

where ϕ is the largest possible angle of intersection between the trajectories in the combined beams ($\phi \ll 1$). Taking the following as the average value

$$T = (\sqrt{E_1} - \sqrt{E_2})^2 + \frac{1}{2}\varphi^2\sqrt{E_1 E_2} .$$

we can re-write the last term in expression (2) in the form

$$\frac{1}{2}\frac{\Delta T}{T} = \frac{1}{2}\sqrt{\frac{E_1}{T}}\frac{\Delta E_1}{E_1} + \frac{1}{2}\sqrt{\frac{E_2}{T}}\cdot\frac{\Delta E_2}{E_2} + \frac{1}{4}\varphi^2\frac{\sqrt{E_1 E_2}}{T} .$$

Thus the minimum collision energy attainable under the conditions of a specific experiment is equal, in the case of strictly monoenergetic beams, to $T_{min} = \phi^2 E/2$ (here $E = E_1 \approx E_2$) and has a 100% uncertainty, contributing thereby 50% to the error in σ.

In the ATOS device the value of T is varied in each measurement cycle by slowing down the ions at the entry to the collision chamber; this reduces E_2 while E_1 remains unchanged. The minimum values of T are obtained when the slowing-down is minimum but not zero, since in order to cut off the background current of protons originating from hydrogen atom stripping in the residual gas outside the collision chamber, a slowing-down potential is always applied to the latter. The resulting debunching of the ion beam prevents the angle ϕ being reduced below $\approx 1^{\circ}(0.02)$.

Hence, to obtain $T_{min} = 1$ eV/nucleon the energy E of particles in the beam should not exceed 5×10^3 eV/nucleon. The energy E has naturally to be made still smaller in order to reduce ΔT and $\Delta\sigma$.

The above considerations relate to the case of strictly monoenergetic beams. The presence of the energy spreads ΔE_1 and ΔE_2 leads to an increase in ΔT and $\Delta\sigma$ so that the greatest contribution to the error $\Delta\sigma/\sigma$ will be made, in our case, by the term $\frac{1}{E}\sqrt{\frac{E_2}{T}} \cdot \frac{\Delta E_2}{E_2}$; this is due to the difference in the degree of energy spread of the beams in the ATOS device: $\Delta E_1 = \pm 0.5\%$, $\Delta E_2 = \pm 2\%$ [3]. Here, too, it is more advantageous to perform measurements at lower values of E.

The reductions necessary (from the above considerations) in the beam particle energy can be made either by slowing down the multi-charge ions at the collision chamber input and protons at the neutralization chamber input or by reducing the beam particle energy during shaping of the beam by the ion source lens systems. In either case the decrease in particle energy can lead to a fall in the intensity of the interacting beams and consequently to a drop in the newly found particle current. As a result, there will be an increase in the measurement time, influencing the value of the first term in expression (2). Let us consider this problem in more detail.

It follows from expression (1) that the reduction in E_1 and E_2 at the given values of the remaining terms in the expression also contributes to an increase in current i_p, thereby reducing the measurement time required to obtain the given measurement error $\Delta i_p/i_p$. In order to evaluate the expected value of this error, let us consider that when we record i_p, we also record at the same time the background proton current i_b formed as a result of hydrogen atom stripping in the residual gas in the collision chamber. The value i_p is determined as the difference between the two measurements: $i_p = I - i_b$, where $I = i_p + i_b$ is the whole current recorded by the detector. (For measurement of i_b the ion beam is switched on.) Under the conditions of measurement in the ATOS device expression (1) can be written in the form

$$i_p \approx 4 \cdot 10^{32} i_1 i_2 \sigma \frac{\sqrt{T}}{E} \tag{3}$$

and the background current will equal (see Ref. [1])

$$i_b \approx 4 \cdot 10^{19} i_1 \sigma_c n \tag{4}$$

where n is the residual gas density in the region of the collision chamber, σ_o the hydrogen atom stripping cross-section in the residual gas. (In these expressions i_1 and i_2 are given in amperes, while i_p and i_b are given in particles/s.) Since $i_b >> i_p$, $\Delta i_p = \Delta I + \Delta I_b \approx 2\Delta i_b$. Hence

$$\frac{\Delta i_p}{i_p} \approx \frac{2\Delta i_b}{i_p} \approx \frac{2\sqrt{i_b t}}{i_p t} \approx 6\cdot 10^{-15}\frac{E}{i_2 \sigma}\sqrt{\frac{\sigma_o P}{i_1 T t}}$$

with the strongest dependence on the multi-charge ion current i_2 and energy E. (P is the residual gas pressure in mmHg and t is the measurement time in seconds.)

By improving the ATOS ion-optic channel of the multi-charge ion beam and the ion-source lens system and redesigning the ion-optic system for slowing down protons at the neutralization chamber input, we produced in the collision chamber stable currents of multi-charge ions sufficient for systematic measurements of σ (see Table 1). The equivalent hydrogen atom current for E_1 = 400 eV passing through the collision chamber is 5×10^{-7} A. The value of 400 eV/nucleon was chosen as optimal for $E_1 \approx E_2$ (where this is allowed by the ratio of masses of the colliding particles) on the basis of measurements for $T \approx 1$ eV/nucleon.

Hydrogen atoms with an energy of 400 eV were obtained by neutralizing the 5-keV protons after they had been slowed down at the neutralization chamber input, while multi-charge ions were obtained by slowing down at the collision chamber input. Considering that $\Delta E_1/E_1 = \pm 0.005$ and $\Delta E_2/E_2 = \pm 0.02$, we find that the contribution of the terms depending on particle energy (the last three terms in expression (2)) to $\Delta\sigma/\sigma$ at T = 1 eV/nucleon is about $\pm$ 30%. (If T is increased to 10 eV/nucleon, the error drops to $\pm$ 10%.)

Substituting into the expression for $\Delta i_p/i_p$ the values $\sigma_o \approx 2 \times 10^{-17}$ cm^2 and $\sigma \approx 1 \times 10^{-14}$ cm^2 [4], $P \approx 2 \times 10^{-9}$ mmHg, $i_1 \approx 5 \times 10^{-7}$, $i_2 \approx 2 \times 10^{-8}$, we obtain for T = 1 eV/nucleon and the measurement time 2 t = 2000 s the value of $\pm$10%. (For T = 10 eV/nucleon we shall accordingly have about 3%.)

Thus the maximum error $\Delta\sigma/\sigma$ in the forthcoming measurements for T = 1 eV/nucleon is expected to be about $\pm$ 40%, decreasing approximately in inverse proportion to the square of the collision energy T.

The remaining three months of the first year of the contract will be devoted to improving the system of determining the absolute intensity of the particle beams passing through the collision chamber so as to minimize the possibility of systematic errors resulting from the need to compare the coefficients of secondary electron emission from the protons and hydrogen atoms when their energy and the degree of purity of the detector plate surface vary.

CONCLUSIONS

In view of the improvements made in the ion-optic and the recording systems of the ATOS device during the first nine months of IAEA Research Contract 2936/RB, and on the basis of analysis of the preliminary experimental results and the possible sources of measurement error, we can affirm that in the forthcoming measurements of charge-exchange cross-sections during collisions by hydrogen atoms with the multi-charge ions of the impurity elements in tokamaks, the maximum error of these measurements for a collision energy of 1 eV/nucleon will be about ± 40%, decreasing approximately in inverse proportion to the square of the collision energy.

REFERENCES

[1] V.A. Belyaev, A.P. Dorovskij, M.M. Dubrovin, A.N. Khlopkin, Report INDC(CCP)-152/GA, IAEA, Vienna, Austria, August, 1980.

[2] BELYAEV, V.A., BREZHNEV, B.G., ERASTOV, E.M., Zh. Eksp. Teor. Fiz. 52, (1967) 1170.

[3] BELYAEV, V.A., DOROVSKIJ, A.P., DUBROVIN, M.M., LAZAREVA, G.A., SOKOLOV, N.I., TERESHKINA, A.G., KHLOPKIN, A.N., SHUROV, O.A., Report IAEh-3363/7, Moscow (1980).

[4] Y. Kaneko, T. Arikawa, Y. Itikawa, T. Iwai, T. Kato, M. Matsuzawa, Y. Nakai, K. Okuno, H. Ryufuku, H. Tawara, T. Watanabe, Preprint, IPPJ-AM-15, Nagoya, Japan, 1980.

Table 1. Multi-charge ion current in microamperes in the ATOS collision chamber for different elements and ion charges

	Ion charge								
	2	3	4	5	6	7	8	9	IO
Ar	0,30	0,40	0,02	0,03	0,I2	0,0I	0,008	0,0I	
Xe	0,04	0,I0	0,04	0,02	0,008	0,008	0,02	0,0I	0,0I
Fe	0,I2	0,08	0,0I	0,02	0,02	0,0I	0,02		
Mo	0,0I	0,02	0,0I		0,02				
Ta	0,0I				0,03				
C	0,04	0,03							

(signed) V.A. Legasov
Academician
Deputy Director, I.V. Kurchatov Institute of Atomic Energy

(signed) N.N. Semasko
Professor, Doctor of Physico-Mathematical Sciences
Chief Scientific Investogator

INFLUENCE OF CHARGE EXCHANGE AND FAST IONS ON IMPURITY RADIATION IN A HOT PLASMA

V.A. Abramov, V.G. Gontis and V.S. Lisitsa
I.V. Kurchatov Institute of Atomic Energy
Moscow, 1982

Currently almost all work on calculating the radiation losses of a thermonuclear plasma in the presence of impurities (see, for example, Refs [1-3]) takes into account only the excitation of multiply charged impurity ions by electrons (below we shall consider only line-radiation losses); the contribution of heavy particles (e.g. protons) to establishment of an ionization balance and to ion excitation is tacitly assumed to be small. This is in fact valid for ionization processes involving multiply charged ions and for the excitation of transitions in which the principal quantum number changes ($\Delta n \neq 0$). Where transitions with $\Delta n = 0$ are concerned, the situation may be just the reverse. In fact, if the values given in Ref. [4] of the cross-sections for excitation by electrons and protons in the case of the Li-like iron ion (Fe XXIV) are used, it is easily seen that the quantities $K_e = \langle v\sigma_e \rangle$ and $K_i = \langle v\sigma_i \rangle$ are equal at a temperature $T = T_e = T_i \cong 2$ keV. As the temperature is increased, K_i continues to grow (while K_e falls), and at $T = 10$ keV K_i exceeds K_e by almost an order of magnitude. Under coronal balance conditions this increase in the rate of ion excitation by heavy particles is compensated to some extent by a reduction, as T_e increases, in the proportion of complex ions having transitions with $\Delta n = 0$ (ion "burn-up"). We shall show, however, that even under conditions where the standard coronal model is applicable allowance for excitation of iron ions by protons leads to a 30% increase in radiation losses in the region $T_e = T_i = 2$ keV. These effects are even more distinct in the case of heavier elements (Mo, W), for which the "burn-up" of complex ions takes place at higher temperatures; a temperature range in which the effect of excitation by protons can appear therefore exists in a thermonuclear plasma.

The role of excitation by protons (deuterons) shows up particularly clearly when the ionization balance of the impurities deviates from a coronal balance. The reasons for such a deviation in a tokamak plasma may be diffusion of the impurities or charge exchange between the impurities and atoms of neutral hydrogen (either residual or introduced into the plasma for supplementary heating) [5]. The radiation losses of a plasma under non-equilibrium conditions are conveniently characterized by the power of radiation $Q(T,T + \Delta T)$ (in terms of one electron and one impurity ion) calculated for the ionization balance existing at a temperature T and for excitation rates K_e and K_i at a temperature $T + \Delta T$. Figure 1 shows the relative increase $R \equiv Q(T,T + \Delta T)/Q(T + \Delta T,o)$ in the radiation losses of a plasma with an iron impurity as a function of T for different degrees of non-equilibrium (magnitude of the parameter $\Delta T/T$). Figure 2 shows the contribution of excitation by protons, which is seen to be dominant. Figure 3 shows the contribution of excitation by protons at different concentrations of neutral atoms. Note that the given situation may occur in almost pure form in the case of sufficiently fast adiabatic compression of the plasma, in which there is no change in the distribution by degrees of ionization for Li-, Be- and B-like ions of the elements with $Z > 20$ within the particle temperature rise time.

In connection with the use of beams of fast neutral particles for plasma heating a great deal of attention has been paid in recent years to the study of non-equilibrium states due to charge exchange between impurities and atomic hydrogen [5–7]. It has been shown that the radiation losses may increase sharply under these conditions, but only if excitation by electrons is taken into account. Taking the excitation by protons into account must substantially enhance this effect. For this reason we calculated the radiation losses for a plasma containing nickel as an impurity (the effect will obviously be similar for all elements of the iron group), taking into account the shift in ionization balance due to charge exchange and excitation of transitions with $\Delta n = 0$ by protons. It was assumed that the parameter $\xi = \frac{n_o}{n_e}$ was equal to 10^{-5} (n_o being the hydrogen atom density and n_e the electron density). The cross-sections for excitation by protons were taken in the form proposed in Ref. [4]. The calculations indicate that for $T_e = T_i = 10$ keV, for instance, the radiation losses are increased by a factor of about 24. If only electron excitation is taken into account, the losses due to the change in ionization balance increase by only a factor of 3.5, i.e. the contribution of excitation by protons is about six times higher than that of excitation by electrons.

The excitation of impurities by heavy particles can also affect the energy losses of fast heavy particles in the plasma, formed by the beam used for plasma heating. In order to assess the importance of these effects let us compare the rate of energy loss $\frac{d\varepsilon}{dt}$ by a fast particle of mass M and energy ε in a plasma with a temperature $T = T_e = T_i$ through Coulomb collisions $(\frac{d\varepsilon}{dt})^{Coul}$ and through impurity excitation $(\frac{d\varepsilon}{dt})^{imp}$ with a given (e.g. average) charge Z and a concentration $c_Z = n_Z/n_e$. The ratio γ of the two quantities under the conditions typical of beam heating $(\frac{\varepsilon}{T}\frac{m_e}{M}) << 1,\ \frac{\varepsilon}{T} >> 1)$ is easily found by means of the expressions for $(\frac{d\varepsilon}{dt})^{Coul}$ given in Ref. [8]:

$$\gamma \equiv \left(\frac{d\varepsilon}{dt}\right)^{\text{кул}} \Big/ \left(\frac{d\varepsilon}{dt}\right)^{\text{имп}} = \lambda \frac{n_e}{n_Z f} \frac{m_e}{M}\left[\frac{2M}{m_i} + \frac{8}{3\sqrt{\pi}}\left(\frac{M}{m_e}\right)\left(\frac{m_e}{M}\frac{\varepsilon}{T}\right)^{3/2}\right] \quad (1)$$

where f is the oscillator strength of a transition with $\Delta n = 0$ for an ion with charge Z.

The quantity γ for conditions typical of a thermonuclear reactor ($T_e = T_i \approx$ 10-20 keV, $n_Z/n_e \leq 10^{-3}$) is usually large when excitation by deuterons and α-particles is taken into account. It is clear, however, that γ falls sharply as the fast-particle velocity decreases, and therefore the ion excitation effect may be stronger when the total energy losses of a fast particle in the plasma are calculated, i.e. it is possible for the profile of power input into the plasma, which is currently calculated without taking the influence of impurity ion excitation into account, to change. In addition, the parameter γ may be close to unity for some contemporary devices in which neutral injection is used for supplementary plasma heating. For instance, in the plasma of the T-11 tokamak ($T_e \sim T_i \sim$ 0.5 keV, $n_e = 3\text{-}5 \times 10^{13}$ cm^{-3}) the typical impurity ions are Mo XXV ($f_{nn'} \sim 1.5$) with a concentration $c_Z = 3 \times 10^{-3}$. At an atom energy ε = 20 keV a considerable proportion of the power input may be wasted on impurity excitation. This effect may also increase because of light impurities in the case of an abrupt shift in their ionization balance resulting from charge exchange with the atoms in the beam.

Thus the foregoing discussion shows that it is now necessary to know the cross-sections for processes of heavy-particle excitation of transitions with $\Delta n = 0$. The calculations performed for the present work are based on the cross-section values given in Ref. [4]. The authors are not aware so far of any experimental data on the cross-sections for such processes. A comparison of the data from Ref. [4] with the results of calculations of the cross-sections based on the model used in Ref. [9] shows that there is a considerable discrepancy in the calculation data (up to one order of magnitude). The authors' calculations of the cross-sections on the basis of the linear trajectory model without the dipole approximation (which was used in Ref. [4]) leads to the following expression for excitation by protons of the transition 2s-2p in a Li-like ion:

$$\sigma_{a.e.} = 4\pi \left(\frac{e^2}{\hbar v} \right)^2 \left(\frac{v}{\omega} \right)^2 f \left(\frac{\omega R_0}{v} \right) \tag{2}$$

where

$$f(\alpha) = \int_0^\infty \frac{dx}{(1+x)^2} \sin^2\left(\sqrt{1+x}\,\alpha\right) \tag{3}$$

$R_o \approx \frac{n^2}{Z}$, ω is the frequency of the transition 2s-2p, and v is the proton velocity. Calculations for specific ions following Eq. (2) give cross-section values lying between the results of Refs [4] and [9], although somewhat closer to those of Ref. [9]. At high energies, however, the accuracy of the linear trajectory model is open to doubt. Hence only the performance in the immediate future of experiments to determine cross-sections for excitation by heavy particles of transitions with $\Delta n = 0$ can provide reliable information and thereby make it possible to establish the importance of the effects discussed above.

REFERENCES

[1] GERVIDS, V.I., KOGAN, V.I., Preprint IAEh-2722 (1976).

[2] Post D.E et al. Atomic and Nuclear Data Tables, 20, 397 (1977).

[3] C. Breton et al. Nucl. Fusion I6, 89I (1976).

[4] BAZYLEV, V.A., CHIBISOV, M.I., Preprint IAEh-3125 (1979).

[5] ABRAMOV, V.A., et al., Pis'ma Zh. Ehksp. Teor. Fiz. 29 (1979) 550.

[6] ZHIDKOV, A.G., et al., Fiz. Plazmy 7 (1981) 443.

[7] J.D. Callen et al., Proceedings of the VIII Intern. Conf. Plasma Phys. Contr. Nucl. Fusion Research, v. 1, p. 775 (1981)

[8] TRUBNIKOV, B.A., in Vopr. Teor. Plazmy, 1, Atomizdat (1973) 98.

[9] VINOGRADOV, A.V., et al., Tr. Fiz. Inst., Akad. Nauk SSSR 119 (1980) 120.

FIGURE CAPTIONS

Fig. 1. Temperature dependence of R.

Fig. 2. Temperature dependence of the contribution of excitation by protons.

Fig. 3. Temperature dependence of the contribution of excitation by protons, taking charge exchange into account (I - $\xi = \frac{n_o}{n_e}$ = 10^{-6} ; 2 - ξ = 3.10^{-6}, 3 - ξ = 10^{-5} ; 4 - ξ = 3.10^{-5} ; 5 - ξ = 10^{-4}).

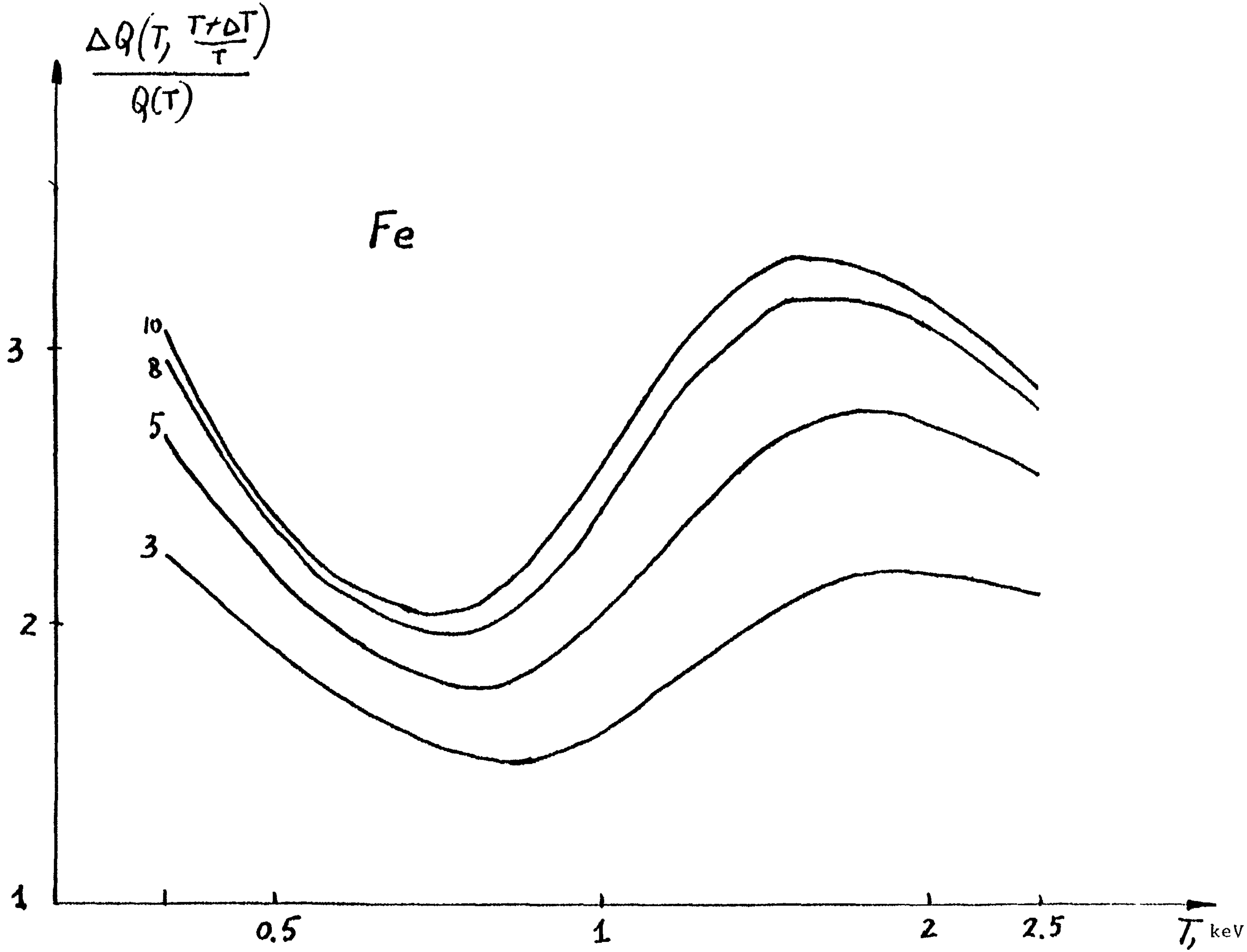


Fig. 1

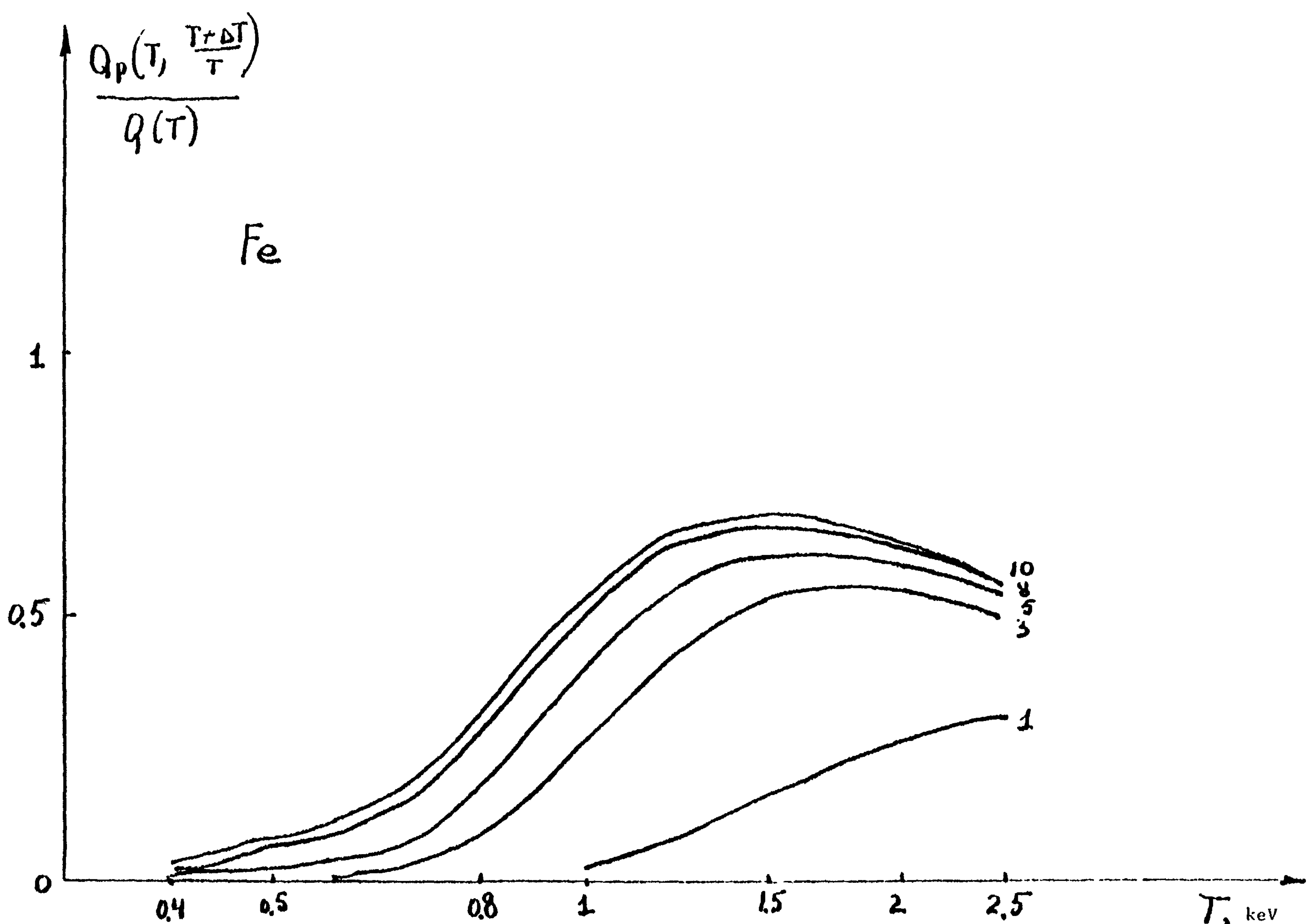


Fig. 2

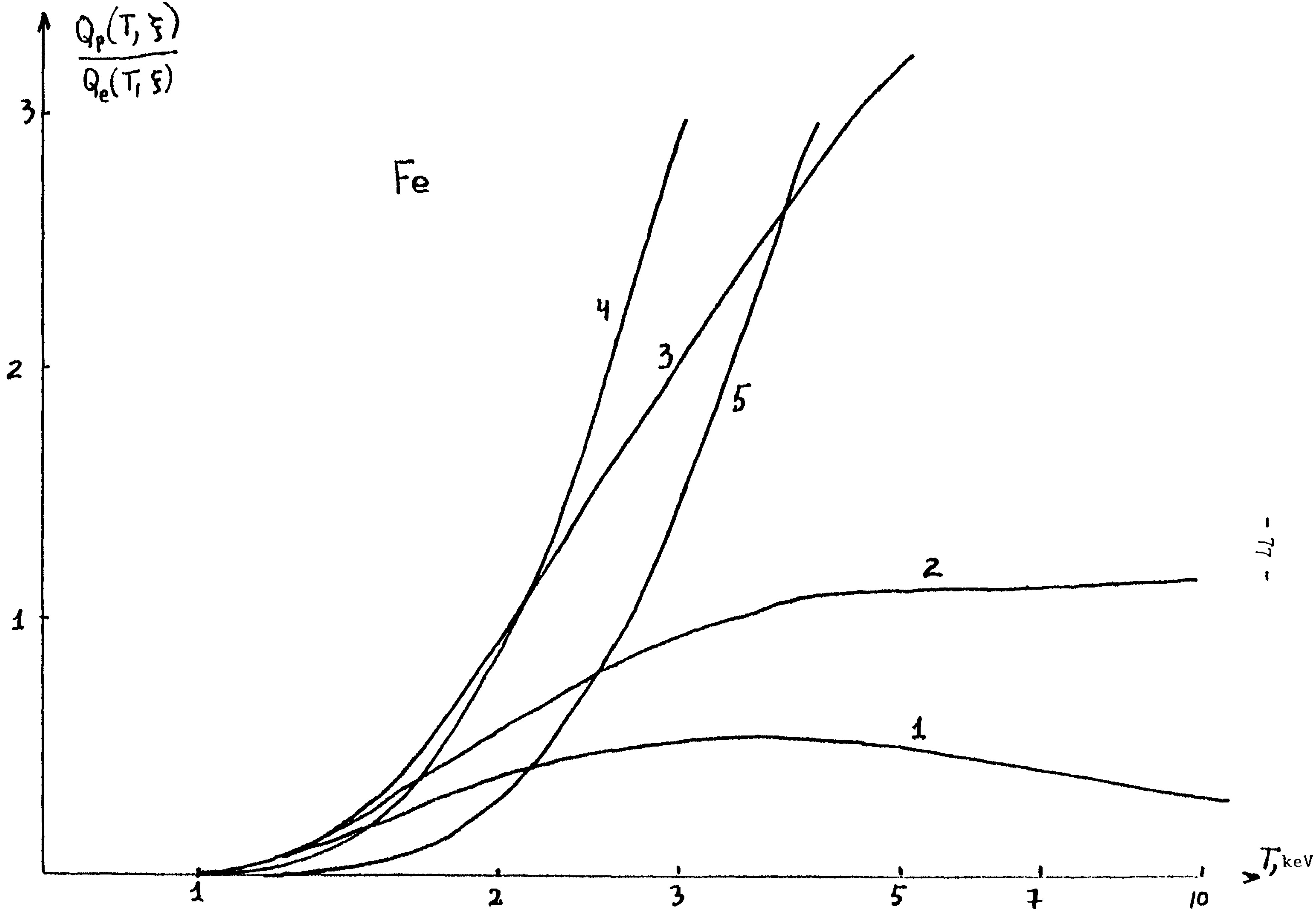


Fig. 3

Appendix 10

Atomic Processes Relevant to Fusion Research

Mathematics Department
Royal Holloway College
(University of London)

1. Staff involved

M.R.C. McDowell, M. Zarcone, S. Nuzzo, M. Gargaud.

2. Current work

a) Evaluation and preparation of electron impact excitation cross section data for atomic hydrogen and helium. A report [1] on data on atomic hydrogen has been produced (in collaboration with Prof. J. Callaway, Luisiana State University). The work on helium is being carried out in collaboration with Dr. A.E. Kingston and others at the Queen's University, Belfast.

b) Classical trajectory Monte-Carlo calculations of electron loss by H atoms colliding with positive ions.

The CTMC models developed by Olson have been generalized to allow the use of model potentials for the ionic electrons. Calculations are in progress for $H - Li^+$, $H - Ar^+$, $H - Ar^{++}$ initially. This work is in collaboration with Dr. G. Peach (University College, London). The model potentials are obtained by fits to the observed spectrum, of the form

$$V(r) = -\frac{q}{r} - \frac{Z}{r}(1 + \delta_1 r + \delta_2 r^2)\, e^{-\gamma r} - \frac{\alpha_d}{2r^4} W_Z(\beta r)$$

where α_d is the static dipole polarizability, $W_Z(X)$ is a cut-off function, and δ_1, δ_2, and β are fitting parameters.

3. Future work

It is intended to undertake detailed close-coupling plus correlation calculations of electron impact excitation of neutral and once ionized carbon and oxygen, starting in October 1982.

REFERENCE

1. J. Callaway and M.R.C. McDowell "What we know and do not know about excitation of atomic hydrogen", submitted in Comm. Atom. Mol. Phys. 1982.

Appendix 11

"Theoretical Study of Charge Exchange, Ionization and Electron Loss-Processes, relevant to Controlled Thermonuclear Research"

R.K. Janev
Institute of Physics, Belgrade, Yugoslavia

1. Capture into excited states hydrogen collisions with highly charged ions

Partial cross sections σ_n and $\sigma_{n\ell}$ for electron capture into specific final principal shells (n) or specific final states (nℓ) in low energy (E $\leq$ 25 keV/amu) collisions of hydrogen atoms with completely stripped ions have been calculated using the multichannel Landau-Zener model, which takes rotational transitions into account. The energy range considered was: 10^{-2}-10^{2} keV/amu. The following completely stripped ions were included in the calculations: Z = 5-10, 13, 14, 18, 19, 20, 22, 24, 26, 29, 30, 36, 40, 42, 54 and 74.

Publications:

1. R.K. Janev, D.S. Belic.
   Final state distributions in the low-energy electron capture reactions of hydrogen atoms with fully stripped ions.
   Phys. Rev. A. (1982, submitted)

2. D.S. Belic, B.H. Bransden, R.K. Janev.
   Total and partial cross sections for electron capture in collisions of hydrogen atoms with completely stripped ions.
   Phys. Rev. A (1982, submitted)

3. R.K. Janev.
   Excited states created in charge transfer collisions between atoms and highly charged ions.
   Physica Scripta (1982, to be published)

2. Ion - Ion collision processes

Charge transfer processes in the low energy ion-ion collisions have been investigated in order to identify their role as a competitive "excitation" and/or "ionization" mechanisms with regard to the corresponding electron-impact processes. Specifically, the resonant two-electron capture and the quasi-resonant one-electron capture were considered.

1. Publications:

R.K. Janev, D.S. Belic.
Double resonant charge exchange in ion-ion collisions.
Phys. Lett. 89A 190 (1982)

2. R.K. Janev, D.S. Belic.
   Quasi-resonant charge exchange collisions between multiply charged ions
   J.Phys. B (1982, in press)

3. Rotational transitions in close ion-atom collisions

The problem of rotationally induced transitions in close ion-atom collisions is treated within the united-atom approximation. The three-state problem ($\sigma \rightarrow \pi, \delta$ transitions) is studied in more details. Trajectory effects (Coulombic or straight-line) has been investigated by using the example of $3d\sigma \rightarrow 3d\pi$, $3d\delta$ transitions, contributing to the $Li^{3+} + H$ $Li^{2+} + H^{+}$ charge-exchange reaction. Transition probabilities as a functions of impact parameter (and center-of-mass scattering angle) has been calculated as well as the corresponding cross sections.

Publication:

T.P. Grozdanov and E.A. Solov'ev
Rotationally induced transitions in close encounters of one-electron collisional systems. The three-state problem.
J.Phys. B (Submitted)

4. Cross section data evaluation

The exciting theoretical cross section data for charge exchange in collisions of hydrogen atoms with multiply charged ions (those which are of direct relevance to magnetic fusion research) have been evaluated. The energy range analyzed was 10 eV to 1 MeV/amu. General criteria for the evaluation of the theoretical data, produced by the methods so far developed, are established. Recommended theoretical charge exchange cross sections for all the considered collision partners are collected.

Publication:

R.K. Janev, P.H. Bransden.
Charge exchange between highly charged ions and atomic hydrogen:
A critical review of theoretical data.
To be published by the IAEA-NDS.

Appendix 12

SUMMARY OF ACTIVITIES ON ATOMIC DATA FOR FUSION AT ORNL, PHYSICS DIVISION

D. H. Crandall, R. A. Phaneuf, F. W. Meyer, D. C. Gregory,
P. M. Griffin, C. F. Barnett, J. W. Hale, H. J. Kim,
C. Bottcher, and consultants specified in this abstract

We have a wide variety of activities in basic experimental and theoretical studies of atomic collisions and in compilation and evaluation of atomic data — all directed at specific fusion interests.

The Controlled Fusion Atomic Data Center is specifically collaborating with IPP-Nagoya, Japan, data center to provide recommended cross sections and rates for excitation of $\Delta n=0$ and $\Delta n=1$ transitions of all ions of C and O. This work is nearly complete and will be part of the present IAEA coordinated research program. This is only part of our longer term effort to update and extend the "Redbook," ORNL-5206 and -5207,[1] which tabulate recommended data for fusion. The principle data missing from the Redbooks is the impurity collisions data which will be included for at least primary impurity species in the new compilations.

Experimental research concentrates on collisions of multicharged ions with atomic hydrogen and with electrons. Experiments on hydrogen employ either a dissociation oven-gas cell type target or neutral beams of H formed by electron capture from H^+ or by detachment from H^-. These H sources are used in conjunction with various sources of multicharged ions — laser ion source,[2] ORNL-PIG,[3] an E-N Tandem,[4] and a planned ECR-type source. Experiments on total electron capture have spanned collision energies from MeV[4] to 10's of eV[5] and are in preparation for energies down to 1 eV. Additional experiments on total electron removal[6] from H and on electron capture to specific final states[7] are pursued.

Electron-multicharged-ion experiments are pursued at ORNL with crossed beams in collaboration with G. H. Dunn and coworkers of the Joint Institute of Laboratory Astrophysics (JILA). Electron impact excitation experiments have demonstrated good agreement with theory in particular cases[8,9] but electron impact ionization experiments have demonstrated dramatic effects due to indirect processes[9,10] (e.g., inner electron excitation followed by autoionization) which are not well predicted by theory. Experiments on electron impact excitation employing new techniques are in planning at JILA and the electron impact ionization experiments are being extended to higher charge states and new species. Another group at ORNL is pursuing experiments on dielectronic recombination employing merged beams and the E-N Tandem.

Nearly all of the present experiments with electrons or H atoms are pursued with the specific intent of testing theoretical predictions. We carry out theoretical studies at ORNL and we interact with a number of theoretical activities at other institutions. A program to develop techniques for including indirect effects in electron impact ionization predictions is in progress[11] in cooperation with M. S. Pindzola of Auburn University and D. C. Griffin of Rollins College. This activity requires calculation of numerous excitation transitions and will have to include recombination resonances[12] so that connections are strong with studies of direct excitation and dielectronic recombination. Electron capture calculations (on which ORNL has collaborated with Heil, Dalgarno, and Bienstock) are directed at low energies[13] where scaling rules and simple predictions fail. New approaches to the problem of electron capture have also been developed.[14]

In addition to these specific activities studying atomic collisions of fusion interest we have direct identification with a group of physicists whose program is development of new diagnostic techniques — presently concentrating on applications of far infrared (FIR) laser systems but also with extensive experience on development of neutral particle analyzers. We also maintain direct interaction with spectroscopic plasma diagnostics and with plasma modelling studies in the Fusion Energy Divison at ORNL.

These references are cited as samples of the work at ORNL, but do not comprise a complete list.

1. C. F. Barnett, J. A. Ray, E. Ricci, M. I. Wilker, E. W. McDaniel, E. W. Thomas, and H. B. Gilbody, Atomic Data for Controlled Fusion Research, ORNL-5206, ORNL-5207, and ORNL-5207R1 (1979).

2. R. A. Phaneuf, Phys. Rev. A 24, 1138 (1981).

3. D. H. Crandall, R. A. Phaneuf, and F. W. Meyer, Phys. Rev. A 19, 504 (1979) and Phys. Rev. A 22, 379 (1980).

4. F. W. Meyer, R. A. Phaneuf, H. J. Kim, P. Hvelplund, and P. H. Stelson, Phys. Rev. A 19, 515 (1979).

5. R. A. Phaneuf, I. Alvarez, F. W. Meyer, and D. H. Crandall, "Electron-Capture in Low-Energy Collisions of C^{q+} and O^{q+} with H and H_2," accepted for Phys. Rev. A (1982).

6. H. J. Kim and F. W. Meyer, Phys. Rev. Lett. 44, 1047 (1980) and additional work submitted to Phys. Rev. A.

7. F. W. Meyer and P. M. Griffin, "Electron Capture and Direct Excitation of $C^{3+}(2p)$ in Collisions with He, H_2, and Xe," completed work in preparation for publication (1982).

8. D. C. Gregory, G. H. Dunn, R. A. Phaneuf, and D. H. Crandall, Phys. Rev. A 20, 410 (1979).

9. D. H. Crandall, Reviews on Electron-Ion Collisions in: Phys. Scripta 23, 153 (1981); p. 595 in the Invited Papers of XII ICPEAC, ed. by S. Datz (North-Holland, 1982); in the "Physics of Ion-Ion and Electron-Ion Collisions," ed. by F. Brouillard and J. W. McGowan (Plenum, 1982); and ORNL/TM-8453, August 1982, and to be in "Atomic Physics of Highly Ionized Atoms," ed. by R. Marrus and J. P. Briand (Plenum, 1983).

10. R. A. Falk, G. H. Dunn, D. C. Griffin, C. Bottcher, D. C. Gregory, D. H. Crandall, and M. S. Pindzola, Phys. Rev. Lett. 47, 494 (1981).

11. D. C. Griffin, C. Bottcher, and M. S. Pindzola, Phys. Rev. A 25, 1374 (1982) and Phys. Rev. A 25, 154 (1982).

12. This work is a sample illustrating importance of recombination resonances in electron impact ionization, but the work was not a part of the ORNL program: K. J. LaGattuta and Y. Hahn, Phys. Rev. A 24, 273 (1981).

13. S. Bienstock, T. G. Heil, C. Bottcher, A. Dalgarno, Phys. Rev. A 25, 2850 (1982). Also, see C. Bottcher and T. G. Heil, Chem. Phys. Lett. 86, 506 (1982).

14. C. Bottcher, Phys. Rev. Lett. 48, 85 (1982).

ELECTRON-ION AND ION-ATOM COLLISIONS RELEVANT TO FUSION AT GIESSEN UNIVERSITY

E. Salzborn

Institut für Kernphysik, Universität Giessen,

D-6300 Giessen

Current work includes the following experiments:

1) Electron impact ionization of multiply charged ions

In a recent series of measurements cross sections $\sigma_{q,q+k}$ with k≥1 for single and multiple ionization of Xe^{q+} ions (q=1,...,5) by electron impact have been measured in a crossed-beams experiment. Although the data are not yet fully evaluated interesting results are being observed. Very important, for an example,is the finding that multiple ionization cross sections may be unexpectedly large, e.g. $\sigma_{1,3}$ reaches values up to $5 \cdot 10^{-17}$ cm^2. The ratio of cross sections $\sigma_{1,3}/\sigma_{1,2}$, taken at electron energies E > 400 eV, approaches the value 0.3. As a consequence, multiple ionization processes should not be neglected in plasma modelling codes,particularly for heavy ions.

2) Transfer-ionization in keV-collisions between multiply charged ions and atoms

A crossed-beam coincidence time-of-flight technique has been used to measure the charge-state distribution of recoil ions created by multiply charged projectile ions which capture one or two electrons in single collisions at keV energies.[1,2,3)

The results of the investigation show the importance of transfer ionization as a contribution to charge-transfer processes: electron capture events were found to cause large shifts in the recoil charge-state distribution toward higher charge states. The dependence of this phenomenon on the charge state of the projectile and the number of transferred electrons was investigated. An overall correlation of the recoil-ion charge states is found with the maximum internal electronic excitation energy available in the collision system. In general, a dependence of the recoil spectra on the projectile kinetic energy has not been observed.

The results of our experiments have several implications. One is that the comparison between theoretical electron capture cross sections and non-coincidence measurements is meaningless if transfer ionization, which theory, in general, does not take into account, gives major contributions to the charge-transfer process. Another implication is that the charge distribution in hot plasmas can be affected since the total ionic and electronic charges are increased by transfer-ionization processes in ion-atom collisions.

1) W.Groh, A.Müller, C.Achenbach, A.S.Schlachter, and E.Salzborn, Phys. Lett. 85A, 77 (1981)

2) W.Groh, A.S.Schlachter, A.Müller, and E.Salzborn, J. Phys. B: At.Mol.Phys. 15, L207 (1982)

3) E.Salzborn, W.Groh, A.Müller and A.S.Schlachter, Proc. of the Symposium on Production and Physics of Highly Charged Ions, Stockholm (June 1-5, 1982), to be published in Physica Scripta.

Experimental investigations of collisions between Multiply charged ions and atoms

Institute of Physics
University of Aarhus
Dk 8000 Aarhus C

1. The following persons have contributed to our research programme: L.H.Andersen, S.Bjørnelund, H.Damsgaard, M.Frost, F.Fukusawa, H.K.Haugen, P.Hvelplund, H.Knudsen, and E.Samsøe.

2. Summary of current work

(a) Electron capture in collisions with H and He

Electron capture has been measured at velocities $v \gtrsim v_0$ for charge states from 2 to 25. Scaling rules are developed on the basis of the Bohr-Lindhard theory. In the near future, more work on atomic hydrogen will be undertaken.

(b) Capture into specific n,l states

The formation of excited states resulting from electron capture by Au^{q+} (q from 12 to 18, $v = 2 v_0$) colliding with H_2, has been measured by means of optical methods. Reasonable agreement with CTMC and UDWA calculations is obtained.

(c) Ionization in collisions with He

Single and double ionization cross sections have been measured for a large number of ions at different energies and charge states by a time-of-flight technique. Good agreement is found with the dipole close-coupling theory of Janev.

(d) Studies of target ionization and electron capture have been carried out through measurements of charge analyzed projectiles and target ions in coincidence for Au^{q+} projectiles at 100-keV/amu (q = 5-21) colliding with a helium target. Partial cross sections where the charge state of both collision partners is specified both before and after the collisions are found. Single electron capture accompanied by ejection of a second electron is found to be of significant importance with a cross section as large as 10^{-15} cm^2.

(e) In order to investigate the process

$$Au^{q+} + He \rightarrow Au^{(q-1)+} + He^{++} + e$$

in further detail, we have just started electron spectroscopy measurements.

Electron spectra showing pronounced peaks indicate that double capture to autoionizing states plays a significant role in the process of double ionization.

Review articles

1. Electron capture and target ionization by medium and high-velocity multiply charged ions. H.Knudsen, Invited paper, 12th ICPEAC, p.657, North-Holland 1982

2. Experimental investigations of electron capture by highly charged ions of medium velocities. H.Knudsen, P.Hvelplund, L.H.Andersen, S.Bjørnelund, M.Frost, H.K.Haugen, and E. Samsøe, Physica Scripta (to be published)

PROGRESS REPORT Presented at
the CRP Meeting - IAEA Vienna June 1982.

S. BLIMAN
DRFC - SIG
Centre d'Etudes Nucléaires
85 X - 38041 Grenoble (France)

The main results on the study of collisionnal processes such as ion atom, ion molecule interaction are related.

To total single electron-capture by highly charged ions from different gaseous targets (D_2, He, Ne, Ar, Kr, Xe) at energies from 0.7 to 5 keV/AMU; experimental scaling tendancy is deduced ; the experimental values for charge exchange on H seem to fit fearly well with it.

And to spectroscopic observation of the transitions in the radiative decay following single electron capture from D_2 :

$$X^{q+} + D_2 \longrightarrow X^{(q-1)+}(n,l) + D_2^+$$
$$\downarrow$$
$$X^{(q-1)+} + h\nu$$

where X is C, N, O, Ne.

1)Total single electron capture cross sections.

In the energy range 0.7 5 keV/AMU a great number of collisionnal pairs have been studied. The following ions C^{q+} ($2 \leqslant q \leqslant 6$), N^{q+} ($2 \leqslant q \leqslant 7$) O^{q+} ($2 \leqslant q \leqslant 8$) Ar^{q+} ($2 \leqslant q \leqslant 16$) have been collided with D_2 : at a given charge q, q, q-1 is quasi energy independant. For $q \geqslant 4$, $\sigma_{q,\,q-1}$ seems to be satisfactorily described by

$$\sigma_{q,\,q-1} \simeq (4.00 \pm 0.7) \times 10^{-12} \times \frac{q}{\left[IP(eV)\right]^3}\ cm^2$$

where q is the incident ion charge. I.P (eV) is the target ionization potential (in eV). Thus for H_o, this would give

$$\frac{\sigma(H_o)}{\sigma(H_2)} = \left[\frac{15.45}{13.6}\right]^3$$ useful for the purpose of prediction.

2) Radiation following capture by completely stripped ions;utilizing a simple flowing gas proportionnal counter, it has been possible to measure the X ray emission cross section for Lyman lines and Balmer lines. Within the energy range of the detector ($E > 100$ eV), the emission cross section of Lyman α is

$1.7\ 10^{-15} cm^2$ for C^{5+}

$1.6\ 10^{-15} cm^2$ for N^{6+}

$1.8\ 10^{-15} cm^2$ for O^{7+} ; and $1.8\ 10^{-15} cm^2$ for the Balmer α line of O^{7+},

emissions. These values quasi energy independant amount to 25-30% of the total single electron capture cross section. In the case of Ne the bahaviour is different since the main radiated lines are : Lyman β and Balmer β with values of the emission cross sections

$$\sigma_{X\ \text{Lyman}} = 2.7 \times 10^{-15} cm^2$$
$$\sigma_{X\ \text{Balmer}} = 8 \times 10^{-16} cm^2$$

This departure is also observed when Ne^{10+} collides He, where the ratio of $\sigma_{X\ \text{Lyman}}$ to $\sigma_{X\ \text{Balmer}}$ is 3.5. These results are now under treatment to deduce the n = 2 level population cross section. From these, with the scaling tendancy the cross section of interest in the case of H_o is probably deduceable.

3) Radiation following a one election capture giving a Li-like ion.

Three different ions collide D_2 ; upon capturing one electron, they are left in excited Li-like states. It has been observed that the highest populated levels are : $4\ d^2D$ in the case of C IV

$4\ d^2D$ in the case aof N V

$4s^2S$, $4p^2P^o$, $4d^2D$ and $4\ f^2F^o$ in the case of O VI

The strongest radiated lines are :

$4f \rightarrow 3d$ and $3d \rightarrow 2p$ for O VI

These results are of importance for the evaluation of losses from scrap off layers on hot plasmas.

S. BLIMAN

Appendix 16

Coordinated Research Program on Atomic Data for

Diagnostics of Magnetic Fusion Plasmas

Meeting June 21 - 25, 1982

Comments on electron-impact ionization of ions.

Gordon Dunn

Ionization Cross Sections for Ions

Z = 1 - 10, H - Ne

A "recommended" set of cross sections has been assembled[1] by qualified scientists and distributed. One may quibble over a number of details where no experiments exist and over some choices, but by and large this set might well be accepted until evidence shows error.

Good experiments exist for all but LiIII, BeIV, BIII, BV, CVI, NVII, OVII, OVIII.

Strong excitation-autoionization effects in Li iso-sequence, and effect increases rapidly with Z. This needs further work, e.g. in O^{+5}.

No data exist for F. It's hard to say why when it is a priority species. Work should be done. Predictor formulae should give reasonable values.

Good beam measurements for NeII, NeIV. Trap measurements for other ionization stages.

Z = 11 - 18, Na - Ar

Good beam measurements on NaII, MgII, MgIII, SlII, SlIII, SiIV, ArII, ArIII, ArIV, ArV, ArVI. Trap measurements on other Ar stages. Na iso-sequence shows excitation-autoionization effects which increase rapidly with Z. No theories nor scaling formulas seem to do well with direct process. Resonant inner-shell dielectronic capture - double autoionization also seems important. Branching ratios for autoionization may not agree with theory.

No work on Cl, a priority species.

Z = 19 - 36, K - Kr

Good beam measurements for KII, CaII, TiIV, ZnII, GaII, XeII, XeIII, XeIV, XeVII.

Main points are that:

1. Excitation-autoionization can (and often does) totally (by an order of magnitude) dominate the ionization cross section.

2. d subshells contribute to the direct process in a scaled down manner from s and p shells. Thus, e.g. simple Lotz-type methods can't be used without inventing new coefficients.

Z = 37 - 102, Rb - No

Good beam measurements on RbII, SrII, ZrIV, CdII, XeII, XeIII, XeIV, CsII, BaII, HfIV, TaIV, HgII, HgIII, TlII. Trap measurements on many stages of Xe, Cs, Ba, Hg.

In addition to specific data, main points to learn are much as for Z = 19 - 36:

1. Excitation-autoionization can (and often does) totally (by up to more than an order of magnitude) dominate the ionization cross section.

2. The d and f subshells probably contribute in a scaled down manner from s and p subshells, and the contribution may vary substantially with species. Simple formulae such as Lotz may not be readily applicable without significantly altered coefficients for these subshells.

Sources

Very good recent sources on ionization of ions are:

1. "Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions" by K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston and F. J. Smith. This gives recommended cross sections for all stages of ionization for H - O, and compares with experimental data, frequently used formulae, and "quality" theory.

2. "Empirical Formulas for Ionization Cross Sections of Atomic Ions for Electron Collisions: Critical Review with compilation of Experimental Data," by Y. Itikawa and T. Kato. Gives compilation of experimental data available to authors for Z = 2 - 19 and compares with Lotz and Scaled Coulomb - Born (G & S).

3. "Bibliography on Electron Collisions with Atomic Positive Ions, 1978 thru 1982" by Y. Itikawa. This supplements and updates the earlier version IPPJ-AM-7 by K. Takayanagi and T. Iwai.

Comments

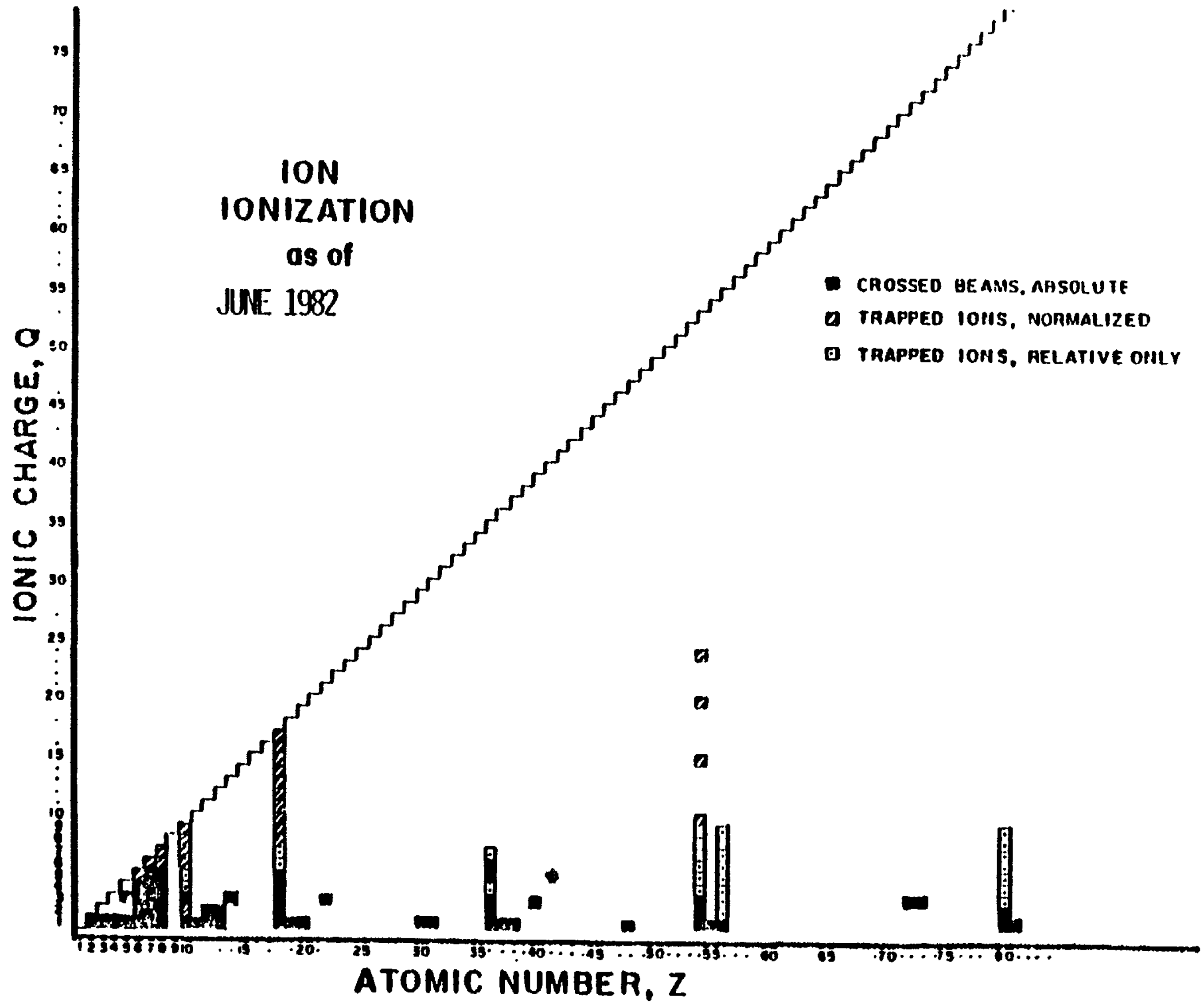
1. With some exceptions which need discussion, (BeII, CIV, BII, CIII) the cross sections "recommended" by Bell et.al. could be adopted for the fusion community for H - O. (Z = 1 - 8).

2. For all Z for which there are beam measurements, a "recommended" cross section could be given based on the measurements.

3. For Z = 9 - 18, a reasonable set of cross sections could possibly be generated based on Lotz, Golden and Sampson (SCB), and McGuire (SPWB),

using more accurate (Moores, Younger, etc.) calculations where available and taking care to scale excitation-autoionization for the sequences where it has been seen to be important (Li, Na, ...). However, more work will be needed to establish experimental validity.

4. For Z > 19 it's very dangerous at this point to generate recommended cross sections except for species on which measurements have been made. More work both theoretically and experimentally needs to be done to establish systematics of subshell contributions and contributions from excitation-autoionization (also resonant excitation/capture -- double autoionization). Some cross sections for high ionization stages corresponding to low Z atom isosequences may be reasonably predicted with care as in comment 3 above.



1	H	47	Ag	93	Np
2	He	48	Cd	94	Pu
3	Li	49	In	95	Am
4	Be	50	Sn	96	Cm
5	B	51	Sb	97	Bk
6	C	52	Te	98	Cf
7	N	53	I	99	E
8	O	54	Xe	100	Fm
9	F	55	Cs	101	Mv
10	Ne	56	Ba	102	No
11	Na	57	La		
12	Mg	58	Ce		
13	Al	59	Pr		
14	Si	60	Nd		
15	P	61	Pm		
16	S	62	Sm		
17	Cl	63	Eu		
18	A	64	Gd		
19	K	65	Tb		
20	Ca	66	Dy		
21	Sc	67	Ho		
22	Ti	68	Er		
23	V	69	Tm		
24	Cr	70	Yb		
25	Mn	71	Lu		
26	Fe	72	Hf		
27	Co	73	Ta		
28	Ni	74	W		
29	Cu	75	Re		
30	Zn	76	Os		
31	Ga	77	Ir		
32	Ge	78	Pt		
33	As	79	Au		
34	Se	80	Hg		
35	Br	81	Tl		
36	Kr	82	Pb		
37	Rb	83	Bi		
38	Sr	84	Po		
39	Y	85	At		
40	Zr	86	Rn		
41	Nb	87	Fr		
42	Mo	88	Ra		
43	Tc	89	Ac		
44	Ru	90	Th		
45	Rh	91	Pa		
46	Pd	92	U		

Appendix 17

Review of Data Requirements and their Priorities

A. Lorenz

In proceeding with the work of this CRP, we should as far as it is possible, strive to satisfy the requirements which have been identified by the fusion community, and put the emphasis on those reactants and processes which have the highest priority.

For this purpose we can use the results of the IAEA survey, which I sent out earlier this year. Actually there is no significant difference from the recommended priorities assigned at the 1980 Paris meeting, and the survey also reflects the recommendation of the IFRC Subcommittee on A+M Data which confined the scope of priority data to: electron impact ionization, electron excitation and electron capture. The results of the IAEA survey are shown in Table 1.

I realize of course, that it would be impossible for this CRP to consider the data for all of the process/reactant pairs given in Table 1. Rearranging and condensing the information from the questionnaire, by listing the reactant group in their order of priority for the high priority processes, namely: electron excitation, ionization and capture, and dielectronic recombination we obtain a priority-ordered list given in Table 2.

Selecting the reactant groups for each of the priority processes which have priorities between 1.0 and 1.5, it can be seen that for electron excitation, ionization and capture the reactant priorities are the same for all three priority processes, namely:

First priority :	C, O, Ti and Fe
Second priority:	Al, Cr and Ni
Third priority :	H, D, T and He

Dielectronic recombination, which was given a high priority rating at the 1980 Paris Meeting, has also been rated with high priority in the IAEA survey. To the extent that it will be possible for the CRP to consider the data for this process, we should restrict our emphasis to the three reactant groups listed above including the impurity group consisting of Cu, Zr, Mo and W.

Other processes and reactants having lower priorities, may be considered as time permits in the course of subsequent meetings of this CRP.

Table I

PROCESS/REACTANT PRIORITIES DERIVED FROM QUESTIONNAIRE ANALYSIS

Reactants \ Processes	Electron Excitation	Electron Ionization	H+D Ionization	Electron Capture (a)	Electron Capture (b)	Electron Capture (c)	Radiative Recombination	Dielectronic Recombination
Group 1: H,D,T	1.3	1.4	1.3	1.3	2.2	1.6	1.6	
Group 2a: C,O,Ti,Fe	1.1	1.1	1.3	1.1	2.3	1.9	1.5	1.3
Group 2b: Al,Cr,Ni	1.2	1.2	2.0	1.3	2.8	2.4	1.7	1.5
Group 2c: B,N,F,Si,Cl	2.1	2.0	2.3	2.0	2.8	2.4	2.2	2.1
Group 3: Cu,Zr,Mo,W	1.9	1.9	2.2	2.1	2.7	2.7	2.4	1.1
Group 4: He	1.3	1.3	1.8	1.3	2.0	1.9	1.6	1.8
Group 5a: Ne,Ar,Kr	1.6	1.6	2.3	1.8	2.7	2.5	2.1	1.6
Group 5b: Xe	2.2	2.2	2.3	2.0	2.7	2.7	2.4	2.2
Group 6: Li,Cs	1.9	2.0	2.3	2.2	2.6	2.6	2.1	2.4

Table 2. Priority-ordered List of Required Data.

(Relative priorities are given in parentheses)

Electron Excitation	Electron Ionization	Electron Capture $(A^{q+} + H^{0} \quad A^{(q-1)+} + H^{+})$	Dielectronic Recombination
C, O, Ti, Fe (1.1)	C, O, Ti, Fe (1.1)	C, O, Ti, Fe (1.1)	
Al, Cr, Ni (1.2)	Al, Cr, Ni (1.2)	Al, Cr, Ni (1.3)	Cu, Zr, Mo, W (1.1)
H, D, T, He (1.3)	H, D, T, He (1.3-1.4)	H, D, T, He (1.3)	C, O, Ti, Fe (1.3)
Ne, Ar, Kr (1.6)	Ne, Ar, Kr (1.6)	Ne, Ar, Kr (1.8)	Al, Cr, Ni (1.5)
Cu, Zr, Mo, W, Li, Sc (1.9)	Cu, Zr, Mo, W (1.9)	B, N, F, Si, Cl and Xe (2.0)	Ne, Ar, Kr (1.6)
B, N, F, Si, Cl (2.1)	B, N, F, Si, Cl, Li, Cs (2.0)	Cu, Zr, Mo, W (2.1)	He (1.8)
Xe (2.2)	Xe (2.2)	Li, Cs (2.2)	B, N, F, Si, Cl (2.1)
			Xe (2.2)
			Li, Cs (2.4)