## INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting

International Atomic Energy Agency

on

## Atomic and Molecular Data for Fusion

Culham Laboratory, UK, 1-5 November 1976

SUMMARY REPORT

Edited

by

A. Lorenz Nuclear Data Section International Atomic Energy Agency

February 1977

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#### Abstract

The IAEA Nuclear Data Section convened an Advisory Group Meeting on Atomic and Molecular Data for Fusion at the UKAEA Laboratory at Culham, from 1-5 November 1976. This first international meeting on this topic was attended by 88 scientists, representing both the technical fusion and the academic atomic physics communities, from 18 countries and 2 international organizations.

Twenty-one papers describing atomic and molecular data needs in fusion research and technology, and outlining national programmes and emphasis in this field were presented. Three detailed working group reports identifying requirements and availability of atomic collision data, atomic structure data, and surface interaction data in fusion research were produced by the participants.

The meeting recognized that the needs for atomic and molecular data for the development of fusion research and technology are so large that any one Member State cannot adequately fulfil these needs for the whole world. Thus, not only was it deemed necessary to coordinate the collection of the requirements and the acquisition of the required data on atomic and molecular processes, but also to create a network of data centres for the dissemination of these data to the fusion community. The meeting recommended the formation of an international network of data centres for the compilation and dissemination of atomic and molecular data required for fusion, and recommended that the IAEA Nuclear Data Section be given the responsibility to establish and coordinate this network.

#### I. Meeting Summary

Experience with present-day fusion devices has shown a critical need for numerical data for the detailed understanding of the physical processes which occur in these devices. As the fusion research programs progress toward the design and construction of larger experimental devices, serving as prototype facilities for full-scale fusion reactors, the data requirements will become more severe as other physical processes become important and the required level of understanding becomes more advanced.

This meeting on atomic and molecular (A+M) data for fusion, convened by the IAEA and organized by the Nuclear Data Section, was the first international meeting on this topic. It was attended by 88 scientists, representing both the technical fusion and the academic atomic physics communities, from 18 countries and 2 international organizations. The opening address of the meeting was given by Sir Harry Massey.

The goals of the meeting were to identify specific data requirements, review the national programs, and agree on an international cooperative effort to compile and disseminate atomic and molecular data needed in fusion research and technology. The objectives achieved by this meeting were:

- to bring together experts in the field of fusion research knowledgeable in the requirements and availability of A+M data;
- to list specific A+M data needs, their accuracies and priorities;
- to identify the existence and availability of evaluated and compiled A+M data and compare them with the requirements;
- to identify and discuss measurements, calculations, and compilations required to satisfy the current and near term A+M data needs of fusion research; and
- to formulate specific recommendations on the IAEA programme and international cooperation in this field, and on the coordination of future activities.

To meet these objectives the meeting was organized around two sets of invited review papers covering the status of A+M data, their accuracies and priorities on one hand (Session A) and the national programmes and emphasis on the other (Session B) (<u>Appendix I</u>). The reviews which in themselves are timely technical reports, provided the basis for discussions and preparation of the conclusions and recommendations. The Agenda of the meeting is given in <u>Appendix II</u>, and the list of participants in <u>Appendix III</u>. Following the presentation and discussion of the review and contributed papers in sessions A and B, which took the first two days of the meeting, four working groups met separately on the third and fourth days of the meeting to focus on three atomic and molecular data areas of importance to fusion research and technology, and on international cooperation in this field.

The four working groups

- on international cooperation,
- on atomic collision data,
- on atomic structure data, and
- on surface interaction data

formulated their conclusions and recommendations in the form of working group reports which were discussed in plenary session on the last day of the meeting. These reports are reproduced in their entirety in this summary report of the meeting.

In view of the significance of the overall objectives, achievements and recommendations of this meeting, and because of the interest of the review papers presented at this meeting to the fusion, atomic and astrophysics communities, the meeting strongly recommended that in addition to their dissemination through the IAEA report series, the proceedings of this meeting be published in one of the recognized physics journals having a wide circulation, e.g. Nuclear Fusion or Physics Reports.

#### REPORT OF THE WORKING GROUP ON INTERNATIONAL COOPERATION

#### Working Group Members

Arcipiani, Dr. B.	Hampel, Mr. V.
Barnett, Dr. C.F.	Harrison, Dr. M.F.A. (Chairman)
Decker, Dr. J.	Johnston, Dr. P.
Delcroix, Prof. J.L.	Lorenz, Mr. A.
Ebel, Dr. G.	Schmidt, Dr. J.J.
	Suzuki, Prof. H.

#### Introduction

As outlined in the reports of the technical working groups, the needs for atomic and molecular data for the development of fusion research and technology are so large that it will be very difficult and costly for any one community to respond to these needs on a world-wide scale.

Thus, not only will it be necessary to coordinate the collection of the requirements and the acquisition of the required information on atomic and molecular data which are presently dispersed in the literature, but also to create a network for the dissemination of these data to the fusion community.

#### A. General Recommendations

## A.1 Establishment of an A+M data centre network coordinated by the IAEA/ NDS

The meeting supported the working group recommendation to form an international network of A+M data centres which will compile and disseminate bibliographic and numerical atomic and molecular data required for fusion. The cooperation between these centres should be coordinated by the new atomic and molecular data unit of the IAEA Nuclear Data Section. The centres which will initially form part of this network are listed in <u>Appendix A</u>. The objectives of the centres' cooperative activity should be to set up common operational procedures for the world-wide compilation, evaluation, exchange and dissemination of bibliographic and numerical A+M data required by the fusion community.

Member States participating in the activities of this network are urged to support the national data centres and to provide for the services of scientists to help compile A+M data and forward them to their respective centre. Those Member States which do not have a national centre, are encouraged to provide similar support and forward their data to the international network through the nearest cooperating centre.

#### A.2 Formation of a network of Liaison Officers

In order to provide an efficient channel of communication between the various data producing and data using research groups, it is recommended that the IAEA form a network of liaison officers in all Member States concerned, so as to provide a link for the exchange of information between national centres, the IAEA/NDS and the research laboratories as well as for the coordination of experimental and theoretical research aimed at the determination of A+M data for fusion in different countries. These liaison officers should be key people in key national establishments or data centers conversant with the data requirements of fusion, and also be experienced in at least one of the basic A+M data fields.

Generally, it will be their responsibility to ensure that their national fusion establishments and universities coordinate their A+M activities effectively with the data centre network. Specifically, it will be their responsibility among others, to provide to the IAEA as well as to their national data centres pre-published new data and to identify data needs for inclusion in a bulletin to be published periodically by the IAEA (see Recommendation B.2.3 below).

# A.3 Promotion of interaction between the technical fusion and academic physics communities

Recognizing on the one hand that many of the required data are unavailable, and on the other hand that numerous atomic physics groups in universities and laboratories all over the world have the capability to measure or calculate the required data, the meeting strongly recommends to the IAEA that it foster the interaction between the fusion, atomic physics and astrophysics communities in order to encourage the determination of A+M data for fusion.

#### B. Recommendations to the IAEA/NDS

#### B.1 General Objectives of the IAEA/NDS

In addition to the general tasks of establishing and coordinating the network of A+M data centres, the meeting recommended that IAEA/NDS give priority to the following objectives:

- B.1.1 To compile and publish international computerized indexes to the literature on atomic and molecular collision, structure, and surface interaction data pertinent to fusion research;
- B.1.2 To compile and disseminate in a quarterly bulletin newly measured and/or calculated A+M data and associated information;
- B.1.3 To devise common formats for the compilation and exchange of bibliographic and numerical A+M data among the centre network; and
- B.1.4 To develop standardized computer input and output formats for the systematic compilation and the dissemination of bibliographic and numerical A+M data.

#### B.2 Specific short-range tasks of the IAEA/NDS

B.2.1 Creation of an international bibliographic index for atomic collision data.

IAEA/NDS should coordinate the creation of an international computerized index of references to A+M collision data, with the assistance and input from the A+M data centre network, and the laboratories engaged in fusion research, and publish it by the end of 1978. This index should be patterned after the CINDA\* index and should incorporate the techniques already de-veloped by the IAEA/NDS and by the A+M data centres, and in-corporate all existing compilations of A+M collision data references (see <u>Appendix B</u>), in particular the comprehensive bibliography compiled by the US/ORNL Controlled Fusion Atomic Data Center which covers the open literature for the period 1950-1976.

B.2.2 Consideration of Surface Interaction Data

Surface interaction problems play an important role in the development of fusion technology and there is a great need for the relevant data on surface interactions. The awareness of such data can be provided by a bibliographical index to the literature on surface interaction data as a first step and then finally by compilations and evaluations of the data themselves.

CINDA is a computerized index to the literature on microscopic neutron data published by the IAEA on behalf of the neutron nuclear data centres' network.

- It is therefore recommended that:
- B.2.2.1 A bibliographical index be established covering the world-wide literature on surface interactions from which references to specific surface interaction data could be retrieved. In developing this bibliography the IAEA should make use of bibliographies compiled by existing centres, i.e. the Surface and Vacuum Physics Index in the Federal Republic of Germany, the bibliography on surface studies compiled for the T-20 design in the USSR, and the bibliographic data on surface interaction compiled by the Controlled Fusion Atomic Data Center at the Oak Ridge National Laboratory.
- B.2.2.2 IAEA sponsor work on numerical data compilations and evaluations in those fields of surface interactions where such data are especially needed.
- B.2.3 Publication of an International Bulletin on new A+M Measurements

During the conceptual design of plasma experiments and prototype reactors, a need often exists for atomic and molecular cross section data to aid in the adjusting and maximising of the various physical parameters. In addition, the interpretation of many diagnostic measurements depend on transition probabilities, photon wave-length identification, reaction rates, etc. Throughout the world, atomic scientists are actively engaged in the measurement and computation of atomic data directly related to fusion research. A crucial problem arises in transferring or communicating the current experimental or theoretical results to the international plasma physics community without costly delays. Usually 12-18 months elapse between the completion of an investigation and the publication of the results in a report or in the open literature.

To alleviate this problem it is recommended that IAEA/NDS compile, publish and distribute a quarterly bulletin on newly measured or calculated fusion-related A+M data. The bulletin would be compiled from input provided through the A+M Liaison Officers' network or directly from investigators in the Member States concerned. The bulletin should be patterned after the US "Atomic Data for Fusion" newsletter circulated by the ORNL Controlled Fusion Data Center and the US National Bureau of Standards, whose distribution is principally limited to the US laboratories. In addition, fusion workers are encouraged to communicate to the IAEA/NDS their current data needs which would be included in the quarterly bulletin. It is recommended that this bulletin be established immediately after IAEA/NDS obtains the required staff.

#### B.2.4 International A+M Data Meetings

- B.2.4.1 The IAEA/NDS should convene Consultants' Meetings of representatives of A+M data centres participating in the international cooperation; the first such meeting should take place in 1977. The development of compilation and exchange formats for the international collaboration between the existing centres should be discussed at that meeting. This meeting should also stimulate the short-term efforts recommended by the first Advisory Group Meeting.
- B.2.4.2 A second Advisory Group Meeting on Atomic and Molecular Data for Fusion should be held in 1978, to review the status of national and international activities, to identify new needs for atomic and molecular data and to recommend programmes for future work.

## Appendix A

## MEMBERS OF THE A+M DATA CENTRE NETWORK

<u>Centre Code</u>	Address	Head of Project or Centre
FR/Orsay	Laboratoire Physique des Plasmas Faculte des Sciences d'Orsay Batiment 212 F-91400 Orsay	Prof. J.L. Delcroix
FRG/ZAED	Zentralstelle fuer Atomkernenergie- Dokumentation Kernforschungszentrum D-7514 Eggenstein-Leopoldshafen	Dr. G. Ebel
FRG/Garching	Surface Physics Division Max Planck Institute for Plasma Physics D-8046 Garching bei Muenchen	Dr. H. Vernickel
IAEA/NDS	Nuclear Data Section International Atomic Energy Agency P.O. Box 590 A-1011 Vienna	Dr. J.J. Schmidt
JAP/Nagoya	Atomic Data Study Group Institute for Plasma Physics Nagoya University Nagoya 464, Japan	Prof. H. Suzuki
JAP/JAERI-A+M	Division of Physics Japan Atomic Energy Research Institute Tokai-Mura, Naka-gun Ibaraki-ken 319-11, Japan	Dr. T. Fuketa
UK/Belfast	Computer Centre Queens University Belfast, Bl7 1NN Northern Ireland, UK	Dr. F.J. Smith
us/nbs-At	Data Centers on Atomic Transition Probabilities and Atomic Line Shapes and Shifts Optical Physics Division National Bureau of Standards Washington, D.C. 20234, USA	Dr. W.L. Wiese

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Appendix A

<u>Centre Code</u>	Address	Head of Pro or Centre	oject
US/NBS-EL	Atomic Energy Levels Data Center Optical Physics Division National Bureau of Standards Washington, D.C. 20234, USA	Dr. W.C. M	artin, Jr.
us/nbs-jila	Atomic Collision Cross Section Information Center Joint Institute for Laboratory Astrophysics University of Colorado Boulder, Col. 80302, USA	Dr. E.C. B	eaty
US/ORNL-CTR	Controlled Fusion Atomic Data Center Oak Ridge National Laboratory P.O. Box Y Oak Ridge, Tennessee 37830, USA	Dr. C.F. Ba	arnett
USSR/Kurchatov	Institut Atomnoi Energii I.V. Kurchatova 46 Ulitsa Kurchatova Moscow, D-182, USSR	Dr. Yu.V. 1	Martynenko

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#### Appendix B

### GENERAL DESCRIPTION OF THE PROPOSED BIBLIOGRAPHIC INDEX FOR A+M COLLISION DATA

#### 1. Scope

This index should contain references to all publications on data measurements, calculations, evaluations and reviews of reactions between atoms, molecules, ions, electrons and photons, expressed in terms of cross sections and reaction rates. Excluded from the scope would be plasmasolid interactions, except in the few cases where these phenomena give information about single binary collision. This would also exclude atomic and molecular structure data as these data would require a more sophisticated format, such as spectroscopic notation.

#### 2. Limits of coverage

The index should cover the properties of collisions between electrons, photons, atoms and molecules (including ions) in chemical systems composed of either pure hydrogen (including D and T), or of hydrogen (and/or D, T) plus one or two other elements, such as H+Mo or H+CO. The energy domain covered by the index should not be limited, but a simple specification of the energy or energy range of the referenced data should be given as qualitative information in the index.

#### 3. Formats

The format of the bibliographic index for A+M data which is to be established by IAEA/NDS should integrate as far as possible the formats and information of existing A+M bibliographies, namely those of Dr. C.F. Barnett (US/ORNL), Prof. J.L. Delcroix (FR/Orsay), Dr. E.C. Beaty (US/ /NBS-JILA) and Prof. K. Takayanagi (JAP/Nagoya), and take advantage of the experience gained by these groups. The experience and the methods developed at the IAEA in the development of the CINDA index on neutron reaction data should also be used, recognising, however, the greater complexity of the problem in A+M data. A semi- quantitative description of the collision process according to its initial and final states, energy range, etc. is desirable. If possible, the indexing of any one collision should fit on one line of an appropriate computer print-out format to be sorted according to a number of desirable criteria.

#### 4. Input to the bibliographic index

The input to the bibliographic index should come from the four centres mentioned in paragraph 3, but other centres, (e.g. USSR/Kurchatov, UK/Belfast, etc.) active in compilation, should also contribute to its input. The IAEA should encourage all the contributing centres to computerize their bibliographies using the same format, and send tapes of their files to the IAEA centre. As an initial step the Orsay centre has proposed to collaborate in a joint effort among Western European Member States.

#### 5. Nature of the analysed documents

The index should include references to publications in regular journals, books, review reports (like NBS reports), proceedings of major conferences in the A+M data field (i.e. ICPEAC\* and ICAP\*\*), and to theses if these are readily available, but not to internal reports which would be more or less covered by the proposed bulletin (see section B.2.3 of this Working Group Report).

#### 6. Time-lag

Currently, the time lag between publication and input into the computer file of the France/Orsay bibliographic system varies from about 2 to 12 months because of a lack of man-power (the reading and extracting of information from the literature is made by highly trained scientists who are also pursuing research in the field). It is hoped that international cooperation and help from the IAEA/NDS could reduce this time-lag in the compilation of the international bibliographic index to about three months. In this respect it is recognized that the technical A+M literature from countries such as the USSR and Japan present particular language difficulties; it is therefore recommended that the IAEA/NDS ask the pertinent authorities in these Member States to help provide input to the international A+M data bibliographic index in the accepted English language input.

#### 7. Up-dating

In addition to the regularly published editions of the international bibliographic index, users should have direct access to the computer file which is to be maintained by the IAEA. It is also desirable that the contributing A+M data centres provide IAEA/NDS with up-dates of their own files on magnetic tape every three months. These updates could also be in the form of listings which could be obtained by users directly from the centres. The publication of a supplement to the main issue of the index by the IAEA every six months could be investigated if considered to be economical.

\* International Conference on the Physics of Electronic and Atomic Collisions.

\*\* International Conference on Atomic Physics.

REPORT OF THE WORKING GROUP ON ATOMIC COLLISION DATA

#### Working Group Members

Baluja, Dr. K.L. Brouillard, Dr. F. Greenland, Dr. P.T. Hogan, Dr. J.T. (Chairman) Hvelplund, Mr. P. Joachain, Prof. C.J. McDowell, Prof. M.R.C. McWhirter, Dr. R.W.P. Ohtani, Dr. S. Oepik, Dr. U. Riviere, Dr. A.C. Summers, Dr. H. Tweed, Dr. R.S.

#### Introduction

Composition of the group

This working group is an ad hoc working group that was drawn from the body of meeting participants. The ad hoc nature of our group has resulted in certain areas receiving more attention than others, both for fusion problems and for the assessment of the adequacy of A+M data.

Sources of information available to the group

The following three reports, which survey the needs for A+M data in this field, have been written in the course of the past three years:

- US report of the panel on atomic, molecular and nuclear physics in CTR entitled "Atomic, Molecular and Nuclear Data Needs for CTR", ERDA-39, dated March 29, 1974.
- US report of the "Workshop of Theoretical Aspects of Atomic Physics in Controlled Thermonuclear Research", ERDA 76/106, September 1975.
- IAEA report INDC(NDS)-72/LNA entitled "Survey of Atomic and Molecular Data Needs for Fusion", by A. Lorenz, J. Phillips, J.J. Schmidt and J.R. Lemley, dated January 1976.

Emphasis given in this report to the fusion aspects

The present report complements the coverage given in the three cited reports: it introduces new needs in the area of neutral beam injection and covers some other areas with more detail than the previous reports. The areas of fusion applications that are specifically introduced are: trapping cross-sections for neutral hydrogenic atoms on plasma impurities, cross-sections and rate coefficients needed for the particle and energy balance in tokamak discharge initiation and termination, scrape-off plasma, and divertor layer.

Emphasis given in this report to the A+M data needs -

The authors of the present report take a significantly different view of the relative priorities of specific data needs in the plasma (spectroscopic) diagnostics and impurity radiation areas; here, the rate coefficients for collisional excitation and ionization are seen as the most important needs. The reference to specific groups and specific work is done to clarify the nature of the data needs. This is not meant to exclude other groups or other work, but rather to complement the descriptions given in the reports referred to above. In our final recommendation (paragraph B8) we propose the only practical scheme for making a realistic appraisal of the resources available to attack the problems that we have identified: specialist working parties should be established to make a detailed evaluation of available data and to set priorities for further work.

#### Accuracy considerations

The specification of existing conditions in CTR devices is often poor. For example, the chemical composition of the neutral heating beams that actually enter the plasma has not been determined. Conditions near the plasma edge cannot be measured with precision. The corresponding specifications of data needs must thus be given in broad terms: only approximate ranges of parameter values can be given and the accuracies required in some areas cannot yet be estimated. The accuracy to be aimed at for values of excitation rate coefficients (by electron collision) might reasonably be set at  $\sim \pm 20\%$  (in a few cases better accuracy can be achieved) although there are indications at this time of very large disparities, in some cases as large as a factor of four. The achievement of this accuracy (+ 20%) is probably close to that aimed at for the most sophisticated quantum-mechanical computer codes currently being developed. Similarly, experimental techniques are such that only in the most careful work is this accuracy achieved. An accuracy of about + 10% appears to be possible for ionization rate coefficients in the region of threshold experimental methods. Theoretical methods appear to be more suspect due particularly to the difficulty of taking account of exchange for threshold collisions.

#### A. Fusion Needs for A+M Collision Data

#### 1. Beam Trapping

The fusion needs here are for cross-sections for charge exchange and for impact ionization of neutral hydrogenic atoms colliding with impurity ions in the plasma. The specific ions of interest can be grouped according to their source; for example, cross sections are needed for all states of ionization of particles from:

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Walls (stainless steel): Ni, Cr, Fe
Loosely bound light elements: C, O
Limiters, guard plates: W, Mo
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The relevant energy ranges and required accuracies are further discussed in Review Al, "Atomic and Molecular Data Needs for CTR Beam Injection" by J.T. Hogan. Further analysis of the requirements taking into account negative ion processes are included below; attention is being drawn to the need for detailed understanding of elementary charge transfer and other processes.

The data needs for neutral beam trapping were discussed in Review Al. This review and the bulk of our recommendations have dealt with processes occurring within the plasma. The report INDC(NDS)-72/LNA by Lorenz et al. contains a thorough description of data needs for the neutral beam ion sources, extraction and acceleration systems, and for beam neutralization. We reproduce this information for completeness as <u>Appendix A</u>.

#### 2. Needs for Plasma "Scrape-off" Data

There was no review dedicated to this subject, which covers three distinct areas: the plasma-wall interface in conventional tokamaks with material limiters, the initiation and termination phases of the tokamak discharge, and the processes which figure in the performance of divertortokamaks, such as DITE. This is in fact a newly developing field in fusion, although it requires data that were important to the stellerator work of ten years ago. An exhaustive specification of data needs in this area was not attempted, but rather some suggestions were made to increase the interaction among A+M physicists and those in the fusion area. The needs in this area will be strongly influenced by results of work on such surfacerelated processes as desorption (see the report of the Working Group on Surface Interactions). Data on electron collisions with atoms, ions, and molecules, for atom-atom collisions and for recombination for both hydrogenic species and impurities are most urgently required for the calculation of the particle and energy balance. The conditions prevailing in the edge region of CTR devices can be characterized only approximately: the temperature is less than 50 eV, and the electron densities in the range of  $10^{12}-10^{13}$  cm<sup>-3</sup> have been measured in the near-limiter region of conventional tokamaks. The DITE divertor-tokamak is presently measuring changes effected by operation with a magnetic limiter. Conditions in the edge region in future devices are likely to involve higher temperatures and densities. Specific needs are considered in the listed Recommendations.

#### 3. Plasma Impurities and Cooling

This working group considered some of the collisional processes needed for considerations of plasma impurities and cooling on the basis of the Review Paper A4, "Plasma Impurities and Cooling" by H.W. Drawin.

- 3.1 The data considered in this section are needed for a number of different purposes: the calculation of power loss due to radiation, the determination of impurity concentration, the electron temperature and density, and the ratios of radiation line intensities.
  - 3.1.1 The calculation of the power loss due to radiation by impurity ions. This arises from three distinct processes, viz.line radiation, recombination radiation and bremsstrahlung. Of these, line radiation is by far the largest, especially in the phase of dynamic ionization before the steady-state is reached. The power must be summed over all the lines emitted by the ion, but fortunately only a small number contribute the great majority of the power and the rest can be taken account of by less accurate methods. The calculation of the total power loss requires a large number of different atomic coefficients. Of those that limit the accuracy of this calculation, they are, in the order of their importance:
    - Collisional excitation rate coefficients from ground and metastable levels.
    - Collisional ionization rate coefficients from ground and metastable levels.
    - Recombination rate coefficients.

- 3.1.2 The determination of impurity concentration and the effective Z of the plasma from spectroscopic intensity measurements. This requires much the same data as for 3.1.1 above, but for a restricted set of lines. There is the same need to take account of metastable populations and state of ionization. Data on the excitation rate coefficients is the most important.
- 3.1.3 The determination of the electron temperature from the intensity ratio of suitable line pairs. Although largely superseded by laser scattering this method of estimating the electron temperature may offer advantages where, for example, it is important to check on departures from Maxwellian velocity distribution. The method depends on having good knowledge of the excitation rate coefficients for the chosen lines. Lithium-like and sodium-like lines are particularly suitable although only for the former has the method been developed in practice.
- 3.1.4 The determination of electron density from intensity ratios of suitable line pairs. Some ions such as Be-like ions have metastable levels with suitable radiative lifetimes to render certain line ratios sensitive to the ambient electron density. Such methods have been shown in principle to work, but have not been entirely successful in practice through lack of sufficiently accurate atomic data. Excitation rate coefficients, in particular for Be-like ions, are needed.
- 3.1.5 The ratios of the intensities of the satellite lines of resonance lines, particularly of He-like ions, provide valuable diagnostic possibilities for electron temperature and density. These satellites arise partly through dielectronic recombination and partly through inner shell excitation. Detailed rate coefficients for both processes are required.
- 3.2 The particular ions for which data are required cover a very wide range of elements and ionic charge. The need, therefore, is to make a selection on the basis of priorities, taking account firstly of the immediate straightforward needs of fusion, but also the limitations of present methods of evaluating this data so that a programme can be developed to improve its reliability. At the present time many of the most important quantities (such as the radiated power loss) can only be calculated with an accuracy amounting to a factor four or five. In the long term this is not

acceptable and there is therefore a need to improve the theoretical methods. The only satisfactory way of doing this is to develop a joint theoretical/experimental programme where new theories can be tested in the laboratory at various stages of its development. Such tests réquire, among other methods, spectroscopic measurements on low density plasmas such as those used in fusion research. Thus the cooperation of the fusion physics community is required in solving the problems in atomic physics. One way in which this could be attempted would be to make available a machine capable of producing low density, high temperature plasma (such as a tokamak) for spectroscopic studies. In such cooperative studies it would be essential to start by trying to understand the relatively simpler atomic systems (ions having few - less than five or six - orbital electrons). Detailed excitation studies of complex ions at this stage would certainly be counter-productive. (This is not to deny the need for spectral line classification of the lines of such ions see report by the Working Group on Atomic Structure). In the meantime interim needs for excitation data on these complex ions can be met through use of the very simple g-formula or impact parameter methods with possibly some use of Coulomb-Born approximation. All this can lead to relatively large inaccuracies (up to a factor of 5).

3.3 To satisfy the requirements for plasma impurities and cooling data, there are needs for basic theoretical work that would enable the needed excitation and ionization rates, particularly near threshold, to be obtained for CTR materials by iso-electronic extrapolation. It is felt that a basic understanding of relatively simple systems should be produced at first. Spectroscopic studies on tokamaks are needed to complement the accuracy of direct A+M data for the rate processes important to the fusion problem. (Noble gas discharges have already been usefully employed to do this).

#### B. Recommendations

The recommendations are ordered according to the nature of the reactants and each have been assigned a priority, viz. (1) top priority, urgent; (2) medium priority, should be undertaken when possible; and (3) lower priority, needed but not immediately.

- 1. Charge Transfer
  - 1.1 Theory

Although calculations are performed using a molecular orbital approach for energies up to  $S_i^2 = 0.1$  (i.e. 2.5 keV for H<sup>+</sup> impact), there is no reliable theory that can be used quantitatively. At intermediate energies LCAO models with traveling orbitals sometimes yield reasonable results. At higher energies the Born approximation or variants of it are used, but higher order terms are required. Fundamental theoretical investigation for simple systems is needed with priority 1.

### 1.2 Experiment

Results of relatively high accuracy for capture of electrons by wall ions (Fe<sup>n+</sup>, Ni<sup>n+</sup>, Cr<sup>n+</sup>, etc.) with fast H<sup>o</sup>, D<sup>o</sup>, and possibly T<sup>O</sup> are required for understanding the physics of beam injection. C and O are among the other interesting targets, and all states of ionization should be considered. Metastable states of the incident beam particles need to be considered, as well as other excited states. Injection with negative ions may raise further problems. Most such work will need to be carried out experimentally, but also to be supported by detailed theoretical calculations on simple systems to allow interpolation and isoelectronic extrapolation. Experimental work is already underway on a few such processes at the Oak Ridge National Laboratory, the FOM Institute of Atomic and Molecular Physics in the Netherlands, the Liebig-Universitaet Giessen in the Federal Republic of Germany, the Queen's University in Belfast, and the Université Catholique de Louvain in Belgium.

#### 1.3 Further remarks on charge transfer

Among other places, theoretical studies of merit are being conducted at the University of Bordeaux, Stanford University, Queen's University at Belfast, and by the Indian Association for the Cultivation of Science in Calcutta. We believe that both theoretical and experimental work on these processes should begin with simple systems building on what is already known, and should be considered as priority 1. Theoretical investigations of high energy limits following recent work of Dettman and Leibfried in Germany and Shakeschaft and Spruch in the US, may be practical and should be given priority 2. Further work on bounds on transition probabilities, following Rapp and Storm and Shakeschaft and Spruch should be pursued.

It is important to note that total capture cross sections, ineluding capture into excited states, are also required. At higher energies, capture by He<sup>++</sup> produced in the basic thermonuclear reactions will be important, and data are required on all the above targets and beam particles at energies up to several MeV.

Low-energy charge transfer (below 1 keV) is important for the wall region, and investigations of capture from and into highly excited states needs further work (priority 2).

Charge transfer may also play an important role in the divertor channel and exhaust in actual CTR machines, for example acting as a pump for neutral impurities (priority 2).

### 2. Other Heavy Particle Processes

## 2.1 <u>Ionization of fast neutral hydrogen by highly ionized</u>, particles

This is of great importance and little is known about this process. Theoretical methods are available to calculate total cross sections using distorted wave codes, which should be reliable down to 20 keV (equivalent proton energy) and are being developed, e.g. by the Royal Holloway College - Université Libre de Bruxelles collaboration. However, experimental work is also required, particularly at lower energies since it seems unlikely that accurate theory can soon be developed. This is also of first priority, though it should be stressed that the calculations will be lengthy and expensive.

#### 2.2 Exitation in atom-atom and ion-atom collisions

We consider atom-atom and ion-atom direct inelastic processes of relatively low importance. Results are needed at low energies (below 50 eV) and some experimental groups may be able to tackle these problems. We need to know in more detail precisely what such reactions, including chemical reactions, are likely to be important in CTR work before we can assess the urgency for further investigations (priority 3).

#### 2.3 Ion-ion reactions

Ion-ion reactions are generally expected to be unimportant unless a resonance process is involved. Identification of likely candidates depends on accurate knowledge of adiabatic molecular ion potentials.

#### 2.4 Fundamental ion-atom processes

The data on reactions of  $H^+$ ,  $He^+$ , and  $He^{++}$  on H and He are of fundamental importance in tokamak particle balance. They are perhaps less well-established than is commonly thought and critical evaluation of current data is required (priority 1).

### 3. Excitation of Positive Ions by Electron Impact

This process is of crucial importance both for understanding energy balance and for diagnostic purposes.

Recent advances in theoretical methods make use of large computers and are aimed at calculating excitation rate coefficients accurate to about  $\pm 20\%$ . Comparison between experimental measurements and preliminary results of these calculations are revealing disparities of up to factors of 4. The reasons for these disparities may be that either:

- the theory may be wrong;
- the experiment may be wrong;
- the method of analysing the data to make the comparison may be wrong.

These comparisons are being done for relatively simple ions (specifically Be-like) and we recommend strongly that efforts be confined to the <u>understanding</u> of these relatively simple ions before going on to apply these sophisticated computer methods to more complex atomic systems. Elementary theoretical methods, such as the Coulomb-Born approximation, are thought to be untrustworthy for excitation processes close to threshold, but distorted-wave and close-coupling treatments show promise. A fairly complete listing of the status of theoretical work in this area is attached (<u>Appendix B</u>, by D.M. Cochrane and R.W.P. McWhirter). The development of such new theoretical methods should be encouraged and we recommend that support be given to the major international collaboration in this field particularly between the groups at the Queen's University at Belfast, the Observatoire de Paris at Meudon, the University College London, the Université Libre de Bruxelles, the Royal Holloway College and groups in the USA and the USSR.

The theoretical collision work depends on the production of tractable, accurate wave-functions for the states involved. It may be possible to obtain these as a byproduct of the atomic structure work discussed by another Working Group. This should be given high priority (priority 1). The wave-function codes produced in this, or in other ways, must be developed to the point where the collision physicist can use these with ease.

We believe that, in this work on collisional excitation, comparisons must be made between theory and experiment as a check on the accuracy of the theory, which is the only conceivable means of evaluating the very large number of collisional rate coefficients that are required. Experimental checks on the calculated excitation rate coefficients and crosssections are possible by two methods, viz.

- Quantitative plasma spectroscopy; and
- Crossed-beams experiments.

A listing of published work by both methods is attached as <u>Appendix C</u>. Many more such collisional processes need to be studied by these experimental methods. The former requires the provision of a powerful plasma source for spectroscopic studies. Currently, work is being developed or is established at the Maryland University, the Astrophysics Research Division Culham Laboratory, the US National Bureau of Standards in Washington, the Los Alamos Scientific Laboratory, and Bocham University. The work of all these groups is based on relatively high density theta-pinches but there is an important case for a low density tokamak plasma being used for this work. Another useful experimental check on the theory of collisional excitation is the measurement of radiative transition probabilities between relevant levels and their comparison with the values calculated using the wave-functions developed for the collision physics. Work using beam-foil spectroscopy is likely to prove very valuable in this connection.

Efforts should be directed to obtaining agreement between theory and experiment to within  $\pm$  20% at all energies but this is particularly important close to threshold. Data is required for ions in metastable levels as well as ground levels.

We consider this work on the simple ions (both the development of theoretical methods and the experimental comparisons) to be of the highest priority (priority 1). We recognize the ultimate importance of heavy impurities but there is no hope of understanding the more complex reactions with heavy metal ions until the simple systems are understood.

#### 4. Ionization by Electron Impact

Cross-section values are needed up to two or three times threshold for ground level, metastable level and inner shell ionization for all ions of interest. In cases where it is important the contribution due to autoionization is also needed. Near threshold theoretical methods are unsatisfactory due particularly to the difficulty of taking account of exchange. Errors of up to a factor of 2 have been reported in the threshold region. For ground level and for autoionization near threshold experimental crossed beams methods have proved successful with reported accuracies of + 10%. As these measurements have so far been limited to ions of charge one and two, there is an important need to extend this work to ions of higher charge. Measurements of ionization rate coefficients are also possible by time resolved plasma spectroscopy but with less accuracy. These measurements, however, cover ions in higher stages of ionization. We recommend the extension of this experimental work particularly with crossed beams. It is important also to encourage the development of theoretical methods of calculating cross sections for ionization close to threshold. Accuracies of  $\pm 20\%$  should be aimed at. This work also is of high priority (priority 1).

#### 5. Electron-ion recombination processes

Impurities are expected to reach a condition of steady-state ionization balance in some of the plasma machines currently contemplated. Under these circumstances it is as important to have as good values for recombination rate coefficients as those for ionization. Three interrelated mechanisms of recombination have been identified as important in these circumstances:

- Radiative recombination
- Dielectronic recombination
- Collisional-radiative recombination.

Of these the first is a purely radiative process that may be calculated using the wave-functions discussed in the Atomic Structure Working Group's report. The other two mechanisms involve electron-ion collisions of the general nature of those discussed above in sections B.3 and B.4 of this report. The collisions that matter in recombination are those that involve high quantum levels of the recombining ion. Methods of calculating these rates have been developed but there are no significant experimental checks on them. Measurements on satellite lines promise to be valuable here and we recommend that these be done. At the same time these calculations and experiments form the basis for important diagnostic methods for plasma electron temperature and density through the observation of satellite lines.

### 6. Electron-Atom Collisions

Electron atom excitation and ionization processes are of importance in plasma formation and for diagnostic purposes. Both theoretical and experimental results accurate to about 10% are currently being achieved for simple systems, but little work has been done on heavy atoms. Relativistic effects are important for Z > 20, and can be treated with reasonable success up to  $Z \approx 40$ . Further work on fundamental theory of near-threshold ionization is required (priority 2), and further measurements of ionization cross sections for many elements at all energies are needed to check present empirical formulae. In view of the importance of the electron impact ionization of atomic hydrogen, a remeasurement and reassessment of the processes from ground and metastable states is required (priority 1).

#### 7. Photon-Atom Collisions

The low-photon densities in non-laser induced plasmas imply that only single photon processes are important. Primarily attention should be devoted to photoionization of atoms and ions. Further details are needed on photon energy spectra of current tokamaks and fusion devices before deciding which photo-ionization processes are likely to be important. Provided the wave function codes already mentioned are developed, there are no fundamental theoretical difficulties other than those involved in obtained accurate elastic scattering cross section from excited states of ions. We assess this work to be of priority 3.

Threshold photo-ionization cross sections should be first estimated by extrapolation of oscillator strength states.

#### 8. Further Study

It seems to us essential that small specialist meetings on specific topics, e.g. charge-transfer, electron excitation of positive ions, tokamak spectroscopy etc. should be convened. These should review the current position in their field with respect to fusion applications and recommend priorities for further work. It would be most convenient to hold these as satellite meetings of established international conferences. They should be encouraged where necessary to set up small working parties to evaluate in a critical way the information in their field.

Appendix A

Extract from INDC(NDS)-72/LNA

## Survey of Atomic and Molecular Data Needs for Fusion

A. Lorenz et al, January 1976, IAEA

#### ATOMIC AND MOLECULAR DATA NEEDS IN FUSION TECHNOLOGY

For all indicated reactions the quantities which are of general interest are the reaction cross sections as a function of energy and the reaction rate coefficients as a function of plasma temperature. Additionally the atomic parameters for spontaneous photon emission and absorption processes are required for many of the indicated species.

Since all isotopes of hydrogen may be involved unless specifically stated, the symbol (H) is used to represent any of the isotopes  $H_{\nu}D_{\nu}$  or T. The symbol e is used for electrons, and the symbol X and Z may represent any other heavy particles.

#### PROBLEM AREAS

DATA NEEDS

#### 1. INJECTION SYSTEMS

The designs of some fusion experiments and reactors require injection of neutral material into the plasma (core) either to raise its average temperature (plasma heating) or to supply the nuclear fuel.

Present injection techniques are restricted because little is known about the atomic and molecular collision processes which occur in the injection system. An understanding of the atomic and molecular physics of the hydrogen isotopes and of collision processes with other gases is necessary to provide data for the design of efficient sources of both positive and negative ions, for the efficient conversion of positive and negative ions to neutral atoms, and for efficient trapping of injected material in the fusion plasma.

The physical processes and data requirements which are encountered in injection systems are discussed under the following topics:

- A. Plasma Heating by Injection of Beams of Neutral Particles.
  - 1) Ion Source
  - 2) Ion Extractor and Accelerator
  - 3) Ion Neutralization
  - 4) Trapping of Neutral Species in the Plasma
- B. Plasma Heating by Injection of Particle Clusters.

#### C. Plasma Fueling

- 1) Injection of Neutral Particles
- 2) Injection of Particle Clusters
- 3) Injection of Solid Fuel (Pellets)

At present it is not clear whether injection of neutral particles or particle clusters are likely to be useful methods for fueling a fusion reactor. Therefore the principal discussion of these topics occurs in connection with plasma heating. Both plasma heating and plasma fueling by means of neutral-particle injection involve the processes of ion-production, ionneutralization and subsequent trapping of the neutral particles within the plasma. However the relative importance of the atomic and molecular processes which are involved might be very different depending on the energies and intensities of the beams which are required for the two purposes.

#### PROBLEM AREAS

#### 1A. Heating by Injection of Beams of Neutral Particles

#### 1) Ion Source

The primary objective of the ion source is to produce a particular ion species by collisions of electrons with isotopes by hydrogen. These processes occur normally in competition with ion loss processes such as diffusion, ion recombination, and electron energy loss due to inelastic molecular collisions. In addition, impurities (Z>1) are produced as a result of the interaction of the ions and electrons with the walls and electrodes of the ion source. Together with the desired ion species these impurities may be introduced into the plasma, which they contaminate (see Impurities and Plasma Cooling below).

#### (i) Collisions between electrons and atomic and molecular complexes in various states of vibrational and electronic excitation

Production of positive  $e + (H)_2 \rightarrow (H)_2^+ + e + e$ ions - (typical processes)  $e + (H)_2^+ \rightarrow (H)^+ + (H) + e$  $\rightarrow (H)^+ + (H)^+ + e + e$  $e + (H) \longrightarrow (H)^+ + e + e$ Production of negative  $e + e + (H) \rightarrow (H)^{-} + e$ ions - (typical processes)  $e + (H)_{2} \rightarrow (H)^{+} + (H)^{-} + e$ Production of negative

#### (ii) Some Processes affecting ion species

Ion-molecular reaction	$(H)_2^+ + (H)_2$	$\rightarrow$	$(H)_{3}^{+} + (H)$
Association	D + T	$\rightarrow$	DT
Recombination	(H) + (H) <sup>+</sup> +	wall ->	(H) <sub>2</sub>

#### (iii) Electron energy loss processes

Atomic and molecular excitation	$e + (H) \longrightarrow (H)^* + e$ $e + (H)_2 \longrightarrow (H)_2^* + e$ $e + (H)_2 \longrightarrow (H) + (H)^* + e$
Electron-electron	$e(e_{2}+e_{1}) + e(2, \dots, ) \rightarrow (e+e)_{a}$

collisions

```
(fast)
          (plasma)
                            'thermal
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Electron recombination or detachment processes, which are the reverse reactions for production of positive or negative ions, respectively, except for the energy range involved

#### (iv) Interaction of ions with surfaces

- Reaction kinetics

Some preliminary experiments show that the surfaces of the ion source walls play a dominant role in the production of (H)". A more precise knowledge of the reaction kinetics of  $(H)_2^+$ ,  $(H)^+$  and (H) particles interacting with surfaces contaminated by Cs, Mg, Na and Li in the energy range 5 - 500 eV. is required.

- Sputtering (see 2A and 2B)
- Charge exchange
- Charge exchange processes of hydrogen with impurities (e.g. Fe, Ni, Gr, Cu, C, W and Mo), which may enter the ionizing discharge due to sputtering from the walls and other surfaces.

#### 2) Ion Extractor and Accelerator

Positive and negative ions extracted from the ion source are accelerated to energies ranging from  $\sim 10$  keV to  $\sim 1$  MeV. The ion beam is accelerated in a low density gas diffusing out of the ion source. In addition to the interaction of the accelerated ions with the gas, in which charge exchange, charge stripping, detachment and dissociation can occur, part of the beam interacts with metallic surfaces creating the attendant surface effects, such as sputtering and outgassing, thereby introducing additional impurities.

Secondary electrons, produced in the extractor and accelerator by particle impact and Xrays, can be accelerated back towards the ion source so that additional ion production takes place but at much higher electron energies; the production of X-rays by these electrons may introduce a significant hazzard to health. The presence of arcs in the extractor system introduces collisions with impurity atoms.

#### 3) Ion Neutralization

Energetic neutral particles in the range a) 5 to 100 keV, which present injection concepts envisage, are most efficiently obtained by neutralization of accelerated positive ions in a gas cell.

In about five to ten years, however, larger ъ) experimental devices and prototype fusion reactors may require injected-particle energies ranging between 100 keV and 1 MeV. Several methods have been proposed to obtain intense atomic (H) beams in this energy range for heating and, possibly, fueling such devices. At these energies it will be more desirable to neutralize a beam of negative ions since the neutralizer efficiency is almost independent of ion energy and can be as high as 10 - 20 % in the case of a cesium-vapor-cell neutralizer. The following two methods have been proposed to obtain negative ions:

- use of a conventional positive ion source to produce a low-energy (1.5 keV) beam which is passed through an alkali vapor cell to form the required negative ions,
- development of a suitable negative ion source to produce the negative ions directly.

The negative ions are then accelerated to the desired energy and neutralized by stripping the excess electrons in a suitable target.

(i) <u>Particle interaction in the beam</u> . X is the neutrali	. 2 <b>8</b> r
species.	
Charge exchange $(H)^+ + X \longrightarrow (H) + (X)^+$	
Ionization (H) + X $\longrightarrow$ (H) <sup>+</sup> + X + e	
Detaohment $(H)^{-} + X \longrightarrow (H) + e + X$	
Dissociation $(H)_2^+ + X \longrightarrow (H)^+ + (H) + Y$	

#### (ii) Surface effects

. .+

(H) + surface $\longrightarrow$	radiation emission
$(H)^+$ + surface $\longrightarrow$	electron emission
$(H)^+$ + surface $\longrightarrow$	X-ray production
$(H)^+$ + surface $\longrightarrow$	outgassing

- $(H)^+$  + surface  $\longrightarrow$  sputtering
- (i) Production of neutrals from positive ions typical processes:

Collisions with heavy species:

$$(H)^{+} + X \longrightarrow (H) + X^{+}$$
  
 $(H)_{2}^{+} + X \longrightarrow (H) + (H)^{+} + X$ 

Collisions with electrons:

$$(H)_{2}^{+} + (X^{+} + e) \longrightarrow (H) + (H)^{+} + e + X^{+}$$

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- (ii) Some re-ionization processes:  $(H) + X \longrightarrow$  $(H)^{+} + e + X$ (H) + e ----> (H)<sup>+</sup> + e + e
- Formation of (H) from positive ions and stripping (iii) of (H) to form neutrals in gas or vapor cells.
- Interaction of  $(H)_2^+$ ,  $(H)^+$  ions with Cs, Na and Li in the energy region 0.5 5 keV. Little information is available for collisions of  $(H)_2^+$  and  $(H)_3^+$  ions in these vapors. Needed are the total cross sections, equilibrium fractions, and differential interaction cross sections to form (H)-.
- No information is available concerning the cross section for the formation of D from  $D^+$ ,  $D_2^+$ , and  $D_3^+$  in target plasmas of either deuterium or Li. This may be a mechanism to produce 0.1 to 1 MeV D without resorting to the D cycle.
- Cross sections for the formation of (H) from (H) collisions in gaseous targets of H2, He, N2, O2, Ne, Ar and H20, in energy region between 50 and 300 keV.
- Peak fraction of (H) formed from (H) in energy range 0.1 to 1 MeV.
- Formation of (H) from passage of (H) through target plasma of deuterium or lithium in energy range 0.1 to 1 MeV.
- Stripping of (H) in electromagnetic fields.
#### PROBLEM AREAS

c) Intense beams of ions cause the neutralizer target gas to become partially ionized so that oharge-exchange (etc.) takes place in a plasma. Since "thick target" conditions may prevail in the neutralizer, cascading collisions are important. The balance between charge exchange and ion production are further complicated by the presence of excited atoms and molecules.

d) <u>Trapping in the plasma core.</u> After passing through the confining magnetic field, the injected (neutral) particles must be ionized before significant heating can occur. The importance of various ionization processes depends upon beam energy and plasma temperature.

#### DATA NEEDS

(iv) Charge exchange rates for (H), (H)<sub>2</sub> and (H)<sub>3</sub> in partially ionized neutralizer target gases are required.

(v) It is important to know the rate at which impurity atoms from the ion source enter the plasma confinement region. Required are cross sections for charge-exchange processes of C, N, O, Fe, Ta and Pt atoms with neutralizer gases over the energy range 5 to 100 keV and the rates for these processes in the environment of the neutralizing gas cell.

#### (vi) <u>Typical trapping processes:</u>

For beams < 50 keV:  

$$(\underline{H})(\underline{h})(\underline{h}) + (\underline{H})^{+}(\underline{h}) \rightarrow (\underline{H})^{+}(\underline{h})$$

At higher beam energies:

$$(\underline{H})(\underline{beam}) + (\underline{H})^{+}(\underline{plasma}) \longrightarrow (\underline{H})^{+}(\underline{trapped}) + \underline{e} + (\underline{H})^{+}.$$

(The underscores indicate energetic particles.)

(vii) Processes which result in trapping of heavy-ion impurities from the ion source within the plasma.

# LIST OF REFERENCES TO CALCULATIONS OF CROSS-SECTIONS FOR THE EXCITATION OF POSITIVE IONS

Compiled by

D.M. Cochrane and R.W.P. McWhirter

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Appleton Laboratory Astrophysics Research Division Culham

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September 1976



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Science Research Council

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Your ref.	
Our ref.	RWPM/PR
Date	23 September 1976

Dear Colleague

Deirdre Cochrane and I have recently put together a list of references to theoretical calculations of excitation of positive ions (and some atoms) by electron impact. This information should be of interest to astrophysicists interested in the interpretation of spectra and to plasma physicists concerned with the problem of power loss from laboratory plasmas. We hope that you will find the enclosed list useful.

The chart covers all ions of all elements up to Molybdenum and gives access to the numbered foot notes on the accompanying list. Since some of the work is not published a list of the addresses of those contributing to the list is also enclosed. Please contact the addressees for information only when there is a genuine need for data. They too are busy people!

The material enclosed has been prepared with a minimum of editing. There has been no critical selection and a few of the people known to be working in the area did not respond to our enquiries. However, the general response was good and we believe the list will be a useful guide to the available data.

Since the charts were printed a number of additional references have been sent to us. You should therefore mark the following on the chart (the foot notes have been up-dated).

He	I	21.1	He	II	8.5
Be	II	8.6	N	II	2.10
0	II	2.10	0	III	2.10
Al	XI	2.11	Cu	I	21.1

Yours sincerely



R W P McWhirter

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- 1. Dr Derek Banks
  - 1.1 Highley-excited States n→n<sup>f</sup> transitions. Percival I C and Richards D, 1975, Adv. in Atom and Molec.Phys. 11 + references therein.
  - 1.2 The same techniques apply to He<sup>+</sup>, etc, provided the ionisation level is not too extreme, as st. line paths are assumed for the incident electron.
  - 1.3 The same techniques apply to all atoms provided only 1 electron is highly-excited. For  $(n, \ell) \rightarrow (n', \ell')$  transitions we hope to have results within 12 months. Corrections are needed for low  $\ell$ .

### 2. Dr Milan Blaha

- 2.1 Solar Phys. 3, 563 (1968). CB with and without exchange. O Bely and M Blaha.
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- 2.4 Astron. Astrophys. 1, 42 (1969). DW with exchange. Transitions between fine-structure levels. M Blaha.
- 2.5 Phys.Rev.A <u>12</u>, 1076 (1975). Univ. of Maryland Tech. Rep. TR 75-076 (1975). CB without exchange. R U Datla, M Blaha and H-J Kunze.
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- 2.9 Current work. DW without exchange. M Blaha.
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- 2.11 J.Ap.Phys. <u>47</u>, 1426 (1976). Distorted wave calculation. J Davis and K G Whitney.

### 3. Dr J van den Bos

3.1 Born-approximation, excited states: 2<sup>1</sup>S,3<sup>1</sup>S,4<sup>1</sup>S,2<sup>1</sup>P,3<sup>1</sup>P,4<sup>1</sup>P, 3<sup>1</sup>D,4<sup>1</sup>D,4<sup>1</sup>F. Ref: Physica <u>42</u> (1969) 245-261.

### 4. Dr Alan Burgess

- 4.1 Current work. Multi-level close-coupling. R Poet.
- 4.2 Distorted wave. M Frank.
- 4.3 General methods, eg Bethe, ECIP, etc. B Christen-Dahlsgaard.

- 5. Dr Helen Mason All results UCL Distorted wave program.
  - 5.1 H E Mason (1975) Mon.Not.R.astr.Soc. 170, 651.
  - 5.2 H E Mason. Calculations complete no preprints yet (3/4 configurations).
  - 5.3 H E Mason and A K Bhatia (Goddard Space Flight Center) (3 configurations) Calculations complete.
  - 5.4 H E Mason Preprint available.
  - 5.5 H E Mason work planned.
  - 5.6 H E Mason and H Nussbaumer work planned (including configurations in n = 4 complex).

### 6. Professor Philip G Burke

- 6.1 Current work Queens University Belfast. Electron collisions using R-matrix method and taking account of 2s<sup>2</sup> ls 2s2p <sup>3</sup>p lp 2p<sup>2</sup> <sup>3</sup>p l<sub>D</sub> ls levels. P G Burke, K A Berrington, P Dufton, A E Kingston. Also proton collisions for 2s2p<sup>3</sup>P fine structure transitions.
- 6.2 Future work otherwise as for 1 above.

### 7. Professor Alex Dalgarno

7.1 Exploration of relativistic effects using relativistic random phase approximation - He and Be isoelectronic sequences.
C D Lin, W Johnson, A Dalgarno.

### 8. Professor Ronald J W Henry

- 8.1 Have calculated LSU noniterative integral equation method (NIEM) solution of close-coupling 5 levels. W L van Wyngaarden and R J W Henry. J.Phys.B.(June 1976).
- 8.2 Have calculated NIEM 5 level close-coupling. W L van Wyngaarden and R J W Henry. Can.J.Phys. (1976).
- 8.3 Current work NIEM 5 level close-coupling, including resonances. J N Gau, J Callaway, R J W Henry.
- 8.4 Current and planned work NIEM 5 level close-coupling, relativistic effects. J N Gau, J Callaway, R J W Henry.
- 8.5 He II Work completed 1s+2s and 1s+2p; NIEM close-coupling of 1s, 2s, 2p and pseudostates 3s and 3p. R J W Henry and J J Matese, Phys.Rev.A (Oct 76).
- 8.6 Be II <u>Current work</u> 2s→2p; NIEM close-coupling of 2s, 2p and pseudostates 3s, 3p, 3d. J J Matese and R J W Henry.

#### 9. Professor C J Joachain

9.1 Electron excitation of H, He, He<sup>+</sup>, Li<sup>+</sup>, Li<sup>++</sup>, using the Eikonal Born series theory and distorted wave methods. Incident electron energies E ≥ 50 eV.

### 10. Dr M Klapisch

- 10.1 Current work investigation of relativistic effects in Coulomb-Born approximation.
- 10.2 Beginning of work use of R Matrix Package of Berrington, Burke et al. Comp.Phys. Com. 8, 149 (1974).

### 11. Professor M R C McDowell

- 11.1 DWPO I, II, III, published H,He<sup>+</sup>. Rest unpublished. McDowell, M R C, Morgan, L A, Myerscough, V P.
- 11.2 DWPO I,II. Results for H and He<sup>+</sup> published. For 3≤ Z≤10 in McDowell M.R.C., Morgan L.A., Myerscough V.P. and Scott T. Submitted to J.Phys.B.
- 11.3 DWPO I, II and Unitarised: Resonance transition; Kennedy J, Myerscough V P and McDowell M R C. Submitted to J.Phys.B.
- 11.4 Close-Coupling-Pseudo-State-DW. Published H, He II in progress. Callaway J, Morgan L A, McDowell M R C.
- 11.5 a. Simplified c.c.(equivalent exchange potentials). Bransden B H, Joachain C J, McDowell M R C. In progress.
  b. Double Distorted Wave.
  K.L. Baluja, L.A. Morgan, M.K.C. McDowell. In progress.

### 12. Dr David L Moores

- 12.1 Scattering of electrons by Mg<sup>+</sup> and Ca<sup>+</sup>; Burke code 2- and 3-state close coupling; H-Fock target wave functions with P G Burke. J.Phys.B <u>2</u>, 161-73 (1970).
- 12.2 4-state close coupling "The scattering of electrons by Na Atoms" with D W Norcross. J.Phys.B 5, 1482-1505 (1972).
- 12.3 With D W Norcross and V B Sheorey. J.Phys.B.7, 371-5 (1974) "Scattering from excited states of Na"
- 12.4 The scattering of electrons by K atoms. J.Phys.B (in the press; proofs returned).
- 12.5 Current work; "IMPACT" with C Mendoza.

13. Dr Hannelore Saraph

- 13.1 Seaton M J, Roy.Astron.Soc.<u>170</u>, 1975, pp.475-86 (excitation of forbidden lines, CC,CI).
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- 13.3 Pradhan A K, J.Phys.B.9, 1976, 433-443 (excitation of forbidden lines, CC, CI). Also: Pradhan, A K, Mon.Not.RAS, 1976, in press. Detailed resonance analysis for (O II) <sup>2D</sup><sub>3/2</sub> -<sup>2D</sup><sub>5/2</sub>, <sup>2D</sup><sub>y</sub> -<sup>2P</sup><sub>y</sub>, and preliminary results for S II.
- 13.4 Jackson A and Pradhan A K, work nearing completion, CC, CI, resonance analysis.
- 13.5 Hayes M, work nearing completion, CC, DW, CI.
- 13.6 Pradhan A K, excitation of forbidden lines; work started CC, CI, DW.
- 13.7 Storey P, DW, CI, work near completion.
- (CC: Close coupling, DW: Distorted wave, CI: Configuration interaction)

### 14. Dr David W Norcross

- 14.1 UCL DW Program, JILA version,9 config. target (five LS terms) for He sequence ions,11 config. target (14 LS terms) for Be sequence ions.
- 14.2 Model potential close-coupling.

#### 15. Dr Harry Nussbaumer

- 15.1 Nussbaumer H, Osterbrook D E, 1970, Ap.J. 161, 811.
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- 15.3 Flower D R, Pineau des Forêts G, 1973, Astron.Astrophys. 24, 181. Nussbaumer H, 1973, Astron.Astrophys. 27, 303.
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- 15.6 Flower D R, 1971, J.Phys.B. 4, 697. Loulergue M, Nussbaumer H, 1975, Astron.Astrophys., in press.
- 15.7 Loulergue M, Nussbaumer H, in connection with a study on solar active regions, H E Mason will study the Fe<sup>+1</sup> 1 ≥ 20 for flare investigations. Fe<sup>+19</sup> will be studied by either Mason or Loulergue and Nussbaumer.
- 15.8 Mühlethaler H P, in progress.

- 15.9 Flower D R, Nussbaumer H, 1975, Astron.Astrophys.(in press) or unpublished (N III, Ne VI).
- 15.10 Flower D R, Launay J M, 1973, Astron.Astrophys. 29, 321.
- 15.11 Malinovsky M, 1975, Astron.Astrophys. 43, 101.
- 16. Dr W Derek Robb
  - 16.1 Current Work R-matrix Close Coupling, CBO and DW, All levels from ls, 2s and 2p with some n = 3 orbitals and CI - W D Robb, J B Mann and J M Peek.
  - 16.2 Work Complete Close-coupling, Coulomb Born with exchange (CBO) and Distorted Wave (DW) with exchange, lowest 5 levels, rates calculated -W D Robb, J B Mann and J M Peek.
  - 16.3 Work Complete Coulomb Born with exchange. All n = 2 levels and some n = 3 levels J B Mann.

  - 16.5 Work Completed Close-coupling R-matrix Lowest levels CI where necessary - W D Robb.
  - 16.6 Work Completed Coulomb Born with exchange Threshold to high energy rates calculated some CI. J B Mann.

### 17. Dr Mike J Roberts

- 17.1 Differential cross section for excitation of H. A classical path T-matrix approx. valid, at best, for high angle scattering only -No good for total x sections.
- 17.2 I intend to investigate the excitation of hydrogenic ions with similar technique.
- 17.3 Calculation of orientation parameters for excitation of optical levels.

### 18. Dr Aaron Temkin

- 18.1 Goddard program distorted wave. Uses exchange approx. for exact initial stale wave function. Bhatia and Temkin (to be submitted for publication) (He isoelectronic ions).
- 18.2 Program being developed at Goddard uses exchange approx. for 3 electron ions (as in 1) in distorted wave. M Ali (Howard Univ) and A K Bhatia.
- 18.3 Uses exchange approx. in distorted wave for arbitrary ion. Program being developed by M Pindzola (NRC fellow at Goddard) and A K Bhatia. Application currently being made to C, Si as indicated. Chief element of program is not to assume orthogonality of scattered orbital to bound orbitals!
- 18.4 Current work UCL distorted wave computer programme. Work being done by A K Bhatia. In the case of Si IX and S XI with the collaboration of H E Mason.

- 19. Dr Eleonore Trefftz
  - 19.1 B-like 2s<sup>2</sup>2p<sup>2</sup>P-2s2p<sup>2</sup> <sup>4</sup>P, UCL Impact program, as exercise for using Impact; further aim: relativistic effects. E Trefftz, C W Dankwort.

# 20. Dr Donald G Truhlar

- 20.1 Planned work Close coupling calculations. D G Truhlar and M E Riley.
- 20.2 Planned work Close coupling calculations. D G Truhlar.

# 21. Prof Kenneth Smith

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21.1 Current work - Multiconfiguration close-coupling approximation. K Smith and S J Wade. - 39 -Contributors' Addresses

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References to Plasma Measurements and to Crossed Beam Measurements

A list of references to measurements of cross sections and rates for electron impact excitation in positive ions has been assembled. Those references appearing before December 1974 were obtained from the Bibliography of Low Energy Electron and Photon Cross Section Data by Lee J. Kieffer.\* The remainder result from a search of the literature appearing between January 1975 and the middle of 1976. The references were not subject to critical selection, and it is possible that a few were overlooked.

The measurements may be divided into classes: plasma measurements and crossed beam measurements. The former are rate coefficient measurements made primarily in multiply ionized species. The crossed beam measurements are forethe excitation cross sections of spectral lines. In some instances, that type of cross section is used to obtain a level excitation cross section. With one notable and encouraging exception (ref. 15), the crossed beam measurements are for singly ionized species. Unfortunately, the two classes overlap for only one transition.

The accompanying chart presents the available data in a convenient form. It gives access to the numbered references on the list. Note that isoelectronic sequences follow diagonals.

Lee J. Kieffer, Bibliography of Low Energy Electron and Photon Cross Section Data NBS Special Publication 426, U.S. Government Printing Office, Washington 1976.

Element	Ion									
	I (0)	II (1)	III (2)	IV (3)	V (4)	VI (5)	VII (6)	VIII (7)	IX (8)	X (9)
H 1 He 2 Li 3		18,19,20,21,22								
<u>Be 4</u> B 5 C 6					5,9,12					
<u>N 7</u> 0 8 F 9	 Neutr			8	1,11,15 8	5 11	4,5	5		
Ne 10 Na 11 Mg 12	als Not	77	7	7	7	7	7,8,13	6,7,10,11	5	
A1 13 Si 14	; Consid								8	
P         15           S         16           C1         17	1ered									
<u>A 18</u> <u>K 19</u> Ca 20		26		· · · · · · · · · · · · · · · · · · ·				2		
Sc 21 Ti 22										
Cr 24 Mn 25 Fe 26									3	2

Compiled by W.L. Rowan, NBS, Washington, D.C.

For heavier elements, the following data sources are available: Kr II  $\rightarrow 26$ ; Ba II  $\rightarrow 14, 16, 24$ ; Hg II  $\rightarrow 17$ .

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1.	B.C. Boland, F.C. Jahoda, T.J.L. Jones and R.W.P. McWhirter, J. Phys. <u>B</u> : <u>Atom. Molec</u> . <u>Phys</u> . 3, 1134 (1970)
2.	R.U. Datla, H.J. Kunze, D. Petrini, <u>Phys</u> . <u>Rev</u> . <u>A</u> <u>6</u> , 38 (1972)
3.	R.U. Datla, M. Blaha, H.J. Kunze, <u>Phys. Rev. A</u> 12, 1076 (1975)
4•	R.C. Elton and W.W. Koeppendoerfer, Phys. <u>Rev</u> . <u>160</u> , 194 (1967)
5•	W. Engelhardt, W. Koeppendoerfer, and J. Sommer, Phys. Rev. A 6, 1908 (1972)
6.	G.N. Haddad and R.W.P. McWhirter, J. Phys. B: Atom. Molec. Phys. 6, 715 (1973)
7•	Einar Hinnov, <u>JOSA</u> <u>56</u> , 1179 (1966) , <u>JOSA</u> <u>57</u> , 1392 (1966)
8.	W.D. Johnston III and H.J. Kunze, Phys. Rev. A 4, 962 (1971)
9•	H.J. Kunze, A.H. Gabriel, Hans R. Griem, Phys. <u>Rev</u> . <u>165</u> , 267 (1968)
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- 15. J.N. Bradbury, T.E. Sharp, B. Mass and R.N. Varney, <u>Nuclear Instruments</u> and <u>Methods 110</u>, 75 (1973)
- 16. D.H. Crandall, P.O. Taylor, and G.H. Dunn Phys. Rev. A 10, 141 (1974)
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- 18. N.R. Daly and R.E. Powell, Phys. Rev. Lett. 19, 1165 (1967)
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   V.A. Kelman, <u>Sov. Phys. JETP</u>, <u>USSR</u> (English Translation) <u>40</u>, 249 (1974)

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- 23. V.A. Kelman and A.I. Imre, Optics and Spectroscopy USA 38, 709 (1975)
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### REPORT OF THE WORKING GROUP ON THE REQUIREMENTS OF ATOMIC STRUCTURE DATA

Working Group Members

Bromage, Mr. G.E. Drawin, Dr. H.W. (Chairman) Fawcett, Mr. B.C. Martinson, Prof. I. Wiese, Dr. W.L.

### Introduction

The working group has examined the status of atomic structure data with respect to the needs of Thermonuclear Fusion Research Programs. It is evident that there are major gaps in the data and that many immediate, as well as long term, needs exist: we focused especially on the very serious implications of heavy ion impurities in high-temperature plasmas, for example, radiative energy losses, which have been well described in the literature (see e.g. Review Paper A4). We deliberately excluded from discussion molecular structure problems, which may become important in the future. The subject has been subdivided into the following four data areas:

Wavelengths and energy levels, Atomic transition probabilities, Line shapes, Radiative excitation, ionization and recombination processes.

For each of these categories we addressed three topics, namely:

Data requirements and justifications. Assessment of the existing data compilations. Recommendations to IAEA.

### A. Data Requirements and Justification

### 1. Wavelength Data and Energy Levels

### Data required

1.1 Identification of the most intense lines in the spectra of elements heavier than nickel, in all stages of ionization, for all elements used as wall and limiter materials in fusion devices.

#### Reasons

Wavelengths of these lines, mostly not yet available are needed for basic identification of presence and ionization states of impurities.

### Data required

1.2 Identification of the spectra of highly ionized impurity elements in spectral regions conveniently access-' ible to experiments, including forbidden lines.

1.3 Detailed identification of spectra arising from transitions involving the most important configurations, for all impurity elements encountered in fusion research.

1.4 Attention should also be paid to the following more specific points:

- i) wavelengths of K and L x-ray transitions of highly ionized impurity elements as a function of ion charge state
- ii) wavelengths of dielectronic-recombination "satellite" lines
- iii) energy levels for autoionizing states
- iv) ionization energies

## 2. Atomic Transition Probabilities

2.1 Determination of the atomic transition probabilities of resonance and other prominent lines for highly ionized species of all those elements used as wall and limiter materials in fusion devices.

2.2 Determination of atomic transition probabilities of light element impurities (C,N,O) with high accuracy (5-10%) and covering essentially the complete spectrum.

2.3 Atomic transition probabilities of medium to high accuracy (10-25%)for medium atomic weight elements used as wall materials (Cr,Fe,Ni).

#### Reasons

Important for diagnostic purposes, for example via measurement of Doppler widths of lines in the visible or near ultraviolet.

Detailed knowledge provides valuable support for wave functions calculations and hence for calculations of oscillator strengths and excitation cross-section.

Needed for independent determination of stage of ionization of impurities.

Needed especially for diagnostics, and partly for plasma modelling.

Needed for presently used approaches to the heavy ion impurity problem, both for measurements of impurity concentrations as well as modelling of the radiative power losses.

Required (a) to select most suitable lines for impurity diagnostics, including spatial and temporal distributions of species in plasma, (b) to obtain detailed modelling of impurities for plasma energy balance, e.g. for laser and electron beam-induced high density plasmas ("laser fusion").

Similar to above, e.g. for diagnostics (including applications of the branching ratio technique), plasma modelling, determination of impurity levels and radiative power losses of plasmas deviating from corona regime, to check theory regarding target wavefunctions.

# Data required

#### Reasons

2.4 Determination of autoionization probabilities.

2.5 Atomic transition probabilities for forbidden lines of highly ionized species with relatively long as well as short wavelengths. Knowledge is required for calculation of dielectronic recombination coefficients, ionization balance, radiation energy losses, and plasma modelling.

(a) Needed for selecting suitable lines for Doppler ion temperature diagnostics, (b) also required for plasma modelling (e.g. in calculating the population densities of excited levels of ions having metastable levels and hence in predicting their spectra, power loss, etc.)

### 3. Line Shapes

3.1 Line profiles, especially Stark broadening parameters.

Plasma diagnostics; solution of radiative transfer problems, especially for high density plasma; plasma modelling.

3.2 Influence of strong magnetic and electric fields on line profiles, emission spectra, and dielectronic recombination. Plasma diagnostics; solution of radiative transfer problems, especially for high density plasma; plasma modelling.

### 4. Radiative Excitation, Ionization and Recombination Processes

4.1 Influence of radiation fields on atomic structure, photon excitation and ionization processes.

4.2 Recombination mechanisms:

- i) radiative
- ii) dielectronic
- iii) collisional-radiative

Ionization processes in the presence of strong laser radiation fields; plasma modelling.

Plasma modelling, energy loss calculations, plasma diagnostics (e.g. satellite lines). Special attention should be given to the influence of strong magnetic fields on the recombination coefficients, and especially on the dielectronic recombination coefficients. In the field of wavelengths and atomic energy data compilations the following principal tabulations are available:

- Atomic Energy Levels, Vols. 1,2,3, published by the NBS, Washington, 1949, 1952, 1959, and supplements on CI - CVI, NI - NVII, OI, HI, DI, TI, SII - SIIV. Also, a new series of NBS compilations appearing in J. Phys. Chem. Ref. Data: FeI - FeXXVI, CrI - CrXXIV, (MnI - MnXXV in preparation).
- Revised Multiplet Tables, published by the NBS, Washington, 1945.
- Atomic and ionic emission lines below 2000 A, H through Kr, by R.L. Kelly and I.J. Palumbo, Naval Research Laboratory, Washington, 1973.
- Wavelengths and Classifications of Emission Lines, Z 28, by
   B.C. Fawcett, Atomic Data and Nuclear Data Tables, <u>16</u>, (1975)
   135-164.

Other useful publications are:

- Bibliographies on atomic energy levels and spectra, through June 1975, by NBS, Washington.
- Critical bibliography by Prof. Edlen, Lund University, published in the book "Beam-Foil Spectroscopy", I.A. Sellin and D.J. Pegg, Eds., Plenum Press, 1976.
- Atomic Energy Levels and Grotrian Diagrams, Vol. I, H through P XV by S. Bashkin and J.O. Stoner, Jr., North-Holland, Amsterdam, 1975.

In the field of atomic transition probabilities the following principal tabulations are available:

- Atomic Transition Probabilities Vol. I (H through Ne), Vol. II (Na through Ca) published by NBS, Washington, 1966 and 1969, and supplements on Sc, Ti.

These tabulations are being complemented by the NBS bibliographies on Atomic Transition Probabilities, NBS Spec. Publ. 320, and Supplements I and II. In the field of Line Shapes Data the following principal tabulation exists: Spectral Line Broadening by Plasmas, by H.R. Griem, Academic Press, 1974. This book is complemented by the NBS - bibliography on Atomic Line Shapes and Shifts, NBS - Spec. Publ. 366, and Suppls. I and II (1972, 1974, 1975). For the other subject areas no critical data compilations exist. However, original work in the field of dielectronic recombination is being done in several laboratories (see e.g. Review Paper A4).

It is the opinion of the members of the Working Group that with respect to the requirements for Fusion Research the aforementioned compilations contain the following serious shortcomings:

- The three major atomic energy data compilations are rather incomplete with respect to the highly ionized heavy atoms. Furthermore, the compilation of Bashkin and Stoner only deals with the light elements up to phosphorus, and that of Kelly and Palumbo goes up to krypton and deals only with wavelengths in the vacuum ultra-violet region. These later compilations rely to a large part on the earlier mentioned atomic energy level compilations.
- Similarly, in the field of atomic transition probabilities the two major compilations are seriously deficient on highly ionized species. Most of the data on such ions have been obtained since then.
- On the subject of line shapes, the book of Griem only contains data for neutral and singly ionized species.

### C. Recommendations to IAEA

On the basis of the assessments in Secs. A. and B. the members of the Working Group recommend that experimental and theoretical work on atomic structure centered on highly ionized species of heavy element impurities, as well as the updating and extension of compilations, should be given very high priority. Specifically:

### 1. Level structure of highly ionized systems

We recommend continued and increased efforts for their investigation. This should be pursued through theoretical calculations and especially through spectroscopic studies of highly ionized plasmas generated for instance in Tokamaks, theta-pinches, laser-produced plasmas, vacuum sparks, and beam foil sources. In particular, a more complete description of atomic energy levels is desirable, which should include the percentage composition of the levels.

### 2. Wave length compilations

Actual situations require substantial improvement. The description of atomic energy levels in terms of their composition as adopted by the National Bureau of Standards should become standard for the sake of easy comparison of data from different sources.

#### 3. Radial parts of the wavefunctions

We recommend their tabulation further; Slater radial integrals computed by Hartree-Fock methods should be tabulated along with empirically adjusted Slater integrals for use by theoretical groups calculating atomic quantities like transition probabilities and cross-sections. Work of this kind needs accurate wavefunctions and term compositions. It is often of interest to study many members of the same iso-electronic sequence, up to high degrees of ionization. The radial parts of the wavefunctions are needed in simple parametric form to permit easy calculation of radial integrals. Since the tabulation of multiconfiguration wavefunctions for all systems of interest is likely to be costly and typographically impossible, it would be desirable to have available programs ready for use to produce the data requirements.

## 4. Determination of atomic transition probabilities

In this area the most promising approaches for determining data primarily theoretical calculations and beam foil spectroscopy - should be vigorously applied. Advanced calculational methods should provide the bulk of the data, with experimental work providing mainly key check points. Since the experiments have not yet reached the area of very highly ionized species of primary interest for fusion plasma diagnostics, special efforts should be made to proceed in this direction. Also, full use should be made of systematic trends and regularities in atomic oscillator strengths. It is very desirable that the data have high accuracy, approaching the 10% level.

### 5. Compilation of atomic transition probabilities

Their compilations urgently need to be updated and extended to include all ionic species of interest to the fusion research programme. Especially important is an update of the tabulations of the principal light element impurities C, N, O, Al and Si.

### 6. Line shapes

Theoretical and experimental work should be concentrated on two specific subjects:

6.1 Determination of Stark broadening parameters for highly ionized species, which are especially needed for high-density plasmas generated by lasers.

6.2 Influence of strong magnetic and turbulent electric fields on the profiles of Doppler broadened lines used for ion temperature measurements in lower density plasmas.

### 7. Stark broadening

Critical data compilations of relevant parameters should be initiated as soon as a significant body of data becomes available.

### 8. Recombination processes

In this field work should be concentrated on the following four areas:

- 8.1 Measurement of the intensities and wavelengths of satellite lines due to dielectronic recombination.
- 8.2 Calculation of recombination rate coefficients, including dielectronic recombination, and their experimental verification.
- 8.3 As soon as sufficient data are available, a critical compilation should be undertaken.
- 8.4 Further studies of autoionization, dielectronic and collisional radiative recombination to high Rydberg states in the presence of intense magnetic fields.

REPORT OF THE WORKING GROUP ON SURFACE INTERACTION DATA FOR FUSION DEVICES

### Working Group Members

Anderson, Dr. H.H. Boschi, Dr. A. Bottiger, Mr. J. Erents, Dr. S.K. Krebs, Prof. K.H. Martinez, Dr. J. Martynenko, Dr. Yu.V. McCracken, Dr. G.M. (Chairman) Nakai, Dr. Y. Navinsek, Dr. B. Pocs, Dr. L. Riccato, Dr. A. Vernickel, Dr. H. Waelbroeck, Dr. F. Watkins, Dr. J.

#### Introduction

Plasmas in magnetic containment devices are confined for relatively short times so that in any practical system the material walls surrounding the plasma will be subjected to bombardment by energetic ions and atoms, ultraviolet radiation and neutrons. The flux of these particles to the wall will result in the release of impurities into the plasma by a number of mechanisms. These impurities are known to have a deleterious effect on the plasma resulting most importantly in large energy losses by radiation. The input information which is required for surface interaction studies is the flux and energy distribution of the particles to the wall. Such studies aim to provide the fluxes and energies (and other relevant parameters) of the impurities re-entering the plasma. These data can then be used together with data on atomic reaction rates to estimate the concentrations of impurities in the plasma and hence the energy loss rates from the plasma. The data required from the surface physicist is thus dependent on the fluxes arriving at the walls and on the parameters which are relevant to the atomic collision processes of the impurity flux from the wall. Because these different areas are so interdependent, a number of iterative stages will obviously be required before it is clear what are the most important mechanisms for impurity production, and therefore what accuracies are required. Although some estimates of particle fluxes to the wall in reactors may be made on rather general grounds, particle fluxes in contemporary plasma containment devices are not well known.

The present working party has considered the role of surfaces primarily from the point of view of the effects of impurities and of plasma recycling. An equally important aspect is the erosion and radiation damage, which may affect the mechanical integrity of the first wall. There are both immediate and long term needs for the understanding of first wall interactions. We have considered the materials which are of primary importance and also studied the underlying physics of the surface interaction concerned.

### A. Particle Surface Interactions

There are many particle surface interactions which may be relevant to the problems of controlled fusion and these have been outlined in a number of different reports. In our review of the interactions of importance we have relied to a large extent on the Review Paper A2 prepared for the advisory group meeting by Dr. H. Vernickel. In his paper he discusses the role which these processes play in the different types of plasma containment devices. We list below the processes, the energy ranges of the primary particles, and the parameters most of interest. The fluxes of particles to the wall in reactors have been summarized in the proceedings of an earlier IAEA workshop.\* Note that hydrogen is used as shorthand for all the hydrogen isotopes.

### 1. Reflection of hydrogen and helium

Primary energy: 10 eV to 10 keV

Data to be measured: reflection coefficient, energy and angular distributions, charge state, excitation state

Important parameters: angle of incidence, surface structure

### 2. Accommodation of hydrogen atoms

Primary energy: 1 eV to 100 eV Data to be measured: accommodation coefficient

### 3. Trapping of hydrogen and helium

Primary energy: 100 eV to 100 keV (hydrogen), 3.5 MeV (helium) Data to be measured: trapping coefficient Important parameters: angle of incidence, temperature, dose, influence of radiation damage

Nuclear Fusion, Special Supplement on Fusion Reactor Design Problems, p. 472, 1974.

#### 4. Detrapping processes for hydrogen and helium

These processes concern thermal and beam induced desorption of trapped gas

Primary energy: 10 eV to 100 keV

Data to be measured: detrapping cross-sections, energy distribution

Important parameters: angle of incidence, target temperature, influence of radiation damage

### 5. Sputtering by hydrogen, helium, and "impurities"

Energy: from threshold to 100 keV

Data to be measured: yields, angular and energy distribution of sputtered material, chemical composition of sputtered material

Important parameters: angle of incidence, temperature for multicomponent surfaces

### 6. Blistering by hydrogen and helium

Energy: 1 keV to 100 keV (hydrogen) or 3,5 MeV (helium)

Data to be measured: critical dose

Important parameters: energy and angular distributions of incident particles (simultaneous He and H bombardment, see also discussion on synergistic effects)

Most important aspect: does blistering or exfoliation contribute to wall erosion for high dose bombardment, and if so, under what conditions? Yields, size of particles, and composition

#### 7. Desorption by ions (hydrogen, helium, impurities)

Primary energy: from threshold to  $\sim 100 \text{ keV}$ 

Data to be measured: cross-section, charge state, excitation state, energy distribution

Important parameters: angle of incidence, surface damage, surface composition

### 8. Desorption by electrons

Primary energy: from threshold to 100 keV

Data to be measured: cross-section, charge state, excitation state Important parameters: surface damage, surface composition

### 9. Desorption by photons

Energy: 5 eV to 100 keV Data to be measured: cross-section, charge state Important parameter: surface damage

#### 10. Chemical reactions of hydrogen atoms and ions

Data to be measured: reaction probability

Important parameters: energy of hydrogen atom, surface temperature, effect of surface contamination, flux density of incident particles

### 11. Secondary electron emission due to ions and electrons

Primary energy: 10 eV to 100 keV Data to be measured: coefficients Important parameters: angle of incidence, surface composition

### 12. Arcing

Little direct evidence of arcing has been published, but both unipolar and power arcs may play a role in the region outside limiters and at divertor targets

### 13. Energy loss

Energy loss for hydrogen and helium are necessary for theoretical predictions and interpolations concerning the earlier points 1, 2, 4, 5, 6 and 11.

### B. Surface Materials of Interest

Since there are so many different criteria determining the wall material it is not always possible to specify the ideal material from the point of view of the surface interactions. Some decoupling of the two requirements for surface interactions and structural materials may be obtained by use of surface coatings or liners. The materials of interest fall into five broad categories.

### 1. Stainless steels and Inconels

These are of particular interest as being the constructional materials of present generation and the next generation machines, e.g. P.L.T., T.F.T.R., T.10, T.20, J.E.T., J.T.60. The most commonly used alloys are stainless steels 304L and 316LN and Inconel 600 and 625.

#### 2. Refractory materials e.g. Mo, Nb, V, W and alloys

These are used in present machines as limiters and may possibly be used in high temperature commercial reactors. However, the high atomic number (z), particularly of tungsten, and high cost are disadvantages.

### 3. Low z materials e.g. C, SiC, B4C, A1203, Be, BeO, BN

These materials may reduce the total radiation because of their low atomic number and some have been used in tokamaks already with encouraging results. However, chemical effects leading to impurities have been shown to be serious in some cases, e.g. carbon.

### 4. Trapping materials

In applications where large fluxes of ions have to be pumped, e.g. in divertors, metals which react chemically with hydrogen are being used. Exemples are Ti, Zr.

### 5. Coatings

This heading covers the use of thin coatings of materials on top of structural materials. These coatings may either be of the materials mentioned above, e.g. low z materials, or of thin metal films. The latter are of interest because in practical devices thin films are produced in the course of operation due to evaporation, sputtering, etc. The wall of many plasma containment devices has been observed to be covered with a layer of molybdenum from the limiter.

### C. Characterization of Surfaces

Many of the surface properties of interest are very sensitive to the surface conditions, in particular to surface composition and structure. Thus the importance of surface characterization is emphasized. Three aspects of the problem, can be considered.

### 1. The source of the materials

Since the composition and structure, particularly of alloys, can vary with manufacturer, a common source of these materials for investigations of surface properties would be very valuable. It is suggested that this might be coordinated through the designers of large machines e.g. T.F.T.R., J.E.T., and T.20 and J.T.60.

### 2. Surface preparation

The cleaning techniques, both liquid chemical cleaning and discharge cleaning, have an important bearing on the surface composition and hence on surface properties. Discharge cleaning techniques are still at a very empirical stage and the development of these techniques is important. In particular, direct measurements of the efficiency of different techniques and their comparison, is an important element in the surface interaction program. The importance of working on materials characteristic of real plasma devices is emphasized, and efforts should be made to characterize the wall materials in machines after discharge cleaning and operation in order that surface interaction data may be obtained on relevant technological surfaces as well as pure materials.

### 3. Measurement of composition and structure

The direct measurement of composition and structure of the surfaces on which surface interactions are being studied is important. It was noted that surface composition and structure will change during bombardment by ion beams. This can be particularly important in the case of multi-component alloys where preferential sputtering can take place. Thus the composition may depend on the bombardment dose rate and possibly on the rate of replacement of the preferentially sputtered material from the bulk by thermal or radiation enhanced diffusion.

#### D. Accuracies

Because of the strongly interactive nature of the plasma and wall processes and the many approximations used in the simulation of the wall, it was not considered possible to give estimates of the accuracies required from computer modelling. Ultimately it is hoped to undertake sensitivity analysis using computer modelling which would allow accuracies to be specified.

Accuracies which should be obtainable experimentally were discussed and the following estimates suggested:

-	Particle	reflection	coefficients	(backscattering)	) <u>+</u> 20%

- Energy reflection coefficients <u>+</u> 20%

- Sputtering yields

-	when measured for a particular sample of defined preparation and composition	<u>+</u> 10%
-	for materials of the same nominal com-	

within a factor of 2

It is noted however, that although absolute yields will change due to variations in binding energy the trends with parameters such as energy and angle of incidence should be reproducible to within  $\pm 20\%$ .

position in different laboratories

*****	Secondary Electron Emission	±	20%
-	Desorption cross-sections	<u>+</u>	50%

An extension of the range of parameters investigated as outlined in Section A, and a more thorough understanding of the fundamental processes are considered to be more important than more accurate measurements.

### E. Priorities

The working group did not undertake to formulate a detailed list of priorities. Since there had been a previous study by consultants to the IAEA who included it, their recommendations are listed in <u>Appendix A</u>. It is clear that priorities are to some extent subjective and they will change as new ideas and methods of operation arise. To take an obvious example, if a satisfactory low z wall material is developed, no further data on heavy metals will be required, except for neutral injection. However, within these limitations there were some broad areas in which it was felt that emphasis was required:

- Measurements at low energies < 3 keV
- Data on materials used in next generation machines e.g. stainless steels and inconels as in Section C
- Data on desorption processes and cleaning methods relative to the removal of surface impurities by ions, electrons and photons.

### F. Data Compilation and Evaluation

Three stages in theprocess can be distinguished

- Bibliography
- Data compilation
- Data evaluation

Only two attempts to collect data were identified by the working group, these were:

- the Vacuum and Surface Physics Index produced by the IPP Garching, FRG, which produces a monthly bibliography covering the field of interest to fusion, within the wider vacuum field. This is carried out in collaboration with the ZAED and the IUVSTA.\* No compilation or evaluation of data is attempted but computer-aided literature searches can be undertaken.
- the Controlled Fusion Atomic Data Centre at ORNL. This annotated bibliographical file includes surface interaction data as well as gas phase atomic collisions. Difficulties have been found in attempting to evaluate surface data since little attention has been paid to surface characterization. Data compilation in some areas of surface interactions have been undertaken.

It was considered that, although many difficulties in evaluating data occur in some areas of surface interactions, data compilation should be relatively straightforward. In particular data for low energy, light ion interactions is relatively limited and so the task of compilation will not be overwhelming. Such a compilation would make clear the extent of scatter of the data and the areas where more data are required. The following surface interactions were those considered to be ones in which it would be possible and useful to carry out compilation and evaluation:

- Sputtering
- Backscattering coefficients
- Desorption cross-sections by ions, electrons and photons
- Thermal desorption of adsorbed gases and release of implanted gas
- Secondary electron emission by ions and electrons
- Stopping power measurements and ranges
- Chemical interaction yields by ions and atoms

Computerization of the data, as in the atomic physics field, should be examined.

### G. Special Areas of Surface Interactions

A number of special problems arise in particular techniques. These were not discussed in detail but note was taken that in some cases additional surface data might be required for a full understanding.

IUVSTA = International Union for Vacuum Science Technique and Applications.

### 1. Pellet injection

It is clear that if pellet injection is used as a method of refuelling plasmas the process of ablation will require investigation. A qualitative idea of the processes involved is probably best acquired by direct observation of ablation in plasmas. However, fundamental data on sputtering and secondary electron emission from solid hydrogen surfaces will be required.

### 2. Heating techniques

Both r.f. heating and neutral injection may give rise to local particle fluxes and energies much higher than observed in ohmically heated plasmas. In our assessment of the energy range of interest in different phenomena we have tried to include these effects. However, more detailed information on the fluxes and energies to be expected would be valuable. Heavy metal impurities in the beam could be important.

### 3. Cold gas blanket and gas puffing

The special conditions at the wall, which will be of interest, have not been adequately assessed. They might include recombination phenomena and diffusion into the bulk materials.

#### H. Conclusions

# Survey of surface interactions, tabulation of relevant parameters, priorities

Surface interactions of importance in fusion have been surveyed and the processes, energies and other parameters of interest have been tabulated. Assessment of priority areas has been included. Another evaluation of priorities has been examined and there is general agreement with its conclusions.

### 2. Characterization of surfaces

One of the major problems in assessing surface interaction data is the one of adequately characterizing the surface and proposals have been put forward as to how this situation can be improved. Emphasis has been put on using materials of direct relevance to the fusion programme and on the use of well defined and relevant surface preparation techniques. However, further understanding of the fundamental physics is also required in many areas.

### 3. Data compilation and evaluation

Despite the difficulties, there are some areas of surface interaction where the underlying physics is well enough understood to make data compilation and evaluation a worthwhile exercise. These areas include sputtering, backscattering, secondary electron emission (by ions and electrons), energy loss measurements, desorption cross-sections (by electrons and ions) and chemical interaction yields. In other areas which include blistering, arcing and synergistic effects, the underlying physics is not well enough understood to make compilation or evaluation very fruitful at the present stage. However, properly annoted bibliographies in these areas are required.

### I. Recommendations

It is recommended that

- 1. The two data centres at present preparing bibliographies in the area of surface interactions (and others if they exist) discuss ways in which the work may be coordinated and possibly integrated. That the IAEA consider playing a role in the dissemination of the bibliographies produced.
- 2. That compilation and evaluation of data in the field of surface interactions for fusion be initiated by the IAEA starting with the specific areas identified as being suitable.
- 3. Further assessments of needs and priorities in the surface interaction field should be carried out at regular intervals.
# Priority List of Surface Interactions of Importance in Fusion Devices

From the recommendations of a panel of consultants to the IAEA Vienna, November 1975. The indicated priorities and urgencies were estimated by three consultants.

The consultants listed a number of surface effect processes of importance to fusion. Each was rated on its priority and when the information might be available.

Priority:	High	→	1	Urgency:	Near term	(0-2 years)→1
	Medium	$\rightarrow$	2		Medium term	(2-4 years)→ 2
	Low	→	3		Long term	( 4 years)→ 3

Proc	cess	Priority	Urgency		
1.	Sputtering:	(a)	Physical; liberation of mate- rial due to beam of particles	1,1,1	2,2.5,3
		(b)	Chemical; non-momentum trans- fer	1,1,1	2,2,2.5
2.	Desorption; re				
		(a) (b) (c) (d)	Ions Electrons Photons Thermal effects	1,2,2 2,3,3 2,2,3 1,2,2	2,2,3 1,1,3 2,3,3 1.5,2,3
3.	Blistering by	(a) (b)	Alphas Hydrogen isotopes	1.5,2,3	1,3,3
4.	Backscattering	1,2,2	2,2,2		
5•	Trapping and r	2,2,2	2,2,2		
6.	Pellet refuell electrons with	2,2,2	2,3,3		
7•	Impurity contr cleaning	1,1,1	1,2,1		
8.	Chemical react z materials	1,2,2	2,2,3		
9•	Combined effec plus large the	1,1.5,2	3,3,3		

# Advisory Group Meeting on Atomic and Molecular Data for Fusion

#### REVIEW TOPICS AND REVIEWERS

#### Introductory Papers

- Overall Appraisal of A+M Data for Fusion, Present and Future (M.F.A. Harrison)
- 2. Proposed IAEA Programme on A+M Data for Fusion (J.J. Schmidt and A. Lorenz, IAEA)

#### A. Data Needs, Priorities and Accuracies

- 1. Beam Injection (J.T. Hogan, ORNL, US)
- 2. Plasma Surface Interaction (H. Vernickel, IPP, FRG)
- 3. Plasma Modelling (M.L. Watkins, Culham Laboratory, UK)
- Plasma Impurities and Cooling (H.W. Drawin, Fontenay-aux-Roses, France)
- 5. Plasma Diagnostics (R.W.P. McWhirter, ARD(SRC) Culham Laboratory, UK)

#### B. National Programmes and Emphasis

- 1. France (J.L. Delcroix, Centre d'Orsay)
- 2. Federal Republic of Germany (F. Waelbroeck, KFA Juelich)
- 3. Japan (H. Suzuki, Nagoya University, Nagoya)
- 4. USSR (Yu.V. Martynenko, Kurchatov Institute, Moscow)
- 5. United Kingdom (M.F.A. Harrison, Culham Laboratory)
- 6. United States (C.F. Barnett, ORNL)

IAEA Advisory Group Meeting on

Atomic and Molecular Data for Fusion

Culham Laboratory, 1-5 November 1976

# Meeting Agenda

### Monday, 1 November

- Opening of the meeting
- Welcome on behalf of IAEA: J.J. Schmidt
- Welcome on behalf of Culham: R.S. Pease
- Opening address: Sir Harry Massey
- Meeting organization: A. Lorenz
  Meeting schedule and organization
  - Appointment of session chairmen and working group chairmen

First presentation session: C.F. Barnett, chairman

- First introductory paper
   "The Role of Atomic and Molecular Processes in Fusion Research", M.F.A. Harrison
- <u>Second introductory paper</u> "Proposed IAEA Programme on A+M Data for Fusion", J.J. Schmidt
- <u>Review Paper Al</u> "Data Needs, Priorities and Accuracies for Beam Injection", J.T. Hogan
- <u>Review Paper A2</u>
   "Data Needs, Priorities and Accuracies for Plasma Surface Interactions", H. Vernickel
- <u>lst Contributed Paper to topic A2</u> "Blistering of Stainless Steel by He<sup>+</sup> Ions", B. Navinsek
- <u>2nd Contributed Paper to topic A2</u> "Investigation of Sputtering and Secondary Ion Yield from Metals under Bombardment of Noble Gases", H. Krebs
- <u>Review Paper A3</u>
   "Data Needs, Priorities and Accuracies for Plasma Modelling", M.L. Watkins

- First Contributed Paper to topics A3 and A4 "Survey on the Scattering of Electron by Atoms", C. Joachain
- Panel Discussion of Technical Objectives (Drs. Barnett, Afrosimov, Hogan, McCracken and Drawin, panelists and Dr. Harrison, moderator)

#### Tuesday, 2 November

- <u>Review Paper A4</u> "Data Needs, Priorities and Accuracies in Considerations of Plasma Impurities and Cooling", H.W. Drawin
- <u>Second Contributed Paper to topics A3 and A4</u> "Cross Section Data Including Atoms and Ions in the Highly Excited Rydberg States", S. Ohtani
- <u>Review Paper A5</u> "Data Needs, Priorities and Accuracies for Plasma Diagnostics", R.W.P. McWhirter
- <u>lst Contributed Paper to topic A5</u>
   "Techniques for the Calculation of Atomic Data Required for Plasma Diagnostics", H.E. Saraph
- <u>2nd Contributed Paper to topic A5</u> "Measurements of Atomic Transition Probabilities in Highly Ionized Atoms by Fast Ion Beams", I. Martinson

Second presentation session: H. Suzuki

- <u>Review Paper Bl</u> "National Programmes and Emphasis in France", J.L. Delcroix
- <u>Review Paper B2</u>
   "National Programmes and Emphasis in the Federal Republic of Germany", F. Waelbroeck
- <u>Review Paper B3</u> "National Programmes and Emphasis in Japan", H. Suzuki
- <u>Contributed Paper to topic B3</u> "Activities on Atomic and Molecular Data in JAERI", Y. Nakai (JAERI)
- <u>Review Paper B4</u> "National Programmes and Emphasis in the USSR", Yu.V. Martynenko

- <u>Review Paper B5</u> "National Programmes and Emphasis in the United Kingdom" M.F.A. Harrison
- <u>Contributed Paper to topic B5</u> "(Storage and Retrieval of Bibliographic and Numerical Atomic and Molecular Data at the Queen's University in Belfast)", F.J. Smith
- <u>Review Paper B6</u> "National Programmes and Emphasis in the USA", C.F. Barnett
- <u>Contributed Paper to topic B6</u> "Atomic Physics Program of the Division of Physical Research of ERDA", J.V. Martinez
- <u>Contributed Paper to topic B6</u> "Atomic Data Compilation and Evaluation Programmes at NBS", W.L. Wiese
- <u>Contributed Paper to topic B6</u> "Activities of the Management Research Project at the Lawrence Livermore Laboratory", V. Hampel
- Panel Discussion of Technical Objectives (same panelists and moderator as on Monday) and organization of working groups

#### Wednesday, 3 November

- Working group meetings throughout the day

## Thursday, 4 November

- Working group meetings. Working groups to finalize their draft reports
- Culham laboratory tour

#### Friday. 5 November

- Plenary Session: Discussion and Approval of Working Group Reports

ANNEX III

- 73 -

IAEA ADVISORY GROUP MEETING ON ATOMIC AND MOLECULAR DATA FOR FUSION

CULHAM LABORATORY, 1-5 NOVEMBER 1976

#### LIST OF PARTICIPANTS

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