



International Atomic Energy Agency

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**INTERNATIONAL NUCLEAR DATA COMMITTEE**

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**FIFTH MEETING OF THE IFRC SUBCOMMITTEE ON  
ATOMIC AND MOLECULAR DATA FOR FUSION**

**IAEA Headquarters, Vienna  
7-8 October 1988**

**SUMMARY REPORT**

**NDS LIBRARY COPY**

**Edited by R.K. Janev**

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

**Fifth Meeting of the IFRC Subcommittee on  
Atomic and Molecular Data for Fusion**

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**SUMMARY REPORT**

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### Abstract

The IAEA Atomic and Molecular (A+M) Data Unit convened the Fifth meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC) in Vienna, Austria, on 7 and 8 October 1988. The current IAEA activity in the field of A+M for fusion was reviewed, and specific recommendations were made regarding this activity in the next two year period.

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## I. Summary of the Meeting

The Fifth meeting of the IFRC Subcommittee on Atomic and Molecular (A+M) for Fusion was convened at the IAEA Headquarters in Vienna, Austria, on 7-8 October 1988. The Meeting was attended by all members of the Subcommittee, except for Dr. N. Shikazono who was substituted by Dr. Y. Nakai, and Dr. V. Abramov. Dr. R.H. McKnight, the future successor of Dr. D.H. Crandall as member of the Subcommittee, also attended the meeting. The list of meeting participants is given in Appendix 1. The adopted agenda of the meeting is given in Appendix 2. The meeting was chaired by Dr. A. Lorenz.

On the basis of the Report of the A+M Data Unit (see Appendix 3), the IFRC Subcommittee reviewed the ongoing IAEA programme in the field of A+M data for fusion and discussed the future activities of the Unit and the Atomic Data Centre Network (A+M/DCN) in this area. The most important issues on which the discussions were focussed and appropriate recommendations made, were the following:

- Status of the numerical data base and data management and exchange systems,
- Near- and long-term priorities in the A+M data evaluation work,
- Plasma-wall interaction data for fusion,
- Status and management of the bibliographic data base,
- A+M data publications, and
- A+M Data Unit manpower.

A summary of the discussions on the above issues is given in the next Section, while the conclusions and recommendations of the Subcommittee are given in Section III. A list of immediate actions which should be taken for implementing the Subcommittee recommendations is given in Section IV of this Report.

The main conclusions of the meeting can be summarized as follows:

- 1) The conditions for creation of an international bank of recommended numerical A+M data for fusion (evaluated data, accepted exchange format and data management system) now exist, and the creation of such a data bank is underway and should be pursued as a top-priority activity by the A+M Data Unit and the A+M Data Centre Network.
- 2) The near- and long-term priorities in the A+M data compilation and evaluation efforts should reflect the A+M data requirements for the current large tokamak experiments and the designs of the next-step fusion devices (such as ITER, NET, TIBER II, OTR etc.), and inclusion data on the fundamental plasma-wall interaction processes should be explored.
- 3) The existing co-ordination of DCN activities and the collaboration with the fusion community should further be strengthened in the areas of recommended data validation, further development of the data exchange system and identification of A+M data needs for the ongoing and envisaged fusion experiments.
- 4) The Agency's programmes in the field of A+M data for fusion are viable and follow the needs of the world fusion programme for such data. In order to continue to fulfill its basic functions and, in particular, to build the A+M numerical data base, it is appropriate to increase the manpower of the IAEA A+M Data Unit.

## II. Meeting Proceedings

### 1. Opening

The meeting was opened by Prof. V.A. Konshin, Director of the IAEA Division of Physical and Chemical Sciences. In his opening talk, Prof. Konshin emphasized the important place of the A+M data activity in the Agency's fusion related programmes. The efforts of the IFRC Subcommittee in advising the Agency on its programmes in the area of A+M data for fusion were highly appreciated. Prof. Konshin stressed the increased role of the IFRC and the Subcommittee in advising the IAEA Director General on fusion related matters after the recent discontinuation of the IAEA Scientific Advisory Council.

### 2. A+M Data Unit Report

The Head of the IAEA A+M Data Unit reported on the Unit's activities during the last two year period, described the status of the ongoing programmes, and proposed programmes for the A+M Data Unit's activity in the next period. The full text of the Report is given in Appendix 3. The report was approved and the Data Unit activity was assessed as highly successful. The discussion then continued along the points and the issues raised in the Report.

### 3. A+M Data Exchange System

The participants expressed the opinion that the adoption of ALADDIN as international A+M data exchange format is an important step forward in the way of creating the IAEA A+M numerical data base and for the data management and exchange. It was stressed that ALADDIN should be put into operation as soon as possible in data evaluation and management practices of A+M data centres. The fusion users should be strongly encouraged to write ALADDIN interfaces to their codes. Questions on whether ALADDIN can also be used for handling also spectroscopic and plasma-wall interaction data were answered positively.

The idea of creating an ALADDIN users Network (ALUN) was discussed (in particular, its structure, tasks, its relation to the A+M DCN, meetings, etc). While creation of ALUN was found useful, establishment of an ALADDIN Newsletter was considered premature. Electronic communication among the ALUN members was suggested instead.

### 4. Numerical Data Base

The existing body of recommended A+M data for fusion (see Appendix 4), was found to form a relatively small part of the A+M data which are presently available and in use in fusion application codes. The participants of the meeting stressed the necessity for intensification of the data evaluation efforts within the A+M DCN (and beyond), and for collecting, up-dating and ALADDIN-formatting the data bases currently used in fusion laboratories by the IAEA A+M Data Unit.

The Subcommittee members reiterated their earlier statement that the DCN should continue to recommend A+M data for fusion, but these data should pass an additional validation procedure before being recommended by the IAEA, and officially disseminated or published. The validation procedure should include also validation by fusion A+M data users to check the utility and adequacy of data presentation.

5. Plasma-wall interaction (PWI) data for fusion

After discussion, it was decided to include particle-wall interaction (PWI) data evaluation in an exploratory manner, within the near-term activity of the A+M data unit. The gas-phase collision data, however, will still remain the first priority for the A+M Data Unit. The PWI data activity should be restricted to fundamental processes only and be strongly related to the needs of current research and reviewed by the Subcommittee. The specific programmes in this area are left to be defined by the IAEA Advisory Group Meeting (AGM) planned for April/May 1989. Prof. Miyahara was asked to act as a liaison officer in establishing the nature and structure of the AGM and co-ordinating with the Subcommittee. It has been emphasized that the PWI data should be stored and disseminated in the ALADDIN format.

The planned AGM on PWI data for fusion was also discussed, both with respect to its scope and structure of participants. It was suggested that the future IAEA PWI data meetings be organized in conjunction with some major international meetings in this area (satellite meetings), such as the International Conference on Plasma-Wall Interactions.

6. Near- and long-term priorities in A+M data evaluation

The meeting discussed the near- and long-term priorities for the A+M data evaluation work. Although the wall and structural materials in the current fusion experiments and design concepts are undergoing relatively rapid changes, a consensus was reached regarding the most important plasma impurities for the envisaged next fusion experiments. Some of these impurities are also machine-invariable. It was also emphasized that the data bases for the basic plasma constituents including helium should be completed as soon as possible. Completion of the data for iron ions and building a data base for the plasma edge carbon- and oxygen-containing molecules were considered also as high near-term priorities. Although data for some PWI processes (e.g. self-sputtering, redeposition, particle release) have a high priority in the current fusion research, the PWI activity was classified as a long-term priority.

7. Other topics discussed

The meeting discussed in detail also the following topics:

- Collaboration within the Data Centre Network,
- ITER related activities of A+M Data Unit and DCN,
- Publication of A+M data in "Nuclear Fusion" and establishment of a regular Nucl. Fusion Supplement for A+M data,
- Status of the bibliographic data base,
- Meetings schedule for 1989-1990,
- Joint IAEA/ICTP (Trieste) workshop on Computational Methods in Atomic Collision Physics,
- A+M Data Unit manpower,
- Collaboration within the IAEA fusion related programmes.

The conclusions of these discussions and the Subcommittee recommendations regarding these subjects are given in the next Section.

## 8. Other matters

The Subcommittee members welcomed Dr. R.H. McKnight as a new Subcommittee member from the USA, replacing Dr. D.H. Crandall. Dr. McKnight was elected as new Chairman of the Subcommittee, with Crandall providing the necessary consultancy.

The meeting was adjourned at 12:30 on October 8.

## III. Conclusions, Endorsements and Recommendations

### 1. Assessment of the IAEA A+M Data Unit Activity

The Report on the IAEA A+M Data Unit Activities since the last IFRC Subcommittee meeting (September 1986) was accepted. The IFRC Subcommittee praised, in the highest terms, the work, initiatives and achievements of the IAEA A+M Data Unit within the last year and fully endorsed the programme and activities of the Unit.

### 2. A+M Numerical Data Base and Data Evaluation Activity

- 2.1. The Subcommittee reiterates its earlier statement, that the creation of a numerical data base (NDB) of recommended data for fusion continues to remain the highest priority of the IAEA A+M Data Unit activity. The first task along this direction should be the storage and dissemination of the existing recommended data in the established ALADDIN format, including provisions for computerized requests for the data.
- 2.2. Prior to dissemination, any set of recommended data should pass a practical validation procedure, for checks of correctness, accuracy and adequacy in fusion application codes. This procedure should be determined in each separate case by the IAEA A+M Data Unit and should include extensive consultations with the DCN members, leading A+M experts and A+M data plasma users.
- 2.3. The existing body of A+M data for fusion is much more extensive than is presently reflected in evaluated and recommended data base. The IFRC Subcommittee urges the Atomic Data Centres for Fusion to intensify their data evaluation work and the A+M Data Unit to assist in the co-ordination of data evaluation efforts, and their possible extension outside the Data Centre Network.
- 2.4. The Subcommittee recommends that, apart from the NDB of recommended A+M data, the IAEA A+M Data Unit (AMDU) assembles, maintains and distributes (on request) the specific-purpose A+M data bases (Libraries) which are comprehensive, more or less complete and in use in major fusion laboratories (PPPL, JET, Culham, JT-60/JAERI, D III-D, Kurchatov, Cadarache, Garching, Jülich). These A+M data libraries should be also put into ALADDIN format, and continuously (or periodically) replaced by the corresponding IAEA recommended data, when these become available.



### 3. ALADDIN Data Exchange System

- 3.1. The Subcommittee endorsed the use of the ALADDIN system as the base for management and exchange of A+M data for fusion on an international basis. The finalization of the first, agreed upon working version of ALADDIN and its implementation into the existing body of recommended A+M data for fusion is the most urgent task of the IAEA AMDU, and the Atomic Data Centre Network.
- 3.2. The fusion A+M data users are strongly encouraged to introduce ALADDIN interfaces to their codes, and to use the ALADDIN format when creating their own specific-purpose A+M data libraries and interactive systems.
- 3.3. The IAEA A+M Data Unit is responsible for maintaining the standard version of ALADDIN, organization and co-ordination of the activities related to the development of the ALADDIN data management and exchange system (changes and extensions of ALADDIN dictionaries, supporting software, etc.) and for prompt dissemination of updated versions of the system to all ALADDIN users. R. Hulse should be consulted before any substantial changes are introduced into ALADDIN and to co-operate in its future developments.
- 3.4. The Subcommittee supports the idea of the formation of an ALADDIN Users Network as a forum for endorsing all the necessary changes in the ALADDIN system, regular reviews of the status and the needs for ALADDIN development, and adoption of upgraded versions of ALADDIN. The core of this Network constitutes the A+M Data Centre Network and the major fusion laboratories which use A+M data in ALADDIN format or ALADDIN interfaces to their codes. The Aladdin Network is open to all A+M evaluated data producers and users. When necessary, the regular DCN meetings may be extended by representatives from the Aladdin Network.
- 3.5. It is suggested that the communication within the Aladdin Network be effectuated through coded electronic mail. Creation of an ALADDIN Newsletter for this purpose could be considered at a later stage, if necessities dictate.

### 4. Co-ordinated Research Programme on A+M Data for Fusion Edge Plasmas

- 4.1. The Subcommittee endorsed the objectives, programme and participants' structure of the initiated three year CRP on A+M data for fusion edge plasmas. The main emphasis within the CRP should be on data for  $H_2(H_2^+)$ , hydrocarbons and carbon oxides.
- 4.2. The evaluated data resulting from the work within this CRP should be promptly introduced in the NDB and made available to the users. Both the interim results (following the annual meetings of CRP participants) and the final results of the CRP should be published in an adequate form.

5. Plasma-Wall Interaction Data for Fusion

- 5.1. Having in mind the progress made by the A+M Data Unit during the last year in constituting the NDB for gas-phase A+M processes, and the urgent needs for plasma-wall interaction (PWI) data in the current fusion research and ITER design, the IFRC Subcommittee endorses the initiative of the A+M Data Unit to explore and identify programmes for data evaluation on PWI processes and creation of a PWI numerical data base. The gas-phase A+M data activity still remains the first priority of the A+M Data Unit. The PWI data activity of the IAEA A+M Data Unit will be focussed on the fundamental PWI processes. This activity, however, should also be closely related to the needs in current fusion research and to ITER design requirements.
- 5.2. The PWI numerical data base should use ALADDIN for data management and exchange. For this purpose, the IAEA A+M Data Unit should develop adequate extensions of ALADDIN structure and dictionaries.
- 5.3. The Subcommittee endorsed the Advisory Group Meeting (AGM) on PWI processes and data for fusion, planned for April/May 1989, as well as its scope and objectives. The list of participants should be widened by E. Thomas (GIT, USA) and representatives from France (Marseille).

The AGM should define in more specific terms the objectives, methods and priorities of the IAEA A+M Data Unit activities in the PWI data area, particularly with respect to the ITER needs.

- 5.4. In order to co-ordinate the A+M Data Unit activity in this field with the ongoing world activities in the PWI area (international meetings, co-operation programmes, etc), a Co-ordination committee is to be established (suggested members: V.A. Abramov, R. Behrisch, W. Gauster, M.F.A. Harrison, R.K. Janev, A. Miyahara) with A. Miyahara acting as a liaison officer.

6. Near- and Long-Term Data Evaluation Priorities

- 6.1. The data evaluation and recommendation work of the A+M Data Unit and Atomic Data Centre Network should be focussed on A+M data most urgently required by the fusion community. In implementing this recommendation, the A+M Data Unit and the A+M DCN should also take into account the actual availability of the A+M data, in order to produce as complete as possible recommended A+M data subsets.

On the basis of these criteria, the following priorities are established:

6.2. Near-term priorities (1-2 years)

- a) Completion of the data base for e,  $H^+$ -H,  $H_2$ ,  $H_2^+$  processes (including isotopic variations)
- b) Completion of the data base for e,  $H^+$ ,  $H_2$ , H-He,  $He^+$ ,  $He^{2+}$  processes

- c) Completion of data base for  $\text{Fe}^{q+}$ -e, H,  $\text{H}_2$ , He processes
- d) Data base for e,  $\text{H}^+$ , H -  $\text{C}_k\text{H}_n$ ,  $\text{CO}_k$ ,  $\text{O}(\text{O}_2)$  and OH processes

### 6.3. Long-term priorities

- a) Plasma edge processes (other than those included in 6.2)
- b) Data for e- $\text{A}^{q+}$ ,  $\text{A}^{q+}$ -H,  $\text{H}_2$ , He processes (A=Ti, Cr, Ni)
- c) Data for e- $\text{A}^{q+}$ ,  $\text{A}^{q+}$ -H,  $\text{H}_2$ , He processes (A=Be, B, Si, W)
- d) Plasma-wall interaction processes (as specified at the AGM '89)

## 7. ITER Related Activities

- 7.1. The Subcommittee endorses the organization of a small experts' meeting on the establishment and validation of a recommended data base for energetic hydrogen beam penetration in reactor -(ITER-)-like plasmas. The results of this meeting should be made available to the ITER-Team.
- 7.2. ITER related PWI data activities at the A+M Data Unit should be considered and defined at the AGM meeting in April/May 1989.

## 8. Data Centre Network

- 8.1. The Subcommittee praised the efforts of the Data Centre Network (DCN) in supporting the A+M Data Unit (AMDU) activities. The DCN continues to be instrumental particularly in establishing and practical implementation of ALADDIN, and in the areas of data evaluation and validation.
- 8.2. The DCN and AMDU are responsible for the quality and utility of the produced recommended data. New sets of recommended data should first be discussed at regular DCN meetings, where a validation procedure for each data set should also be suggested.
- 8.3. The recently expressed interest of several newly formed A+M data centers (CRAAMD in China, A+M/ENEA in Bologna, A+M/NDC in Obninsk and other laboratories (LLNL, Cadarache)) for a closer collaboration with the A+M DCN was welcomed by the IFRC Subcommittee. The proper membership to the A+M DCN should be defined by the involvement of each A+M data center or unit in the compilation and evaluation work on A+M data for fusion and by the commitments to contribute to the A+M data programmes co-ordinated by the IAEA Data Unit.

## 9. A+M Data Publication

- 9.1. The Subcommittee supports the IAEA AMDU initiative for creation of journal-level possibilities for publication of A+M data for fusion resulting from the ongoing research in atomic physics laboratories, and from the co-ordinated research programmes or experts meetings organized by the IAEA AMDU. The following publication activities are endorsed.

- 9.2. Introduction of a permanent section "Atomic and Plasma-Wall (particle-surface) Interaction Data for Fusion" in the regular issues of the IAEA journal "Nuclear Fusion". This Section will constitute about 10-15% of the "Nucl. Fusion" volume. Only data on fundamental processes should be published, with minimum methodological description. R.K. Janev was proposed to be co-opted in the journal's Editorial Board and to act as Co-editor for the A+M data section. The necessary advertising of the Section should be undertaken in the atomic physics community.
- 9.3. A "Nuclear Fusion Supplement on A+M Data" is to be established as a regular refereed journal-level publication, with frequency of one issue per year. Each volume should contain coherent material related to the A+M and PWI data for fusion. The A+M Supplement will have an Editorial Board (recommended members: R.K. Janev, H.-W. Drawin, R.A. Phaneuf, A. Miyahara, R. Behrisch) which will be responsible for the quality of published material.
- 9.4. The Subcommittee endorses the publication of the IAEA recommended A+M and PWI data for fusion in book-format, with numerical, graphical and analytic-fit presentation of the data. Each volume of the IAEA Book Series on A+M and PWI recommended data for fusion should contain only well established, highly accurate and well formatted data sets. The IAEA AMDU and the IFRC Subcommittee will be jointly responsible for the quality and the presentation of the data, contained in each volume of the series.

#### 10. Bibliographic Data Base

- 10.1. The Subcommittee expressed the opinion that the coverage of bibliographic A+M data for fusion in the Bulletin is at present adequate. The publication frequency of the Bulletin should remain two issues per year.
- 10.2. The decision for publication of the next volume of CIAMDA is postponed until the next Subcommittee meeting (in 1990).

#### 11. IAEA A+M Data Meetings for the Period 1989-1991

- 11.1. The Subcommittee adopted the following list of A+M data meetings for the period 1989-1990.

##### 1989:

- 1) SM on A+M data base for H-beam penetration (March/April)
- 2) AGM on PWI data for fusion (April/May)
- 3) Review of the A+M data for fusion edge plasmas (SM) and of the DCN activities (CM)

##### 1990:

- 1) Data status and requirements for fusion: AGM on medium- and high- Z impurities, and SM/CM on PWI data
- 2) Review of the A+M data for edge plasmas (RCM) and DCN programmes (CM, TCM)

- 11.2. The Subcommittee considered that a Technical Committee Meeting might be organized in 1991 to review the A+M data status and needs for fusion.
- 11.3. In order to minimize meeting travels, meetings should be suitably grouped, and then combined under one broader title, as and if appropriate.
12. Joint IAEA/ICTP Workshop on Computational Methods in Atomic Collision Physics
  - 12.1. The Subcommittee endorsed the organization of a joint IAEA/ICTP (Trieste) Workshop on "Computational Methods in Atomic Collision Physics", in order to enlarge the atomic physics computational base for production of A+M data for fusion.
  - 12.2. The Subcommittee recommended to shorten the presently foreseen four-year repetition rate of this Workshop to two years.
13. Subcommittee Interaction with IFRC and Co-ordination of AMDU Activity with Other IAEA Fusion Related Programmes
  - 13.1. Since the IAEA Scientific Advisory Council has recently been discontinued, and thereby the role of the IFRC in advising the Agency's Director General on fusion related matters has increased, it was felt that the interaction of the Subcommittee with the IFRC should also increase.
  - 13.2. This interaction should be maintained through frequent informative contacts of the Subcommittee members with the IFRC members, and through regular annual reports of the IFRC Subcommittee Chairman together with the A+M Data Unit on the A+M data activities for fusion to the IFRC.
  - 13.3. The A+M Data Unit activity should be brought into a closer correlation with the other fusion related IAEA activities, conducted by the IAEA Physics and Advanced Nuclear Power Technology Sections. This should particularly include co-ordination of meeting activities.
14. A+M Data Unit Manpower
  - 14.1. The current A+M Data Unit staff consists of two professionals and one secretary. With respect to the period before September 1987, the increase in Data Unit manpower is only 1/2 full-time professional.
  - 14.2. In order to pursue the new A+M Data Unit programmes, which are essential for fulfilling the Unit's basic functions, particularly to build the numerical data base and the data management and exchange system, the Subcommittee recognizes that the increase of A+M Data Unit manpower is of crucial importance.
  - 14.3. The Subcommittee strongly recommends to the IAEA to increase during 1989 the A+M Data Unit staff by one P-3 level professional, having an adequate atomic physics/PWI and computer science/programming

knowledge. This recommendation should be conveyed to the IFRC and the IAEA management.

14.4. The A+M Data Unit may also partly satisfy the need for manpower by accepting cost-free experts from A+M data centres or research laboratories, as well as through the IAEA fellowship programme.

14.5. The Nuclear Data Section is requested to investigate all possibilities for the implementation of recommendations 14.3. and 14.4.

15. Subcommittee Membership and New Chairman

15.1. Due to his new responsibilities in US DOE, Dr. D.H. Crandall will not be able to serve further as member of the IFRC Subcommittee. In this capacity he will be replaced by Dr. Ronald McKnight from the Office of Fusion of US DOE.

15.2. The responsibilities of the IFRC Subcommittee Chairman will be assumed by R. McKnight, and D. Crandall will provide him consultancy, when necessary.

15.3. The Subcommittee cordially thanked Dr. H.W. Drawin for his outstanding Chairmanship during the period between the 3rd and 5th Subcommittee meetings.

16. Next IFRC Subcommittee Meeting

The next IFRC Subcommittee Meeting is scheduled for 1990.

IV. List of Actions

<u>Action</u>	<u>Responsible</u>	<u>Target Date</u>
1. Finalization of ALADDIN Data Storage and Exchange System and formation of ALADDIN Users Network	AMDU	March 1989
2. Establishment of a validation procedure for recommended data (within the ALADDIN system) and its application to the existing recommended data	AMDU	April 1989
3. Extension of ALADDIN structure and dictionaries to incorporate PWI data	AMDU	May 1989
4. Storage and dissemination of all existing recommended and validated A+M data in ALADDIN form	AMDU	June 1989
5. Assembling and ALADDIN-formatting of specific-purpose A+M Data libraries	AMDU	August 1989
6. Advertising the A+M Data Section in "Nucl. Fusion" and "Nucl. Fusion Supplement on A+M Data" in Atomic Physics community	AMDU "Nucl. Fusion"	Continuing
7. Recommendation letter to the IAEA DG for increase of A+M Data Unit staff by one P-3 professional during 1989. Information to be done through the IFRC	Subcommittee Chairman	Nov/Dec. 1988
8. Investigate all possibilities to increase the professional manpower of the A+M Data Unit	Head, Nuclear Data Section	End 1989

Appendix 1

Fifth Meeting of the IFRC Subcommittee on Atomic and  
Molecular Data for Fusion

IAEA Headquarters, Vienna, Austria,  
7, 8 October 1988

(Meeting Room A-19-72)

LIST OF PARTICIPANTS

<u>Name</u>	<u>Institute</u>
Dr. D.H. Crandall	Division of Applied Plasma Physics, ER-542, GTN, U.S. Department of Energy, Washington, D.C. 20545, U.S.A.
Dr. H.-W. Drawin	Dépt. de Recherches sur la Fusion Contrôlée, Association EURATOM-CEA sur la Fusion, Centre d'Etudes Nucléaires de Cadarache, BP No. 1, F-13115 St. Paul-lez-Durance, France
Dr. M.F.A. Harrison	Culham Laboratory, UK Atomic Energy Authority, Abingdon, Oxon. OX14 3DB, United Kingdom
Dr. R.H. McKnight (Observer)	Division of Applied Plasma Physics, ER-542, GTN, U.S. Department of Energy, Washington, D.C. 20545, U.S.A.
Dr. A. Miyahara	Institute of Plasma Physics, Nagoya University, Furoo-cho, Chikusa-ku, Nagoya-shi 464, Japan
Dr. Y. Nakai (Substitute for Dr. N. Shikazono)	Nuclear Data Center, Japan Atomic Energy Research Institute (JAERI), Tokai-Mura Naka-Gun, Ibaraki-Ken 319-11, Japan
Dr. R.K. Janev	Nuclear Data Section, IAEA, Vienna, Austria
Dr. A. Lorenz	Nuclear Data Section, IAEA, Vienna, Austria
Dr. J.J. Schmidt	Nuclear Data Section, IAEA, Vienna, Austria
Mr. J.J. Smith	Nuclear Data Section, IAEA, Vienna, Austria



Fifth Meeting of the IFRC Subcommittee on A+M Data for Fusion

IAEA Headquarters, Vienna, Austria  
7-8 October, 1988

The Meeting started on Friday, 7 October at 9:30 am, and ended on Saturday, 8 October about noon and was held in Conference Room A-1972 in the Vienna International Centre.

MEETING AGENDA

1. Introductory Items

- Opening of the Meeting
- Selection of Chairman
- Adoption of Agenda
- Subcommittee Membership

2. Review of the Current IAEA A+M Data Activities

- 2.1. Report on the A+M Data activities since last Subcommittee meeting
- 2.2. Results of July 1987 SM on A+M Data for Plasma Edge Studies
- 2.3. Results of the May'88 Consultants and Specialists Meetings
- 2.4. Status of the CRP on A+M data for fusion edge plasmas
- 2.5. CM/SM on data base for neutral beam penetration in ITER (March, 1989) (initiation)
- 2.6. AGM on particle-surface interaction processes for fusion (April, 1989) (initiation)
- 2.7. Joint IAEA/ICTP workshop on computational method in atomic collision physics (initiation)
- 2.8. Other activities:

- Conferences attended (with a review talk):

- IX ESCAMPIG, (Lisbon)
- 4th Int. Conf. on Phys. Multiply Charged Ions (Grenoble)

- Data parametrization:  $\sigma_{ion}$ ,  $\sigma_{cx}$  in  $C^{9+}$ ,  $O^{9+}$  - H, H<sub>2</sub>, He collision

3. Status of Numerical Data Base and Exchange Format

- 3.1. The existing IAEA A+M recommended data base
- 3.2. Status of data storage and exchange system (ALADDIN)
- 3.3. A+M Data Exchange Network, "ALADDIN" Newsletter

4. Status of Bibliographic Data Base

- 4.1. Scope of data coverage
- 4.2. A+M Bulletin production; frequency
- 4.3. Next CIAMDA (1990 ?); frequency

5. Near- and Long-term Programme of the IAEA A+M Data Activities

- 5.1. Near-term priorities in data evaluation/production (gas-phase collisions, spectroscopic data)
- 5.2. Long-term priorities in data evaluation/production (gas-phase collisions, spectroscopic data)
- 5.3. Plasma-wall interaction processes (scope, programme, methods and procedures)
- 5.4. A+M Data Unit and Data Center Network Programme for 1989-91
- 5.5. Meetings for 1989-91/92.

6. IAEA A+M Data Activity and Relation to ITER Design Needs

- 6.1. Collaboration with IFRC and connections with plasma physics community
- 6.2. IAEA A+M Data programme and relation to ITER

7. Data Publication

- 7.1. IAEA Series on Recommended A+M Data for Fusion
  - a) A+M data series: format, content
  - b) PWI data series
- 7.2. Publication of a regular "Nuclear Fusion" Supplement on A+M Data for Fusion

8. A+M Data Unit Manpower

- Current manpower
- Required manpower for the new programmes

9. Next Meetings

- IFRC Subcommittee meeting
- Data Center Network meeting

Report on the IAEA A+M Data Unit Activities  
in the Period September 1987 - September 1988

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I. Introductory Remarks

During the first half of the reporting period, the IAEA A+M Data Unit was operating with reduced manpower (1.5 professionals). Despite that fact, the Unit was able to carry out some of its basic functions: the publication of the International Bibliographic Bulletin on Atomic and Molecular (A+M) Data for Fusion, co-ordination of the Atomic Data Centre Network (DCN) activities and organization of experts' meetings for assessment of the A+M data status and needs in certain areas of fusion research. In September 1987, the position of the Head of A+M Data Unit was filled, and the Unit started to operate with two professionals and one secretary.

In accordance with the Terms of Reference and the priorities established by the IFRC Subcommittee, the activities of the IAEA A+M Data Unit in the reporting period, and particularly after September 1987, were focused on the following objectives:

- 1) establishment of the IAEA A+M numerical data storage exchange system, (acceptable for both data producers and users),
- 2) establishment of the IAEA numerical recommended data base (in a format compatible with the interfaces of fusion application codes),
- 3) strengthening the interaction of the IAEA A+M Data Unit with both atomic physics and fusion communities for stimulation of fusion relevant data production and their implementation in current fusion research.

Besides the activities oriented towards achievement of these objectives, the IAEA A+M Data Unit during the reporting period continued to perform all its "traditional" activities, such as the co-ordinating function within the Data Centre Network, compilation and publication of bibliographic A+M data and initiated a Co-ordinated Research Programme on "Atomic and Molecular Data for Fusion Edge Plasmas".

The results and the status of these activities are described below.

II. Status of the A+M numerical data storage and exchange system

In order to resolve the problem of efficient data transmission between the national data centres, the IAEA A+M data Unit as a central place for storage and dissemination of recommended A+M data, and the fusion laboratories, as well as the interface of these data with the fusion modelling and diagnostic codes, an appropriate and unique data exchange system has to be

adopted. The prior attempts to introduce EXFOR were unsuccessful because of complexity of its structure and format and because of its incompatibility with the large diversity of atomic processes.

The Consultants' Meeting on "Atomic Data Base and Fusion Applications Interface", organized by the Unit in May 1988, had the objective of adopting a unique A+M data exchange system, acceptable for both data centres and fusion A+M data users.

The meeting was successful and the system ALADDIN, developed by R. Hulse at the Princeton Plasma Physics Laboratory, was adopted. The Summary Report on this meeting is given in Attachment 1.1.

ALADDIN has already been tested in most of the data centres (ORNL, Nagoya, JAERI, GAPHYOR, Belfast, IAEA) and proved to be very adequate. The representatives at the meeting from the major fusion laboratories (JFT, Garching, Jülich, JT-60) made commitments to interface their modelling/diagnostics codes with ALADDIN. The ALADDIN dictionaries have also been worked out although some minor details are still under discussion.

The issuing of an ALADDIN Manual could be expected by the end of this year. At that time all the available recommended A+M data should also be stored in the IAEA numerical data base. Volume 1 of the ORNL Red Book series, which should be finished by the end of this year, will also be in the ALADDIN format.

The ALADDIN structure and format is open to further developments. Such developments are envisaged both in the area of supporting software and in the dictionaries (to accommodate new types of data such as spectroscopic data, plasma-wall interaction data, composite processes, etc.).

The co-ordination of the development of the data storage and exchange system, maintenance and distribution of the standard and up-dated versions of ALADDIN will be a responsibility of the IAEA A+M Data Unit. In order to fulfill this task, the Unit intends to initiate the creation of an ALADDIN Users Network. The core structure of this Network will consist of:

- A+M Data Centre Network,
- major fusion laboratories using A+M data,
- other atomic and plasma physics laboratories actively involved in A+M data production, use or management (such as JILA, Livermore, Los Alamos, ENEA (Bologna), Obninsk, Lebedev Physical Institute, etc.).

The communication within the ALADDIN Users Network will be provided through a regular ALADDIN Newsletter, which will also serve to announce and communicate possible changes or additions in the ALADDIN system (structure, dictionaries, supporting subroutines, etc.). The ALADDIN Newsletter will be published by the IAEA A+M Data Unit.

The ALADDIN Users Network will have regular meetings, jointly or in close connection with the A+M Data Centre Network Meetings, for assessment of ALADDIN developments, agreement on changes in the system and its components, and for taking other decisions on similar matters.

### III. Status of the recommended A+M numerical data base

The existing body of A+M numerical data for fusion, recommended by an international body with involvement of the IAEA (e.g. the Data Centre Network, or IAEA Advisory Group Meetings) includes:

- 1) Recommended data for electron-impact ionization of all atoms in almost all stages of ionization from hydrogen to uranium (Belfast Data Centre).
- 2) Recommended data for electron-impact excitation and ionization of  $C^{9+}$  and  $O^{9+}$  ions and for ionization and charge exchange processes of these ions in collisions with H,  $H_2$  and He (ORNL Data Centre).
- 3) Recommended data for electron impact excitation and ionization of  $Fe^{9+}$  ions and for charge exchange of these ions (with  $q \geq 5$ ) on H,  $H_2$  and He. (Nucl. Fusion Supplement, 1987).

A detailed list of the recommended data sources is given in Attachment 2. There is a much broader spectrum of other data in the areas of both atomic collision processes and particle-surface interaction processes recommended by the national data centres, but with no recommendation from an international experts' forum. Some of these data (e.g. the backscattering and sputtering data from Garching, as amended in the latest publications of the Nagoya Data Centre) are tacitly used in practice as recommended data. A critical evaluation of the status of these data and their formal recommendation for use in fusion research is a task which should be undertaken urgently. Otherwise, confusion might be created in the A+M data users community, and the basic role of the IAEA in this field will be unfulfilled. The initiative of the IAEA A+M Data Unit to undertake an organized activity on evaluation of particle-surface interaction data was inspired partly by this idea.

In order to achieve a completion of the recommended A+M data base for carbon and oxygen ions, particularly for the recombination and state-selective electron capture processes, the IAEA A+M Data Unit convened a Specialists' Meeting on the "Carbon and Oxygen Collision Data for Fusion Plasma Research" (May 1988, Vienna). Besides a precise assessment of the data status, and quality of the data, the meeting contributed also to the enlargement of the data base for these ions through original contributions presented at the meeting, as well as through some follow-ups from the meeting in the data production area. The results of this meeting are given in the Meeting Summary Report (see Attachment 3), and will be published as a Topical Issue of "Physica Scripta" by the end of this year.

It is felt that the evaluation work leading to recommendation of particular sets of recommended data for fusion is still not adequately well organized and co-ordinated. This is partly because of manpower shortage in the data centers, but also because of lack of specific guidelines about the priorities for the A+M data needs for fusion. The IFRC Subcommittee may be instrumental in removing the latter obstacle by setting clear priorities in the data evaluation work.

#### IV. Coordinate Research Programmes

The July 1987 Specialists' Meeting on "Atomic and Molecular Data for Fusion Plasma Edge Studies" was extremely useful in assessing the A+M data status and requirements for the plasma edge region and suggesting actions for the future A+M work in this area. As follow-ups of this meeting, two review articles were written, one for the "Comments in At. Mol. Phys." (by H. Tawara and R.A. Phaneuf) to bring to the attention of atomic physics community the needs of specific A+M data for plasma edge studies, and the other for "Nuclear Fusion" (by R.K. Janev, M.F.A. Harrison and H.-W. Drawin) to provide information to fusion community about the existing A+M data base for the processes occurring in this plasma region.

As a further follow-up of this Meeting, a three year Co-ordinated Research Programme (CRP) on "Atomic and Molecular Data for Fusion Edge Plasmas" was initiated at the beginning of 1988, with a starting date of October 1, 1988. The CRP programme and objectives are described in Attachment 4. The CRP participants are:

- 1) F. Brouillard, (Louvain-la-Neuve, Belgium)
- 2) S. Trajmar, (JPL, Pasadena, USA)
- 3) H. Winter, (Vienna, Austria)
- 4) W. Wiese, (NBS, Washington, USA)
- 5) P.S. Krstić, (Belgrade, Yugoslavia)
- 6) I. Cadez, (Belgrade, Yugoslavia)
- \* 7) A. Salin, (Bordeaux, France)
- \* 8) F. Linder, (Kaiserslautern, FRG)
- \* 9) V. McKoy, (CIT, Pasadena, USA)
- # 10) V. Abramov, (Kurchatov Inst. Moscow, USSR)
- # 11) H. Tawara, (Nagoya Univ., Nagoya, Japan)
- 12) Vacant

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\* proposal submitted, under consideration

# proposal not yet submitted, but commitment exists

A Specialists' Meeting is planned for September 1989 to review the first year results of this CRP. Apart from the experts from the above list, a much larger number of potential participants will be informed about the meeting by the end of this year and invited to participate with A+M data contributions on the processes within the scope of the CRP.

Regular meetings of this type will be organized each year during the CRP period. It is expected that the response of atomic physics community will be as enthusiastic as in the case of the May 1988 carbon and oxygen meeting, and that the number of contributors to this CRP will be much larger than the number of its official participants.

#### V. ITER Related Activities

The Head of the A+M Data Unit was invited to attend the ITER Meeting on Heating and Current Drive Issues (June 13-17, 1988, Garching) and to participate in the workshop organized during that Meeting on the assessment of A+M data base for neutral hydrogen beam penetration in ITER plasmas. For that

purpose, the A+M Data Unit prepared a complete set of the required atomic data which includes:

- electron loss cross section for hydrogen atoms in ground and excited states in collisions by protons, carbon, oxygen and iron ions in all stages of ionization;
- proton-impact excitation of ground state hydrogen atoms into  $n=2,3,4,5$  states by proton and impurity (any  $A^{q+}$ ) ions, as well as transitions between the excited states;
- electron-impact excitation of ground state hydrogen and  $n - n'$  transitions;
- radiative decay probabilities.

The prepared set of data is probably the best one at present, but it contains also data with uncertainties which may influence the accuracy of beam stopping cross section calculations. This holds particularly for the impurity-impact excitations of  $n \geq 3$  states and the  $n - n'$  transitions. In the multi-step ionization scheme of penetrating H-atoms, these processes play a very important role.

In order to resolve these uncertainties in the data base for neutral hydrogen beam penetration in reactor-type plasmas, the IAEA A+M Data Unit proposed to the Head of the Physics Group of the ITER Team organization an experts' meeting in March 1989 for establishing the most accurate data base for the hydrogen beam penetration problem. An appropriate data production activity would be undertaken before the meeting in order to provide the required (and presently missing) information on some of the processes involved. The meeting should end-up with a complete set of recommended data for calculation of the energetic beam penetration in reactor type plasmas. The correspondence between the IAEA A+M Data Unit and the Physics Group of ITER Team is attached (see Attachment 5).

A Consultants'/Specialists' Meeting devoted to this problem has been included in the Units' programme for the next year. A number of potential participants in this action have already been consulted and the formal organizational steps will be taken in the immediate future.

## VI. Particle-Surface Interaction Data for Fusion

Preparative work has been undertaken towards the initiation of organized data evaluation efforts in the area of particle-surface interaction (PSI) data for fusion, and the inclusion of recommended PSI data in the A+M numerical data base. A small, informal meeting was held in Garching on July 14, 1988 (present: R. Behrisch, J. Bohdansky, M.F.A. Harrison, R.K. Janev) to investigate and discuss the practical possibilities, the scope and the methods of such an activity. The possible connections of this activity with ITER PSI data needs and R+D programmes were also discussed. It was found that because of the critical importance of these data for the ongoing fusion research programmes, the existence of a considerable data base for PSI processes which is not adequately evaluated and put into a unique format and because of

increasing demands for new PSI data, an activity of the IAEA in this field, similar to the one for A+M gas-phase data would be extremely useful.

The scope, objectives and potential participants of the planned IAEA Advisory Group Meeting (April/May 1989) on the PSI data for fusion was also elaborated (see Attachment 6).

The work on the PSI Dictionary within the ALADDIN format has also been started.

#### VII. Joint IAEA/ICTP Workshop on Computational Methods in Atomic Collision Physics

In order to strengthen the interaction with the atomic physics community and stimulate the A+M data production for fusion, an initiative has been put forward for organization of a Workshop/Training Course jointly with the International Centre for Theoretical Physics (ICTP) in Trieste, on the Computational Methods in Atomic Collision Physics. The underlying idea of this undertaking is to make available the existing codes for A+M data calculations to laboratories throughout the world (particularly in the developing countries) and to enlarge the number of A+M data producers. The atomic physicists in developed countries, either from financial (expensive computer time) or scientific reasons, are more and more reluctant to participate in programmes the only aim of which is data production (unless someone pays directly for such work). On the other-hand, the recent developments in computer technology (PC's mini-computers) made these computational tools (with significantly increased capabilities) accessible also to the laboratories in developing countries. An adequate channel for transfer of the A+M computational software and knowledge to the A+M laboratories of developing countries, is organization of a regular workshop through the ICTP. Through an appropriate tailoring of the programmes of these workshop, as well as through different post-workshop activities, one can achieve an enlargement of the computational base for A+M data for fusion.

The IAEA A+M Data Unit proposal for this workshop is given in Attachment No. 7. The ICTP has already considered this proposal and took a positive attitude with respect to it. However, different constraints within the ICTP (general policies, budget, time-schedules) have limited the frequency of these workshops to one in four years (the first being scheduled for 1992), instead of one in two years, as proposed.

The idea of the Workshop was widely accepted by many A+M physicists from both developed and developing countries.

#### VIII. Publication of a Regular Supplement to "Nuclear Fusion" on A+M Data for Fusion

Another difficulty encountered in the process of involvement of A+M physicists in A+M data production activities is the absence of adequate journal for publication of data obtained by well known theoretical or experimental methods. In majority of cases, articles containing such data do not contribute to the extension of existing fundamental knowledge, and the



standard physical journals are reluctant to publish such articles. On the other hand, specialized journals for data publication (At. Data Nucl. Data Tables, and J. Phys. Chem. Ref. Data) require comprehensiveness and a certain degree of finalization of a data set (recommended data). These criteria cannot be met by the results of a normal A+M data production work, which should be dynamic and responsive to the fusion A+M data demands.

In order to resolve this problem, the IAEA A+M Data Unit has recently put forward a proposal for publication of a regular Supplement to "Nuclear Fusion", devoted completely to publication of A+M data for fusion. This Supplement should have all characteristics of a regular journal (refereeing, regularity, volume numeration for referencing, etc.). The proposal (see Attachment 8) was discussed at a meeting with the Editor of "Nuclear Fusion" and the representatives of the IAEA Publication Division. Within the existing financial constraints, the following solution was found as the most acceptable at present:

- a) Establishment of a regular "Nuclear Fusion" Supplement on A+M Data for Fusion, with the all journal characteristics, with a frequency of appearance one volume per year, and number of pages around 200. The cost of the publication of this Supplement will be accommodated within the regular budget of the IAEA Nuclear Data Section.
- b) Establishment of a special Section in "Nuclear Fusion" devoted to publication of articles on A+M Data for Fusion. This Section should be about 15% of the total journal volume.

The proposal should be endorsed by the Agency's Publication Committee and (possibly) the Editorial Board of "Nuclear Fusion", but no difficulties are expected.

The Supplement will also be a medium for publication of the results of different meetings on A+M data for fusion.

#### IX. Collaboration with the National A+M Data Centres and Extension of the DCN

In performing most of its basic activities, the IAEA A+M Data Unit strongly relies on a close collaboration with the national A+M data centres, and on their active participation in the programmes defined jointly or by the IFRC Subcommittee. We believe that through such collaborative approach, the co-ordinating function of the IAEA A+M Data Unit within the A+M Data Centre Network (DCN) will be more effectively and more productively fulfilled.

The collaboration with the A+M DCN was most pronouncely manifested in the organization and the work of the May '88 Consultants' and Specialists' Meetings and the actions that followed thereafter. The data centres enthusiastically accepted ALADDIN, started to implement it in their data bases, and actively collaborated in the formulation of ALADDIN dictionaries.

In the area of data evaluation activity direct collaboration between the ORNL and Nagoya data centres, and the IAEA A+M Data Unit was initiated (evaluation of the state-selective electron capture data for  $C^{9+}$ ,  $O^{9+}$  - H,  $H_2$ , He collisions). Similar collaboration between the ORNL data centre and

the A+M Data Unit was undertaken on the problem of creating new, physically better founded analytical fits for the charge exchange and ionization cross sections in  $C^{9+}$ ,  $O^{9+}$  - H,  $H_2$ , He collisions.

In October 1987, the A+M Data Unit organized the 7th Meeting of the A+M Data Centre Network (hosted by the ORNL data centre), at which, among other items, the future data compilation and evaluation programmes were discussed and co-ordinated.

It is a pleasure to report that during 1987 the Chinese Research Association on A+M Data (CRAAMD) was established, which immediately expressed the wish to be included in the A+M DCN. Already at the 7th A+M DCN Meeting in Oak Ridge, CRAAMD presented its plans in the field of A+M data for fusion. CRAAMD also volunteered to the next A+M DCN Meeting in Beijing.

An active interest in the A+M data for fusion was recently expressed also by the ENEA Centre in Bologna. Representatives of this centre attended the 7th A+M DCN Meeting and the May '88 Consultants' Meeting on the "Atomic Data Base and Fusion Applications Interface".

Interest for participation in the work of A+M DCN and, in general, for participation in the other IAEA A+M data programmes, have been also recently expressed by other institutions (Livermore, Obninsk).

#### X. Bibliographic Data Base

The building-up of the IAEA Bibliographic Data Base has been continued during the reporting period. The main new element in the bibliographic data activity is the reduced frequency of publication of the A+M data Bulletin (two issues per year) during the past two years. This decision, taken at the last Subcommittee meeting, was based mostly on financial and manpower shortage arguments. There are indications that the informative functions of the Bulletin has been substantially weakened by its rarified publication. The six months period between two consecutive Bulletin issues is too long a period for a publication aimed to provide information on the availability of new A+M data for the current research in fusion and atomic physics areas. The delay in the transmission of this information is even longer, since the input from the national data centres also includes a certain delay-time. Reinstatement of the earlier publication frequency of the Bulletin (four items per year) seems to be necessary in order for the Bulletin to fulfil its basic function.

The content of the Bulletin is almost entirely based on the input received from the ORNL Atomic Data Centre for Fusion. Comparison with the much broader GAPHYOR bibliographic data base shows that some low-energy processes involving molecular species, which have recently become of interest to fusion in connection with the kinetics of low-temperature edge plasmas, are not adequately covered in the ORNL bibliographic data base. A reassessment of the methods for improving the completeness of the content of the Bulletin seems to be necessary.

During the reported period, the second volume of the Computerized Index on A+M data for Fusion has been published (CIAMDA '87).

The new bibliographic information stored in the IAEA Bibliographic Data Base is approaching the level for publication of the next volume of the Index. The A+M Data Unit is planning to publish the next volume of CIAMDA in 1990. It would be convenient to establish a regular publication frequency of CIAMDA.

## **XI. Other Activities**

### **1. Interaction with atomic and plasma physics communities**

In order to extend the awareness and interest of the plasma and atomic physics communities of the IAEA A+M data programmes for fusion, and develop closer relations between the IAEA A+M Data Unit with these communities, the Head of the A+M Data Unit attended in 1988 two international meetings, in which the atomic processes of interest to fusion were included in the scope. At these meeting the A+M Data Unit head also delivered invited talks.

The meetings were:

- a) 4th International Conference on the Physics of Multiply Charged Ions (September 12-15, 1988, Grenoble).  
Title of talk: "Atomic Collisions in Fusion Plasmas" (will be published in a Topical Issue of J. de Physique, Paris).
- b) 9th Europhysics Sectional Conference on Atomic and Molecular Physics of Ionized Gases (Sept. 1-3, 1988, Lisbon).  
Title of talk: "Atomic and Molecular Processes in Tokamak Edge Plasmas".

The Head of the A+M Data Unit was also invited to write an article for the "Comments on At. Mol. Phys." on the subject of "Atomic Collisions in Fusion Research". The article should be submitted to the Editor by the end of the year.

The Head of the Unit also received an invitation from the Programme Committee of the 19th International Conference on the Physics of Ionized Gases (July 10-14, 1989) to present an invited review talk on "Elementary Processes in Fusion Plasmas".

### **2. Parametrization of the recommended A+M data for fusion**

The existing Chebishev polynomial fits to the recommended cross section data for electron capture and ionization in  $C^{9+}$ ,  $O^{9+}$  - H,  $H_2$ , He collisions (ORNL Red Book Vol. 5) are inadequate for rate coefficient calculations since they generate the cross section only in a given range. In order to allow for cross section extrapolations outside the prescribed data range, non-polynomial analytic fits are required. In the course of preparations for the storage of these data in the IAEA A+M Numerical Data Base, the A+M Data Unit undertook the effort of constructing such, physically founded, non-polynomial analytic fits for the electron capture and ionization recommended cross section data for the above mentioned system. The simplicity of the fits (i.e. relatively

small number of fitting parameters) and the correct asymptotic behaviour of the fitting functions (both at the high and low collision energies), were taken as basic criteria in constructing the fits. Another criterion was to achieve rms deviations below 10% (i.e. the same or better than in the case of Chebishev polynomial fits). The work has been successful accomplished for the majority of cross sections, and it is expected to be finished by the end of November. All the ionization cross sections can be accurately fitted by only five parameters (as opposed to nine with Chebishev polynomials), and for a given target (and all ions) can be appropriately charge-scaled using the same form of the analytic fit. Due to the more complex nature of the electron capture process (dominant capture to different ionic states in different energy regions), the analytic functions (of basically simple form) contain more fitting parameters (between five and eleven). The cross section data extrapolations using these fits can be extended far in the MeV/amu region (sufficient for fusion applications). The extension of the ionization data by these analytic fits in the low-energy region may be achieved with an acceptable accuracy, but for some electron capture cross sections, new experimental or accurate theoretical data are required in order to specify the correct low-energy cross section behaviour. Details of this work are given in Attachment 9.

The Existing Data Base of  
Recommended Atomic and Molecular Data

Atomic and Molecular Collision Data

1. "Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionisation of Light Atoms and Ions," K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith, Culham Laboratory Report CLM-R216, Abingdon, Oxfordshire, United Kingdom (1982); J. Phys. Chem. Ref. Data 12, 891 (1983).
2. "Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionisation of Light Atoms and Ions: Fluorine to Nickel," M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray, F.J. Smith, Report UKEA, Culham Laboratory, Abingdon, OX14 3DB, Oxfordshire, UK (1986); (to be published in J. Phys. Chem. Ref. Data).
3. "Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions," Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M.S. Pindzola, D.H. Crandall, IPPJ-AM-27 report series of the Institute of Plasma Physics, Nagoya, Japan (1983); At. Data Nucl. Data Tables (ADNDT) 33, 149 (1985).
4. "Recommended Data on Atomic Collision Processes Involving Iron and its Ions," J.G. Hughes (Editor) Nucl. Fusion (NF) (1987), Special Issue (to be published).
5. "Report on Recommended Data (for Electron-Impact Excitation)," K.M. Aggarwal, K.A. Berrington, W.B. Eissner and A.E. Kingston, Atomic Data Workshop, Daresbury Laboratory, United Kingdom (March 1986).
6. "Collisions of Carbon and Oxygen Ions with Electrons, H. H<sub>2</sub>, and He, Atomic Data for Controlled Fusion Research, Vol. V," R.A. Phaneuf, R.K. Janev, M.S. Pindzola (Editors), Report ORNL-6090/V5, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA (1987).
7. "Collisions of H. H<sub>2</sub>, He and Li Atoms and Ions with Atoms and Molecules, Atomic Data for Controlled Fusion Research, Vol. I," C.F. Barnett (Editor), Report ORNL-6086/VI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, USA (in preparation).
8. "Recommended Data for Excitation Rate Coefficients of Helim Atoms and Helim-like Ions by Electron Impact," T. Kato and S. Nakazaki, IPPJ-AM-58 report series of the Institute of Plasma Physics, Nagoya, Japan (1988).
9. "Atomic and Molecular Data for Fusion, Part III - Recommended Cross Sections and Rates for Electron Ionisation of Heavy Atoms and Ions: Copper to Uranium," M.A. Lennon et al., (in preparation - to be published as a Culham Laboratory Report).

Data for Surface Interactions

1. "Data on Backscattering Coefficients of Light Ions from Solids," R. Ito, T. Tabata, N. Itoh, IPPJ-AM-41 report series of the Institute of Plasma Physics, Nagoya, Japan (1985).

2. "Energy Dependence of the Yields of Ion-Induced Sputtering of Monatomic Solids," N. Matsunami, Y. Yamamura, Y. Itikawa, N. Itoh, Y. Kazumata, S. Miyagawa, K. Morita, R. Shimizu, H. Tawara, IPPJ-AM-32 report series of the Institute of Plasma Physics, Nagoya, Japan (1983).
3. "Data Compendium for Plasma-Surface Interactions," R.A. Langley, J. Bohdanský, W. Eckstein, P. Mioduszewski, J. Roth, E. Taglauer, E.W. Thomas, H. Verbeck, K.L. Wilson, Nucl. Fusion (NF), Special Issue (1984).

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