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INDC

INTERNATIONAL NUCLEAR DATA COMMITTEE

Second Meeting of the IFRC Subcommittee
on Atomic and Molecular (A+M) Data for Fusion

IAEA, Vienna, 4-5 November 1982

SUMMARY REPORT

Edited by A. Lorenz
Nuclear Data Section
International Atomic Energy Agency

January 1983

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

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Abstract

The IAEA Nuclear Data Section convened the second meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) in Vienna, Austria, from 4-5 November 1982. Members of this IFRC Subcommittee met to review the IAEA programme on Atomic and Molecular (A+M) Data for Fusion, and made specific recommendations regarding the bibliographic and numerical data centre services to the fusion community.

I. Summary of the meeting

A. Introduction

The second meeting of the IFRC Subcommittee on A+M Data for Fusion was convened at IAEA Headquarters in Vienna, Austria, 4-5 November 1982. The meeting was attended by five of the eight members of Subcommittee and one member substitute, and staff of the IAEA Nuclear Data Section. The list of Participants is given in Appendix 1. The Adopted Agenda is given in Appendix 2. Dr. M.F.A. Harrison chaired the meeting.

B. Conclusions and Recommendations

While a more detailed account of the meeting proceedings is given in Part II of this report, the main conclusions and recommendations made by the Subcommittee are summarized as follows:

The Subcommittee

- Confirmed its own recommendation on the function of the IAEA A+M Data Unit, made at the January 1981 meeting.
- Stressed the importance to assure the completeness of the Agency's A+M bibliographic data file, and recommended that the newly developed capability to perform selective retrievals from that file for customers, be advertised in the A+M Data Bulletin and the Agency's "Nuclear Fusion" journal.
- Commended the A+M Data Unit on the excellence of the A+M Data Bulletin and decided to maintain the existing subject scope of the Bulletin.
- Decided to postpone the publication of a second edition of the index to A+M collision data, CIAMDA, until 1985.
- Strongly endorsed the plan to have the report which resulted from the CRP on Atomic Data for Plasma-Wall Interaction Processes published in the Agency's Nuclear Fusion Journal.
- Reviewed the work of the CRP on A+M Collision Data for Plasma Diagnostics, commended the over-all quality of their first report, and suggested certain guidelines in the further work.
- Reviewed the procedures to arrive at recommended numerical A+M data, and suggested to have the responsibilities for the data assessment, evaluation and recommendation assigned to specific individual groups.
- Identified specific functions, which the A+M Data Unit should perform, with regard to the stimulation and coordination of A+M data assessment and evaluation, and in the dissemination of these data to the fusion research community.

- Recommended that IAEA publicize the availability of recommended data from the IAEA in the Agency's "Nuclear Fusion" journal and in the A+M Data Bulletin.
- Recommended to have the Agency arrange for a critical assessment of the A+M "recombination" data.
- Recommended that the Agency compile an index of bibliographic and numerical A+M data compilations existing in the A+M data centres, and publicize this information in the A+M Data Bulletin.
- Recommended that the A+M Data Centre Network as well as the IFRC Subcommittee itself meet more frequently.

The list of actions which resulted from the meeting is given in Appendix 3.

C. Next Subcommittee meeting

The Subcommittee agreed to have its next meeting in April or May 1984.

II. Meeting Proceedings

A. Subcommittee Membership

The IAEA had been advised informally prior to the meeting that both Dr. P.H. Stone (USA) and Dr. Y.V. Martynenko (USSR) would be replaced on the Subcommittee; neither of them could attend this meeting.

In view of the change in the INDC chairmanship, effective January 1983, the IAEA was asked by the Subcommittee to ask the new INDC chairman (Dr. Seeliger, GDR) to appoint a new INDC representative on the Subcommittee, to replace Dr. Derrien who has represented the INDC during the first two years of the Subcommittee's existence.
(Action # 1).

The current composition of the Subcommittee is given in Appendix 4.

B. IAEA A+M Data Unit Programme Review

In reviewing the programme of the IAEA Data Unit, the Subcommittee confirmed its own recommendation on the functions of the IAEA A+M Data Unit made at the January 1981 meeting (see INDC(SEC)-77/GA, p.2).

Recommendation on the function of the IAEA A+M Data Unit

The overall objective of the IAEA A+M Data Programme is the establishment of an international data centre service to provide the fusion research community with bibliographic data, as embodied in the International Bulletin on Atomic and Molecular Data for Fusion and the CIAMDA index of atomic collision data, and with recommended numerical A+M data of adequate and uniform quality and acceptable accuracy.

In order to achieve these objectives, the Subcommittee recommends to maintain an international co-operative effort with the participation of national and regional A+M data centres for which the IAEA A+M Data Unit acts as a co-ordinating centre.

The progress report of the A+M Data Unit was presented by A. Lorenz (see Appendix 5).

Although the subcommittee felt that attendance by the staff of professional meetings should be more encouraged to include meetings on nuclear fusion, it noted with concern that approximately 50 % of the travel undertaken by the staff to attend meetings or visit laboratories was done at their own expense.

C. Bibliographic A+M Data

1. A+M Bibliographic Data Base (A+M/BDB)

The Subcommittee acknowledged the completion of the A+M/BDB computer system and the conversion of all of the data into one unified data base. It accepted the retrieval capabilities of the A+M/BDB, and recommended that the service of selective retrieval from the A+M/BDB, which can now be provided by the A+M Data Unit to the fusion community, be advertised in the A+M Data Bulletin as well as in the Agency's Nuclear Fusion Journal.

The Subcommittee stressed the importance to assure completeness of the A+M/BDB and recommended that a special effort be made to include in the A+M/BDB all important A+M data review papers, as well as the major references describing mathematical models for the calculation of numerical reaction data (Action # 3). In this regard, it also encouraged comparison of the A+M/BDB content with other bibliographic compilations, and the supplementation of the A+M/BDB input with material which could be obtained from data bases from other data centres (e.g., Gaphyor, ...).

The Subcommittee emphasized the importance to indicate in the A+M/BDB whether data published in an article on plasma-surface interaction is differential with angle (e.g., sputtering coefficient given as a function of incident particle angle), and recommended that this type of information be included in the "comment" of the reviewed article entered in the A+M/BDB.

2. A+M Data Bulletin for Fusion

The Subcommittee commended the Unit on the excellence of the Bulletin, and expressed their satisfaction with its content and over-all appearance.

In the consideration of its general scope, the Subcommittee decided to maintain the existing subject scope of the Bulletin as it is, and did not require to include information specifically related to inertial confinement (i.e., laser fusion) physics, although the Unit is encouraged to collect the data of the latter subject for future compilation.

In order to maintain the fusion relevance criteria used in the publication of the Bulletin up-to-date, an action (Action # 2) was put on all members of the Subcommittee to review the "Fusion Cut-off Criteria for the IAEA Bulletin Input" published in the Summary Report of the first (1981) meeting of the Subcommittee (INDC(SEC)-77/GA, Appendix 8), and advise the A+M Data Unit of desirable changes.

3. CIAMDA

In reviewing the proposed publication of the next issue of CIAMDA (see IAEA A+M Data Unit Progress Report, Appendix 5, para B.4.), the Subcommittee has accepted the suggestion to delay the next publication of CIAMDA at least until 1985.

In discussing the next publication of CIAMDA, the Subcommittee made the following suggestions:

- the next issue of CIAMDA should not have a time cut-off (i.e., not to include information published after a given date)
- give consideration to the publication of a CIAMDA supplement
- not to limit the subject scope of CIAMDA to fusion.

In an effort to promote sales of CIAMDA, the Subcommittee suggested to publicize the book review on CIAMDA written and published in Japan, and asked Dr. Y. Nakai to arrange for the translation of this book review into English, and to send the translation to IAEA (Action # 4).

D. Numerical A+M Data

1. Review of the CRP on Atomic and Molecular Collision Data

The Subcommittee commended the over-all quality of the report of the first meeting of this CRP, (which is to be published as INDC(NDS)-136/GA). As they did not have the time to read the draft report before the meeting, Subcommittee members agreed to review this report and to send their comments to the IAEA and the CRP participants.

In their discussion of the procedures used by the CRP in writing the Working Group Reports, the Subcommittee suggested that the complete body of existing data should be available to the CRP for their assessment. In all cases, the CRP should indicate the selection criteria used in their data assessment, and document their conclusions.

The Subcommittee expressed the opinion that in addition to their contractual commitment with the Agency, the CRP participants task is to perform an assessment and a review of the existing data, and to recommend which data should be measured or calculated, and which data should be evaluated. (See "Procedures to arrive at recommended data" described below).

2. Review of the CRP on Atomic Data for Plasma-Wall Interaction Processes

The Subcommittee commended the IAEA on the results obtained by this CRP and strongly endorsed the plan to publish the final report of this CRP in the Agency's Nuclear Fusion journal. A brief summary of this report is given in Appendix 5 of this report.

3. The IAEA Numerical A+M Data Base

Referring specifically to atomic collision data, the Subcommittee made the following statement concerning the future IAEA numerical A+M data base.

The IAEA numerical data base shall comprise "recommended" data, consisting of appropriately annotated unique data sets for each required species and reaction in the form of cross sections, (Maxwellian averaged) reaction rates, and/or parametric fits on the data, which should be released to the fusion research community in the most suitable and required formats. The data should be presented in tabular and graphical form in hard-copy reports, and in the form of computer listings or tapes.

The discussions concerning the procedures by which data reach the status of "recommended data", resulted in the following summarized "Procedures".

Procedures to arrive at recommended data

The process to generate recommended A+M data consists of a number of sequential procedures. The following procedures to be followed have been recommended by the Subcommittee:

1. The first step is the assessment and review of the data status: this is to be performed by the Agency's CRP, by other groups co-opted by the IAEA (e.g., on recombination), and other non-IAEA efforts. The data resulting from these activities are considered to have the status of: "proposed to be evaluated and/or recommended".

2. The second step is the evaluation of the data: this is to be performed primarily by, or under the auspices of, A+M Data Centres (excluding the IAEA A+M Data Unit). Evaluation, normally implies the existence of more than one experimental data set, and/or existing theoretical techniques. In those cases, where only a single set of data exists, or where data are non-existent and accepted values depend on unique calculational models, the evaluation step may be by-passed. The data resulting from this activity would have the status of "evaluated data".
3. The final step, which consists in the selection of data from among the complete body of evaluated data, and the recommendation of unique data sets for each reaction and species, or unique parametric representations of the data, is to be performed by the Subcommittee, or by experts appointed by the Subcommittee. The data resulting from this final procedure has the status of "recommended data", and should form the data base of recommended A+M data which shall be made available to the user community by the IAEA. In those cases where only one data set exists for a given reaction/species, it can be considered as the best available data, and be designated as "provisionally recommended".

In context of these three steps, the IAEA A+M Data Unit has the following important functions:

1. To stimulate the review, assessment and evaluation of data.
2. During the assessment and evaluation stages, IAEA should inform the atomic physics and fusion communities of on-going and planned data reviews (e.g., by the CRP), or data evaluations (e.g., by the data centres), and solicit data contributions which should be taken into consideration in these activities. These announcements and requests for data should be made in the quarterly Bulletin. (See Action # 8).
3. After data have been recommended, IAEA should publicize the availability of recommended data from the IAEA, in the Agency's "Nuclear Fusion" journal and in the Bulletin.
4. In order to ascertain that the fusion community is supplied with the available recommended data, IAEA should take a strong lead in the international dissemination of A+M data.

4. Assessment of Recombination Data

In view of the critical need for evaluated "recombination" data (including dielectronic as well as two-body recombination), and the existence of a large amount of recombination data, the Subcommittee recommended that this body of data be critically reviewed in a separate effort. Individual members of the Subcommittee are prepared to suggest names of potential reviewers who could be approached by the A+M Data Unit to perform a critical assessment of these data. (See Actions # 6 and # 7).

5. Exchange Format

In order to facilitate the exchange of numerical data between centres, to help maintain a reasonable degree of uniformity and completeness of the information compiled and stored by all participating centres, and to facilitate the evaluation and dissemination of data, the Subcommittee endorsed the development of an exchange format.

6. Terminology

In order to maintain a common usage of terminology in the A+M data field, the Subcommittee confirmed its earlier endorsement and recommended that the data terminology as defined in the "Definition of Terms", given in Appendix 6 of this report, be adhered to.

E. International A+M Data Centre Network

The Subcommittee reviewed its statement on the A+M Data Centre Network (INDC(SEC)-77/GA, p. 9), made at the last Subcommittee meeting, and felt that it was still relevant to the current situation. That statement is reproduced below:

Statement on the International A+M Data Centre Network

Although no formal arrangement exists between the cooperating centres, two informal agreements have been reached at the second A+M Data Centre Meeting, (Fontenay-aux-Roses, May 1980), namely,

- to have an unrestricted exchange of bibliographic and numerical data between centres, and
- to cooperate in the development of a computerized data exchange format.

In addition to endorsing these agreements, the Subcommittee encourages the following long-term arrangements:

- (i) to share a topical or regional responsibility in the collection and compilation of bibliographic and numerical A+M data to ascertain that all available data are compiled with a minimum of duplications,
- (ii) to share the responsibility to evaluate A+M data, either through the auspices of the IAEA or through bilateral agreements,

- (iii) to maintain an international list of data requirements and their priorities, and
- (iv) to establish regional responsibilities for providing services to the user community.

In order to keep the fusion research community currently informed of the A+M data available in the data centres of the network, the Subcommittee recommended that the IAEA compile an index of existing bibliographic and numerical collision and surface interaction data compilations (see Action # 9) on the basis of information received from the data centres, and publicize this information in the Bulletin.

F. Future IAEA A+M Data Meetings

1. A+M Data Centre Network meetings

The decision by the A+M Data Centre Network at their November 1982 meeting (see INDC(NDS)-136/GA) to change to more frequent meetings of the network was endorsed by the Subcommittee; the Subcommittee also recommended that these meetings be held whenever possible adjacent to the IFRC Subcommittee meetings.

2. Meetings of the CRP on Atomic Collision Data

Participants in the CRP meet annually. In order to allow the Subcommittee to evaluate the results of each of these meetings, the Subcommittee suggested that there should be adequate time between each CRP meeting and the next Subcommittee meeting.

3. Small experts meetings

If financially feasible, the Subcommittee endorsed convening small (Consultants') experts meetings on specific technical topics (e.g., recombination).

4. Technical Committee Meetings

The next large meeting, of the type held in Culham (1976) and Paris (1980), was recommended by the Subcommittee to be held in 1985.

5. Next meeting of the IFRC Subcommittee

The next meeting of the IFRC Subcommittee was suggested to take place in April or May 1984, adjacent to the next A+M Data Centre Network meeting. Considerations should be given not to conflict in time with scheduled INTOR meetings or any other larger atomic physics or fusion technology meetings.

Appendix 1

IFRC Subcommittee on Atomic + Molecular Data for Fusion

Meeting 4-5 November 1982

List of Participants

(Members of the Subcommittee are marked by an asterisk)

- | | |
|--|--|
| * Derrien, M.A. | DEDR/DRNR/SEDC/SPNR
Centre d'Etudes Nucleaires
de Cadarache
B.P. No. 1
F-13115 Saint-Paul-Lez-Durance |
| * Drawin, H.W. | Dept. de Recherche sur la Fusion
Association Euratom-C.E.A. sur
la Fusion Controlee
Rue du Panorama, P.O.B. 6
F-92260 Fontenay-aux-Roses |
| Gremillet, D. | IAEA/Nuclear Data Section
A+M Data Unit |
| Nakai, Y.
(Substitute for
Dr. K. Harada) | Division of Physics
Japan Atomic Energy Research
Institute
Tokai-Mura, Naka-Gun
Ibaraki-Ken 319-11, Japan |
| * Harrison, M.F.A. | Culham Laboratory
United Kingdom Atomic Energy Authority
Abingdon, Oxon. OX14 3DB
United Kingdom |
| * Hayakawa, S. | Department of Astrophysics
Nagoya University
Nagoya, Japan |
| Katsonis, K. | IAEA/Nuclear Data Section
A+M Data Unit |
| * Lorenz, A. | IAEA/Nuclear Data Section
A+M Data Unit |
| Schmidt, J.J. | IAEA/Nuclear Data Section |

Second Meeting

IFRC Subcommittee on A+M Data for Fusion

Vienna, 4-5 November 1982

Adopted Agenda

1. Introductory Items

- Selection of Chairman
- Adoption of Agenda
- Subcommittee Membership

2. A+M Data Unit

- 2.1. Programme and function (see last meeting recommendation)
- 2.2. Staff changes
- 2.3. Attendance of non-IAEA Meetings
- 2.4. Other considerations

3. Bibliographic A+M Data

- 3.1. Description of the A+M Bibliographic Data Base System
- 3.2. Status of the A+M bibliographic data base
- 3.3. A+M Data Bulletin and related considerations
- 3.4. Publication of CIAMDA
- 3.5. Selective retrievals from the A+M Bibliographic Data Base
- 3.6. Review of last meeting recommendations

4. Numerical A+M Data

- 4.1. CRP on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas - (Report on the first meeting)
- 4.2. Recommended A+M Collision Data
- 4.3. Considerations of data priorities and evaluation
- 4.4. International numerical data base
- 4.5. A+M Data for Fusion Plasma Modelling
- 4.6. CRP on Atomic Data Pertinent to Plasma-wall Interaction Processes
- 4.7. Review of last meeting recommendations

5. A+M Data Centre Network

- 5.1. Report on the 3rd A+M Data Centre Meeting
- 5.2. Review of last meeting recommendation

6. Future A+M Data Meetings

- 6.1. A+M Data Centre Network Meetings
- 6.2. CRP Meetings
- 6.3. Experts Meetings
- 6.4. Next Advisory Group on A+M Data for Fusion

7. Next meeting of the Subcommittee

Appendix 3

List of Actions

(IAEA = A+M Data Unit of the Nuclear Data Section)

1. IAEA Ask Dr. D. Seeliger, incoming chairman of the INDC, to appoint new INDC representative to the A+M Data subcommittee.
2. All Members Review the "Fusion Cut-off Criteria" described in Appendix 8 of INDC(SEC)-77/GA, and send to IAEA comments and suggestions for changes deemed necessary.
3. Katsonis Approach all known experts and ask them to inform IAEA of all important review papers which should be included in the A+M/BDB.
4. Nakai Arrange for the translation into English of the book review on CIAMDA which has been published in Japan, and send translation to IAEA.
5. All Members Review the report of the first meeting of the atomic collision data CRP (INDC(NDS)-136/GA), and send comments to IAEA and CRP participants.
6. Drawin Send IAEA a list of potential recombination data reviewers.
7. IAEA Approach selected experts on recombination to perform a critical assessment of existing recombination data.
8. Katsonis Introduce a separate section in the Bulletin to inform the readers that evaluations of certain data are being considered, and ask contributions to these efforts. Also inform Bulletin readers that results of evaluation efforts are available at IAEA.
9. IAEA Obtain from all A+M Data Centres, a descriptive list of their bibliographic and numerical data holdings, and publish a combined list in the Bulletin. This list should be updated annually.
10. IAEA Send all Subcommittee members copies of INDC(NDS)-136/GA and the Culham report CLM-R 216 (1982), and the material representing the private communications referred to on page 5 of INDC(NDS)-136/GA.

Appendix 4

IFRC Subcommittee on Atomic + Molecular Data for Fusion

Membership as of November 1982

Derrien, M.A.	INDC Chairman Representative	DEDR/DRNR/SEDC/SPNR Centre d'Etudes Nucleaires de Cadarache B.P. No. 1 F-13115 Saint-Paul-lez-Durance
Drawin, H.W.		Dept. de Recherches sur la Fusion Association Euratom-C.E.A. P.O.B. 6 F-92260 Fontenay-aux-Roses
Harada, K.		Division of Physics Japan Atomic Energy Research Institute Tokai-Mura, Naka-Gun Ibaraki-Ken 319-11, Japan
Harrison, M.F.A.		Culham Laboratory United Kingdom Atomic Energy Authority Abingdon, Oxon. OX14 3DB United Kingdom
Hayakawa, S.		Department of Astrophysics Nagoya University Nagoya, Japan
Lorenz, A.	Scientific Secretary	IAEA/Nuclear Data Section
Martynenko, Yu.V.		Institut Atomnoi Energii I.V. Kurchatova Ploshchad I.V. Kurchatova Moscow D-182, 123182 U.S.S.R.
Stone, P.M.		Applied Plasma Physics Office of Fusion Energy U.S. Department of Energy Washington, D.C. 20545 U.S.A.

Appendix 5

Progress Report of the IAEA A+M Data Unit
for the period February 1981 - October 1982

A. Lorenz

A. A+M Data Unit Staff

1. Staff Changes

Since the last meeting of the A+M Data IFRC Subcommittee, R.A. Langley who was the head of the A+M Data Unit from August 1980 until November 1981, returned to the ORNL in the USA at the end of 1981. Because of the need to introduce a change in the programmatic emphasis in the Nuclear Data Section, at that time, requiring a staff reorganization, A. Lorenz was appointed head of the A+M Data Unit. The other professional staff of the Unit, K. Katsonis and D. Gremillet, has remained the same during this reporting period. Two new clerical staff, K. Sheikh (data processing clerk) and E. Baumgartner (secretary), make up the complement of five in the A+M Data Unit.

2. Attendance of non-IAEA Meetings

External, non-IAEA, meetings attended and laboratories visited by the A+M Data Unit staff, are listed in Annex 1 to this report.

B. Bibliographic A+M Data

1. Status of the A+M Bibliographic Data Base (A+M/BDB)

The A+M Bibliographic Data Base (A+M/BDB) consists of a computerized file of references to publications on atomic and molecular data relevant to fusion. It includes references to atomic collision data, structure and spectra data, surface interaction data and general references pertinent to A+M data for fusion. All reference citations stored in the A+M/BDB are indexed with respect to their content, so as to allow selective retrieval from the data base and the production of special publications (e.g. Quarterly A+M Data Bulletin, CIAMDA, etc.).

The computer system of the A+M/BDB which supersedes all earlier computer programmes generated for the production of the A+M Data Bulletin and of CIAMDA, is now completed, and all bibliographic data which existed in the past in separate files (i.e. CIAMDA and Bulletin) have been cleaned up and converted to the new system. A general description of the A+M/BDB is contained in a separate report presented to this meeting, and the Input and Update Procedures of this system are described in IAEA-NDS-AM-12 (report to be published).

2. Updating of the A+M/BDB

The A+M/BDB is updated quarterly, corresponding to the production of the International Bulletin on A+M Data for Fusion. At the present time, a total of 137 journals are systematically scanned to provide the input for the update; this is supplemented by information received from correspondents and reference citations provided by other centres.

3. Publication of the A+M Data Bulletin

The IAEA Bulletin has continued to be published regularly on a quarterly basis. This year, the Bulletin was issued in February (No. 18), June (No. 19), September (No. 20) and foreseeably in December (No. 21). It is distributed to 1105 scientists in 26 Member States and International organizations.

4. Publication of CIAMDA

The date of the next publication of CIAMDA depends on two factors,

- the status of the CIAMDA 80 sales, and
- the number of new indexation lines entered since the publication of CIAMDA 80.

In addition to the limited number of copies distributed free of charge, the Agency has sold 521 copies in 1980-1981, and 14 copies in 1982; 130 copies are still in stock. Although the total sales for this document are considered good by IAEA standards, it is questionable whether the IAEA Publications Committee will agree to a new publication with 130 copies of the old publication still in stock, unless the new product would be considerably different from the old one. With regard to this point, approximately 660 new reference citations for collision data have been entered into the system since the publication of CIAMDA 80, which is approximately 5 % of the total content of CIAMDA 80. Under these circumstances, a new CIAMDA publication is not warranted at the present time. It is suggested to re-assess the justification to publish a new CIAMDA in two years time (i.e. at the next meeting of the IFRC Subcommittee).

5. Selective Retrievals from the A+M/BDB

To supplement the information published in CIAMDA 80 and in the individual issues of the Bulletin, it is now possible, with the conversion to the A+M/BDB system, to perform selective retrievals from the complete bibliographic data base on request from individual users. Such retrievals would also serve as tests of completion made on the basis of feed-back received from the users. The retrievals could be made on all of the indexed information, including "structure and spectra", "collisions" and "surface interactions". It is proposed to inform the readers of the Bulletin of this new service in each of the future issues of the Bulletin.

C. Numerical A+M Data

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

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

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

With the view to determine more specifically the data types which the CRP should cover and to establish an order of priority among the needed data, the A+M Data Unit, using the recommendations of the May 1980 IAEA Technical Committee Meeting on A+M Data for Fusion (reference: Physica Scripta 23 69 (1981) 206-209), formulated a questionnaire and conducted a survey among the fusion research community. The results of this questionnaire are summarized in the Summary Report of the first meeting of the CRP (INDC(NDS)-136/GA). The emphasis of the CRP is thus based on the initial IFRC subcommittee recommendation and on the results of the Data Priority Questionnaire.

The first meeting of the participants in the IAEA Coordinated Research Programme (CRP) on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas was convened by the IAEA Nuclear Data Section on 21-25 June 1982 at IAEA Headquarters in Vienna. The meeting was chaired by A. Lorenz with the assistance of three co-chairmen: M.R.C. McDowell, H.B. Gilbody and G. Dunn. The Scientific Secretary of the meeting was K. Katsonis.

The CRP reviewed the overall status of electron collision data of importance to the diagnostics of magnetic fusion plasmas. In reviewing these data from the point of view of reliability and presently accepted accuracies, the CRP could identify only certain electron impact ionization data which could be recommended to be used by the fusion community at this time. The accuracy of these data could be taken to be $\pm 10\%$ (see section C.2. below).

The summary report of this meeting (INDC(NDS)-136/GA) will be distributed at the IFRC Subcommittee meeting, and is to be published in November 1982.

2. Recommended A+M Collision Data

The electron impact ionization data proposed to be recommended by the Atomic Collision CRP, consists of the ionization cross sections of all species for $Z = 1-8$, including all ionization stages, generated by the Belfast group, K.L. Bell et al. (published as Culham Laboratory

report CLM-R 216), and for $Z > 8$, of data measured in recent cross-beam measurements. A list of these data (taken from the Summary Report of the CRP Meeting) is given in Table I.

The data for $Z > 8$, which have been identified by the CRP as the best currently available, are proposed to be recommended data, and are not "evaluated data". The $Z = 1-8$ data, generated by the Belfast group are "evaluated", in the sense that these were derived from an assessment of all existing numerical data and complemented by theory.

The ionization data generated by the Belfast group, and published in the CLM-R 216, is part of the Belfast Data base on Atomic and Molecular Physics. This data base is kept up-to-date at Queen's University, Belfast, and at the Daresbury Laboratory.

3. International Numerical Data Base

As a first step in the establishment of an international base for the storage and exchange of numerical A+M collision data, the A+M Data Unit, with the cooperation of the Queen's University Computer Science Department staff, has made the Belfast system operable at the IAEA.

The data stored in this system at IAEA, consists of the evaluated Belfast data ($Z = 1-8$) as published in the CLM-R 216 report, which was transmitted to us from Belfast, and most of the $Z > 8$ data listed in Table I, which will be entered into this system by the A+M Data Unit.

It has been agreed with the Queen's University Computer Science Department to pursue the further development of the system itself, as well as the exchange of data which either Belfast or IAEA adds to the data base.

4. Coordinated Research Programme for the Evaluation of Atomic Data Pertinent to Plasma-wall Interaction Processes (Plasma-Surface Data CRP)

The Plasma-Surface Data CRP, conducted by R.A. Langley, was a one year project which was completed during calendar year 1981. The compendium of data for plasma-surface interaction (summarized in Annex 2) which resulted from this CRP is to be published in a special issue of the Agency's Nuclear Fusion Journal.

5. A+M Data for Fusion Plasma Modelling

A consultants' meeting on Computer Codes for Fusion Research, convened by the IAEA Physics Section in December 1979, identified the appreciable need for atomic physics data used as input to computer codes designed for the computation of fusion plasma models.

In an effort to identify these data users and what data they use, and to initiate an activity which would eventually lead to an atomic data library, providing a common data base for the calculations performed by these modelling groups, the A+M Data Unit sent a circular letter to 60 scientists, identified by the original participants in the 1979 consultants' meeting. The text of that circular letter is included in this report as Appendix 3. The response was 30 %. The information sent back to us has not yet been fully analyzed; in a number of cases new names have been suggested, which will require follow-up letters to be sent.

Table I

Electron Impact Ionization Data Proposed to be Recommended

Z = 1 - 8

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

Z = 9 - 18

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

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

Z = 19 - 102

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

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

A. Meetings attended by A+M staff (Feb. 81 - Oct. 82)

- International Seminar of High-Energy Ion-Atom Collision Processes, Debrecen, Hungary, 17-19 March 1981 (K. Katsonis)
- 9th International Conference on Atomic Collisions in Solids, Lyon, France, 5-10 July 1981 (R.A. Langley)
- XII International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC), Gatlinburg, Tennessee, USA, 15 July - 21 July 1981 (K. Katsonis)
- Xth European Conference on Controlled Fusion and Plasma Physics, Moscow, 14-19 September 1981, (R.A. Langley)
- Symposium on Atomic and Surface Physics (SASP), 7-13 February 1982, Maria Alm-Hintermoos, Austria (K. Katsonis)
- Winter School on Atomic Physics of Hot Plasmas with Application to Fusion Plasma Diagnostics, Les Houches, France, 1-13 March 1982 (K. Katsonis)
- European Sectional Conference on Atomic and Molecular Physics of Ionized Gases (6th ESCAMPIG), Oxford, UK, 1-3 September 1982 (K. Katsonis)

B. Laboratories visited by A+M staff (Feb. 81 - Oct. 82)

- Institute for Plasma Physics, Max-Planck Institute, Garching, FRG, 11-15 May 1981 (R.A. Langley)
- Institute of Physics, Beograd, Yugoslavia, June 1981 (R.A. Langley)
- KFA, Jülich (FRG), Hahn-Meitner Institute (West Berlin), FOM Institute, Amsterdam (The Netherlands), Culham and JET Laboratories, Oxford (UK), Fontenay-aux-Roses (France), 15 June - 2 July 1981 (R.A. Langley)
- Institute of High Temperature of the Academy of Sciences, Moscow, the Kurchatov Institute of Atomic Energy, Moscow, and the Ioffe Institute of the Academy of Sciences, Leningrad, September 1981 (R.A. Langley)
- Visit to the Laboratoire de Physique des Plasmas of the University of Paris, France, 11-13 and 16 January 1982 and to the EURATOM-CEA Association Fusion Laboratory at Fontenay-aux-Roses, France, January 1982 (K. Katsonis)
- Fusion Research Department of CEN Laboratory in Grenoble, France, 15 March 1982 (K. Katsonis)
- Culham Laboratory, JET Joint Undertaking, UK and Royal Holloway College, University of London, Egham Hill, UK, August 1982 (K. Katsonis)
- Institute of Physics, University of Belgrade, Yugoslavia, 28-30 September 1982 (K. Katsonis)

Data Compendium for Plasma-Surface Interactions

Abstract

Reviews of particle-solid processes pertinent to modelling plasma-wall interactions are presented and sets of recommended data are given. Analytic formulas are used where possible otherwise data are presented in the form of tables and graphs. The incident particles considered are e^- , H, D, T, He, C, O and self ions. The materials include the metals: aluminium, copper, molybdenum, stainless steel, titanium and tungsten and the non-metals: carbon and TiC.

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R.A. Langley (IAEA, A+M Data Unit)
2. Light ion reflection from solids
W. Eckstein and H. Verbeek (Max Planck Institut für Plasmaphysik)
3. Hydrogen and helium trapping
K. Wilson (Sandia National Laboratory)
4. Desorption
E. Taglauer (Max Planck Institut für Plasmaphysik)
5. Evaporation
R.A. Langley (IAEA, A+M Data Unit)
6. Sputtering
J. Bohdanský (Max Planck Institut für Plasmaphysik)
7. Chemical effects in sputtering
J. Roth (Max Planck Institut für Plasmaphysik)
8. Blistering
K. Wilson (Sandia National Laboratory)
9. Secondary electron emission
E. Thomas (Georgia Institute of Technology)
10. Unipolar arcing
P. Mioduszewski (Oak Ridge National Laboratory)

Letter addressed to Fusion Plasma Modellers

Dear,

One area in the field of plasma modelling requiring attention which was identified by the participants in the IAEA Consultants' meeting on Computer Codes for Fusion Research, convened in December 1979 at the IAEA in Vienna, is the appreciable need for atomic physics data used as input to computer codes designed for the computation of fusion plasma models. The input to these calculations consists of atomic collision data (e.g. ionization, recombination, charge transfer), atomic structure and spectral data (e.g. energy levels, transition probabilities, oscillator strengths), and plasma-surface interaction data (e.g. sputtering, trapping, sorption). Although these data are now being used for plasma modelling and other fusion research applications, it is recognized by the fusion community that they are incomplete, mostly not known to the desired degree of accuracy, and in some instances lacking altogether.

In response to the general need for reliable and accurate atomic physics data, the IAEA Atomic and Molecular (A+M) Data Unit is currently pursuing a programme for the international coordination of the compilation, evaluation and dissemination of atomic and molecular data for the benefit of fusion technology. One objective of this programme is to promote the collaboration between groups using numerical atomic physics data in plasma modelling calculations so as to develop a common data base for the calculations performed by these groups.

With this letter I would like to ask you if you would be interested to participate in such an informal international exchange of atomic physics data. Initially we intend to collect the input data used by plasma modelling groups and to perform an intercomparison of these data. At the end of this first stage we would distribute the results of this intercomparison to all participating groups. Depending on the outcome of this initial exercise, and on the response from the participating groups, we would consider creating a computerized data base of atomic data specifically designed for plasma modelling calculations. The content and accuracy of such an atomic data library would be gradually improved by parallel evaluation efforts of groups of atomic physics experts coordinated by the IAEA A+M Data Unit.

Should you decide to participate in this exercise, I would appreciate it if you would send me the atomic data currently used by your group in modelling calculations as well as any documentation and published reports that could be useful to us. If this information is available on magnetic tape, please send it to us on tape (9 track, 1600 or 6250 BPI, EBCDIC). In the event that you use polynomial representation of the reaction cross-sections, we would appreciate receiving those as well. If you know of any other groups involved in plasma modelling calculations, which could contribute to this effort, I should appreciate it if you would inform me of their names and addresses. The list of individuals to whom this letter has been sent is enclosed herewith for your information.

encl.

Sincerely yours,

A. Lorenz, Head
Atomic and Molecular
Data Unit

Appendix 6

Definition of Terms

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

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

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

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

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

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

- Experimental data: numerical values resulting from a physics experiment (i.e., measurement)
- Calculated data: numerical values resulting from computation (e.g., calculated from theory)
- Derived data: numerical values calculated from data obtained in the analysis of experimental data (e.g., reaction rates calculated from reaction cross sections)
- Evaluated data: set of numerical values which have resulted from an evaluation (see above)
- Recommended data: set of numerical data, chosen by a recognized body to be recommended as the best set among a set of evaluated data.
- Standard data: set of numerical data established by general agreement as a basis for the measurement of other physical quantities, or set of accurately known data relative to which other data are determined (normalized)
- Provisionally recommended data: set of numerical data, which, because of its uniqueness, is recommended as the best set.