

INTERNATIONAL NUCLEAR DATA COMMITTEE

Minutes of the Third Meeting of the Joint IFRC/INDC

Subcommittee on Atomic and Molecular Data for Fusion

Vienna, 14 April 1978

Compiled by A. Lorenz and R.E. Seamon Nuclear Data Section

International Atomic Energy Agency

April 1978

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria June 1978 78-05248 Minutes of the Third Meeting of the Joint IFRC/INDC Subcommittee on Atomic and Molecular Data for Fusion

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AGENDA

- 1. Adoption of Agenda
- 2. Terms of Reference
- 3. Progress Review

Reports by staff of A+M Data Unit

- a) A+M Data Bulletin
- b) Atomic Collision Data Index
- 4. Technical Evaluation of Current IAEA A+M Data Programme
- 5. Future Course of IAEA A+M Data Programme
 - a) Suggested Programme
 - b) Discussion
 - c) Recommendation
- 6. Timetable for IAEA A+M Data Programme Regularization
- 7. Future Review Procedure
- 8. Summary of Recommendations
- 9. Next Meeting

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List of Meeting Participants

Name (Committee Affiliation)	Present at Meeting in Capacity of	Home Address
E.C. Beaty (IAEA)	Head Atomic and Molecular Data Unit	IAEA, Nuclear Data Section
C.M. Braams (IFRC)	Subcommittee Chairman	FOM-Instituut voor Plasmafysica Rijnhuisen, Jutphaas, The Netherlands
H.W. Drawin (IFRC)	Subcommittee Member	Dept. Phys. Plasmas & Fus. Contr. Association Euratom-C.E.A. sur la Fusion Controlee Rue du Panorama, P.O.B. 6 F-92260 Fontenay-aux-Roses
T. Fuketa (INDC)	Subcommittee Member	Nuclear Data Center Japan Atomic Energy Research Institute Tokai-Mura, Naka-Gun Ibaraki-Ken 319-11 Japan
K. Katsonis (IAEA)	Member Atomic and Molecular Data Unit	IAEA, Nuclear Data Section
A. Lorenz (IAEA)	Scientific Secretary	IAEA, Nuclear Data Section
M.K. Mehta (INDC)	Subcommittee Member	Bhabha Atomic Research Centre Nuclear Physics Division Trombay, Bombay 400 085
J.E. Phillips (IAEA)	Subcommittee Member	IAEA, Physics Section
J.J. Schmidt (IAEA)	Subcommittee Member	IAEA, Nuclear Data Section
R.E. Seamon (IAEA)	Member Atomic and Molecular Data Unit	IAEA, Nuclear Data Section
P.M. Stone*(IFRC)	Subcommittee Member	Division of Magnetic Fusion Energy U.S. Department of Energy Washington, D.C. 20545

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*Attending for J. Decker

Progress Report of the Atomic and Molecular Data Unit

In conformity with the recommendations of the Joint IFRC/INDC Subcommittee on Atomic and Molecular $(A_{+}M)$ Data for Fusion, work during the past year has been devoted to the creation of the International Bulletin on Atomic and Molecular Data for Fusion, the development of an International Index for Atomic Collision Data for Fusion, and to the initiation of an international network of A_+M data centres.

- In connection with the A+M Bulletin, it was reported that the first 1. three issues have been completed and mailed in September and December. 1977 and March, 1978. The fourth issue was ready for press at this meeting. The first issue was sent by surface mail in accordance with the regular IAEA policy. As a result of shipping strikes the overseas delivery of this first issue was considerably delayed. To avoid such delay the second and third issues were sent to overseas addresses by airmail: future issues will also be sent by airmail. In view of the large number of recipients (close to 1000) and the need to keep the mailing costs within reasonable limits, a questionnaire was attached to Bulletin no. 3 asking recipients to confirm their professional interest. It is hoped that it will be possible to reduce the mailing list so that airmail can be used in the future without unduly raising the mailing cost. From the first 50 questionnaires returned in the week of the meeting it could be concluded that the response of the fusion community has been favourable and that the scope of the Bulletin has been found acceptable.
- 2. The project to publish in 1978 an Index to Atomic Collision Data is approximately on schedule. Magnetic tapes with bibliographic data for this project have been received from the Oak Ridge National Laboratory, the Joint Institute for Laboratory Astrophysics and the University of Paris/Orsay. The fourth major source of information will be the data index portion of the A+M Data Bulletin. Contributions are also expected from the Soviet Union and Japan. The three source tapes for the index do not have the same information content and in those cases where the information is the same the coding systems are very different. The tasks to be accomplished for the preparation of the index are as follows:
 - a) Convert the information on each tape to a common coding system and rearrange it so that all information on a given publication can be merged. As a result of this there may be up to four different statements concerning the data content of a single publication.
 - b) Check for and resolve inconsistencies. The number of citations is so large that the checking must be done by computer. How to make the corrections depends upon the type and number of inconsistencies found.
 - c) Eliminate material not relevant to fusion application.

d) Prepare printout in final form for the publication.

Task (a) is essentially complete in the sense that the programming is nearly complete. Task (b) has been addressed only to the extent that the recoding work under (a) was done in such a way as to make the intercomparison relatively easy. Task (c) is being done in several steps. Some references on molecular data of no interest to fusion are eliminated as part of task (a). The final and most difficult step will be to separate the marginally acceptable references from the marginally unacceptable ones. As the large number of citations requires that this separation is done by computer, the principal work will be in defining the rules. Work on the Bulletin is providing some useful experience in establishing such rules. Task (d) is expected to be relatively straightforward. It is planned to provide the final manuscript for the index publication before the end of 1978.

3. A meeting of the Atomic and Molecular (A+M) Data Centre's Network held in May 1977 (see Summary Report INDC(NDS)-88/GB) formulated general plans for future cooperation not only on collision data but also on spectroscopy data and surface interaction data. The basis was laid for getting the information for the 1978 Index. Also agreements were reached to get some assistance with the coverage of Japanese and Russian language literature. Tentative plans were made for another meeting in May of 1978; however, it was decided to postpone the second meeting, pending the regularisation of the IAEA A+M data programme. The principal task for a second meeting of this group would be to make specific plans for long-range cooperation. For this it is essential to anticipate continued IAEA involvement.

Conclusions and Recommendations

1. Concerning the relationship between the Subcommittee and the parent bodies IFRC and INDC the following revised formulation of conclusion 8 of the Second Subcommittee Meeting in May 1977 (INDC(SEC)-63/GA, page 5) was adopted:

"Before recommending a commitment of the NDS, or officially approaching the IAEA in any other way, the Subcommittee should indicate the intended action to the chairmen of INDC and IFRC. Any official approach to an outside organization should be approved by these chairmen".

This reformulation resulted from consultation between the Subcommittee and INDC chairmen.

- 2. Concerning the A+M Bulletin, the following specific actions were requested of the A+M Data Unit:
 - a) Section III (Other Literature, Reviews, etc.) of the Bulletin contains references to papers with data which cannot readily be indexed. Consider the possibility of adding one or two descriptive sentences following each citation. This is not to be considered a priority item, and should not be placed above existing commitments.
 - b) The list of molecules which are considered to be "of fusion interest" should be published in the Bulletin.
 - c) It would be desirable to solicit short articles from experts concerning the data needs of the fusion community for publication in Section VI of the Bulletin.
 - d) The publication of data requests in Section VI is left to the judgement of the A+M Data Unit; the Unit should feel free to secure the assistance of a referee in case of doubt.
 - e) Additional detail concerning each reference in Section II C (Surface Effects) should be provided.
- 3. Concerning the Index to A+M Collision Data, a sample of which was distributed at the meeting, the following remarks were made:
 - a) In lists of atoms and molecules, the atoms should be arranged in order of increasing Z, and the molecules should follow.
 - b) Adhere to the original decision concerning the publication of the full bibliographic citation as stated in the Minutes of the Second Meeting of this Subcommittee (INDC(SEC)-63/GA). If in October there is a draft volume available, the question can be reconsidered at that time.
- 4. The Subcommittee agreed with the four points listed in the "Proposed Future IAEA Programme on Atomic and Molecular Data for Fusion" (<u>Appendix A</u>) with the following comments:

- a) It was understood that the Second A+M Data Centre Meeting and the Second Advisory Group Meeting (of the type held at the UKAEA Culham Laboratory in November 1976) were scheduled for the Spring of 1979, but felt that a better date for these meetings would be late in 1979 or early in 1980.
- b) With regard to the establishment of a data bank of numerical evaluated atomic collision data, the Subcommittee felt that although it was too early to expect the existence of such a file, preliminary formulations of scope and format could be undertaken. It was suggested that the digitized form of C.F. Barnett's et al Compilation of A+M Cross Sections (published in ORNL-5206 in February 1977) together with the digitized version of the Nagoya University data files (when available) could be used advantageously in gaining experience with the design of an A+M evaluated data file, and form an initial basis for such a file.
- c) With regard to the actual evaluated A+M data, it was suggested that the IAEA solicit reviews of specific A+M data topics pertinent to fusion, which topics would form the basis of an evaluated data compilation. It was suggested that recognized form of publication for these reviews should be established so as to offer the appropriate incentive to the review authors.
- 5. The Subcommittee asked the Nuclear Data Section to formulate a detailed plan for the long-term (i.e. beyond the transition date of 1 January 1980) development of the Agency's A+M data programme and submit it to the members of the Subcommittee and the IFRC before 1 July 1978. It was suggested that this plan include the recommended level of effort, including manpower requirements, and relative priorities of the programme components.
- 6. The timetable for regularization of the A+M Data Programme, revised to reflect a more logical sequence of events in the second half of 1978 and to take into account the dates of the May 1978 and August 1978 meetings of the IFRC, and of the October 1978 meeting of the INDC is included as Appendix B.
- 7. Concerning procedures for future review of the Agency's A+M Data Programme, the Subcommittee noted that while its mandate extends through the trial years 1977/78, it would be prepared to offer advice also during the evaluation year 1979, if so requested. For the long range the Subcommittee felt that it would be outside its mandate to propose a future external review procedure.
- 8. The Subcommittee suggested that the IFRC, as the initiator of the A+M Data Programme, at its forthcoming meetings in 1978 take note of the progress of this programme and, in particular, re-confirm the needs of the fusion community for a long-term international A+M data programme for fusion.
- 9. It was agreed that the next meeting of the Subcommittee would be held in Vienna on 2 October 1978.

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Proposed future IAEA programme

on Atomic and Molecular Data for Fusion

The following tasks are proposed for a continued IAEA programme on atomic and molecular data for fusion.

- 1. Continue to review the A+M data requirements for fusion and to convene meetings of the A+M data centre network.
- Continue to publish the International Bulletin on Atomic and Molecular Data for Fusion.
- 3. Maintain the data bank of the bibliographic index on atomic collision data for fusion. The 1978 Index will provide the initial basis for this data bank. It will be supplemented and kept current by input from the cooperating data centres as well as by the information published in the bulletin. Future issues of the index will be published as required. As an additional option the master file could be distributed in machine-readable form to fusion laboratories and cooperating data centres. Since accuracy and completeness of this data bank are very important continuing effort will be required to control and check the input with other data sources.
- 4. Establish a data bank of numerical evaluated atomic collision data for fusion. This is proposed to be a decentralized activity in which the IAEA would be the coordinating and data collecting centre. The evaluated data will be solicited from the cooperating data centres as well as from research groups with pertinent experience in those A+M data required for fusion. The data will be made available to interested fusion laboratories in the form of reports, computer listings or magnetic tapes.

MEMORANDUM

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To: Distribution

31 March 1978 Revised 26 April 1978

From: J.J. Schmidt, Head Nuclear Data Section

Subject: Sequence of events for the regularisation of the Atomic and Molecular (A+M) Data trial programme of the IAEA Nuclear Data Section by 1 January 1978

This memorandum should inform you on the sequence of events preceding regularisation of the IAEA programme on A+M data for fusion by 1 January 1980. This development in order to take effect assumes positive decisions at every single step without anticipating them. It is in conformity with the previous decision (see e.g. document GC(XX)/567, p. 94 f) to implement an IAEA programme on A+M data for fusion for a two-year trial period 1977/78 followed by one year (1979) during which this trial programme is being evaluated by the Agency with respect to its regularisation effective 1 January 1980.

Third Meeting of the Joint IFRC/INDC Subcommittee 14 April 1978 on A+M Data for Fusion (hereinafter referred to as the A+M Data Subcommittee). Tasks: Interim technical evaluation of the work during the trial period 1977/78 and preliminary discussions of the recommended future course of the Agency's programme on A+M data for fusion. 12 - 14 May 1978 9th Meeting of the IFRC. Proposal for the regularisation of the Agency's $A_{\pm}\mathbb{M}$ Summer 1978 data programme, including the regularisation of three professional and two general service staff (hereinafter referred to as regularisation), to be submitted to the IAEA Division of Personnel for review by an internal review committee. End August 1978 10th Meeting of the IFRC. 2 October 1978 Fourth Meeting of the A+M Data Subcommittee. Tasks: Evaluation of the trial period 77/78, recommendations concerning the regularisation and future course of

the Agency's A+M data programme.

Distribution: Prof. C.M. Braams, Chairman Joint IFRC/INDC A+M Data Subcommittee Prof. S. Pease, Chairman IFRC

Dr. W. G. Cross, Chairman INDC

October 1978 Subcommittee recommendation to be approved by parent committees INDC (10th INDC Meeting 4-10 October) and IFRC and thereafter to be submitted to the Director General.

November 1978 Hearing by internal review committee and submission of a recommendation to the Director General.

- Fall 1978 Decision will be taken by the Director General. If positive, the Director General will request the Division of Budget and Finance to include the regularisation of the A+M data programme in the budget (estimate) for 1980.
- December 1978 Consideration of the Agency's future A+M data programme by the Agency's Scientific Advisory Committee.
- April 1979 Recommendation for approval of the regularisation by the Administrative and Budgetary Committee of the IAEA Board of Governors.
- June 1979 Approval of the regularisation by the IAEA Board of Governors.
- September 1979 Approval of the regularisation by the IAEA General Conference.

1 January 1980 If all necessary approvals obtained, start of the regular IAEA programme on atomic and molecular data for fusion.