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International Atomic Energy Agency

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

MINUTES OF THE FIRST MEETING OF THE JOINT IFRC/INDC SUBCOMMITTEE ON ATOMIC AND MOLECULAR DATA FOR FUSION

Culham Laboratory, UK, 5 November 1976

Compiled by

A. Lorenz

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Agenda

1. Subcommittee Membership
2. Terms of Reference
3. Review of Culham Meeting
   Conclusions and Recommendations
4. IAEA A+M Data Programme
5. Future IAEA A+M Data Meetings
6. Dissemination of A+M data publications and information.

1. Subcommittee Membership

Members of the Subcommittee	Present at this meeting
C.M. Braams (Chairman)(IFRC)	C.M. Braams
J. Decker (IFRC)	J. Decker
H.W. Drawin (IFRC)	H.W. Drawin
T. Fuketa (INDC)	H. Suzuki + Y. Nakai (proxy for Fuketa)
Yu.V. Martynenko (IFRC)	Yu.V. Martynenko
M.K. Mehta (INDC)	B. Rose (proxy for Mehta)
J. Phillips (IAEA)	(not present)
J.J. Schmidt (IAEA/INDC)	J.J. Schmidt
G.B. Yankov (INDC)	(not present)

Others attending the meeting

A. Lorenz (IAEA) Advisor to J.J. Schmidt (IAEA)

M.F.A. Harrison (Culham) Observer

The members of the Joint IFRC/INDC Subcommittee on Atomic and Molecular Data for Fusion have been officially appointed by the Director General, by letters dated 18 and 25 October 1976.

2. Terms of Reference

The following terms of reference of this subcommittee were agreed upon:

1. Review the progress and achievements of the IAEA A+M data for fusion programme during the trial period 1977/1978 and assist IAEA in assigning priorities;

2. Stimulate international cooperation in the measurement, compilation, evaluation and dissemination of atomic and molecular data for fusion;

3. Advise the Director General of IAEA on the A+M data programme and in particular whether the trial programme should be converted to a continuing IAEA programme after 1978.

3. Review of Culham Meeting Conclusions and Recommendations

The subcommittee reviewed those points in the Working Group Reports which had direct implications to the IAEA A+M Data for Fusion programme.

A. Discussion on the report of the Working Group on International Co-operation

1. A+M data centre network

a) The question was raised by the subcommittee whether data center cooperation in the A+M data field be based on that which evolved for the neutron data field.

b) In view of the existing specialization of those centres already participating in this international cooperative effort, the subcommittee recommended that the separation of data centre responsibilities be based on topical rather than geographical distribution.

c) The subcommittee recognized the need for regional A+M data centre for Western Europe. Although it recognized that CCDN, the neutron data centre of the NEA/OECD, could become an A+M data centre sometime in the future, it was suggested by the subcommittee that a Western European centre be established under the aegis of the CCE *, and that the subcommittee (Braams) officially approach CCE * (Palumbo) (with copy to Committee of Directors of Associated Laboratories) regarding this suggestion. (Letter from Braams to Palumbo to be drafted by Schmidt).

d) Regarding the recommendation by the working group that IAEA foster the interaction between the fusion and atomic physics communities in order to encourage the determination of A+M data for fusion, it was concluded by the subcommittee that it was a long term objective, and too early to be considered at the present meeting. Schmidt was requested to collect more information on this, and the topic was relegated to the next subcommittee meeting.

e) The Working Group recommendation that IAEA appoint liaison officers in all Member States concerned to provide efficient channels of communications between A+M data users and producers and A+M data centres, was considered by the subcommittee to be premature and it was suggested that it be put on the Agenda of the next meeting.

2. Bibliographic data

a) There was a consensus in the subcommittee that a CINDA-like (neutron) index should be adopted as the bibliographic index

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* Commission des Communantée Européennes.

to atomic reaction data. Although it was deemed feasible to adapt Delcroix's (Orsay) bibliographic compilation to a CINDA-type index, differences in content and format between Barnett's (Oak Ridge) and Delcroix's (Orsay) bibliographies posed certain problems in combining both of these bibliographies into one CINDA-like Index.

b) The "Recent References" bibliographic index, which is used for nuclear structure and decay data, was also mentioned as a possible index for atomic data.

c) In the final analysis the subcommittee concluded that, although a CINDA-type index produced in the form of a book (as described in Appendix 1 of the Working Group Report on International Cooperation) was desirable, the final and detailed decisions should be made by the representatives of the data centres themselves and by the user community.

(Further conclusions and recommendations on the bibliographic index were made under Agenda item 4, see section 4.D below).

B. Discussion on the report of the Working Group on Atomic Collision Data

1. Specialists meeting. It was concluded that the recommendation that small meetings on specific topics be convened (made by this working group, see section 6) was not considered to be pertinent to the Agency's A+M programme during its first two (trial period) years.

2. In general it was agreed that it was necessary to separate the importance and priorities assigned by the technical working groups to specific areas and topics, and the emphasis and priorities to be assigned to the Agency's A+M data programme.

C. Discussion on the report of the Working Group on the Requirements of Atomic Structure Data

1. The question was raised as to the role of the IAEA/NDS in atomic structure data, in view of the continuing and strong programme of the US National Bureau of Standards, and about the extent of NDS-NBS cooperation.

2. It was recommended that IAEA/NDS consider undertaking the compilation of atomic wave functions (in the form of parametric representations allowing for a more complete description of atomic energy levels for improved oscillator strength and collision cross section calculations). Although a limited amount of information has been published in early issues of the Atomic Data Journal, it is basically a new field and a systematic compilation of these parameters have not been undertaken so far. (See Working Group Report, Sections D.1 and 2)

Harrison (Culham) was asked to check with the Belfast group to see if they had these data in their files.

3. In general, it was agreed that IAEA/NDS should review the recommendations made by the subcommittee at this meeting and present an appraisal as to the execution of these recommendations at the next meeting of the joint Subcommittee.

D. Discussion on the report of the Working Group on Surface Interaction Data for Fusion Devices

1. The recommendation by this Working Group for IAEA/NDS to cooperate with existing centres in the preparation and dissemination of bibliographies in the area of surface interactions was noted by the subcommittee, but recommended that IAEA/NDS assess the magnitude of these jobs and investigate the extent to which the work can be delegated to other centres.

2. With regard to compilation of numerical data on surface interaction, it was agreed that numerical data on sputtering, backscattering and desorption (which are amenable to numerical representation) is of significant importance and it was requested of the IAEA/NDS to investigate and assess the magnitude of this effort and inform the subcommittee at its next meeting.

4. IAEA A+M Data Programme

The Subcommittee discussed the "Progress Report on the IAEA Atomic and Molecular Data Programme", included in this report as Appendix A. As any plans beyond 1978 were considered to be outside of the subcommittee's jurisdiction at this point, "Plans for 1979-82" (page 10, Appendix A) were not discussed at this meeting.

A. Plans for 1977-1978

The discussions centered in particular around the six points outlined under "Plans for 1977-78" (page 10, Appendix A). In particular the subcommittee asked for clarification of the fourth point on the formulation of standardized computer input/output formats. As explained by Lorenz (IAEA) formulation of a format does not necessarily mean that a computerized system is programmed and operational, what is meant is that within the initial two years, it is intended to develop a common format for bibliographic and numerical data and to formulate common compilation rules.

B. Publications

The subcommittee discussed a few aspects of A+M data publication; it was suggested that "keywords" be included in journal publications so as to help with the compilers' tasks. It was also suggested that authors be

encouraged to send large sets of data, which usually are not included in journal publications, directly to the data centres. Both of these points were considered worth pursuing in the future.

C. IAEA/NDS A+M Data Unit Composition

At the time of this meeting, the full complement of the A+M Data Unit had been selected, and staffing was expected to be completed in January and February 1977. The staff is to consist of: E.S. Beaty*(from US/ /NBS) as head of the unit, K. Katsonis (from Fontenay), atomic physicist, R. Seamon (from Los Alamos), programmer analyst, and two clerical support staff.

D. Summary of Important Tasks

In addition, the subcommittee reviewed the functions of the IAEA A+M data unit, identified by the Working Group on International Cooperation (see second and third page of working group report).

1. Bibliographic index for collision data

a) Of the computerized indexes which were identified by the Working Group, the subcommittee felt that an "Index for Collision Data" was of prime importance. This index should be composed of the existing compilations of Barnett (Oak Ridge), Delcroix (Orsay), JILA (US/NBS) as well as of supplementary input from Japan (Nagoya) and the USSR (Kurchatov). The index should be in book form, be an index to the literature on A+M collision data, and be addressed to a wide audience (i.e. fusion and academic communities).

b) IAEA/NDS was asked to formulate the nature of the A+M collision data index and present it to the next subcommittee meeting. Based on Wiese's (US/NBS) publications, it was estimated that a minimum of 1500 copies would be required. (On the other hand, the National Bureau of Standards books on atomic energy levels have been published in 8000 copies for volume 1, 7100 copies for volume 2, and 6600 copies for volume 3).

2. Bulletin on latest A+M measurements

The Subcommittee endorsed the quarterly publication of a bulletin on newly measured and calculated A+M data and associated information. The bulletin, composed of input from all interested Member States, would be compiled and disseminated by IAEA/NDS.

3. Exchange of A+M data

The Subcommittee assigned top priority to the formulation of a common system for the exchange of bibliographic and numerical A+M data between centres.

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* To be confirmed.

4. Standardized Computerized Formats

The Subcommittee recommended that

the formulation of standardized computer input and output formats for the storage and dissemination of bibliographic and numerical A+M data be considered at the next scheduled A+M data centres meeting.

E. Additional considerations

1. It was re-emphasized that wave function data should be compiled by IAEA (see section 3.C.2 above).

2. The Subcommittee considered that "dielectronic recombination" forms an important body of data and that it should be compiled. It was recommended that IAEA/NDS write to US/ERDA and UK/Culham to see if anyone could provide a review of dielectronic recombination data.

5. Future IAEA A+M Data Meetings

A. Technical Meetings:

1. A consultants meeting convening representatives of centres and groups participating in the international effort of compilation, evaluation and dissemination of A+M data for fusion to formulate groundrules for their cooperation is planned to be held 9-13 May 1977 in Vienna; a confirmation of these dates will be announced by IAEA/NDS.

2. A second advisory group meeting to review the status of A+M data for fusion, and to assess new needs for A+M data and to recommend actions for future work, is planned to be held in 1978.

B. Joint Subcommittee Meetings:

1. The second meeting of the joint IFRC/INDC Subcommittee is scheduled to be held on 14-15 May 1977 (Saturday and Sunday), immediately following the A+M Data Centres Meeting and preceeding the INDC Meeting, 16-20 May. All three meetings will take place at IAEA Headquarters in Vienna.

(IAEA/NDS is to prepare draft of Subcommittee recommendation on the continuation of IAEA A+M programme beyond the trial programme, and foresee an Agenda Item for this purpose at the May Subcommittee meeting).

2. The third meeting of the Joint IFRC/INDC subcommittee is to be held in close time and place proximity to the second Advisory Group Meeting on A+M Data for Fusion, which is planned to be held in the fall of 1978.

6. Dissemination of A+M data publication and information

The Subcommittee endorsed the proposal by IAEA/NDS to incorporate two distribution categories for the dissemination of A+M data into the existing INDC document distribution system. The following two distribution codes were proposed:

"A" - Distribution code for A+M documents concerning the international effort in the field of A+M data for fusion. This group of recipients consists of INDC and IFRC Committee members, heads of data centres, and key personnel responsible for the measurement, compilation, evaluation and dissemination of A+M data.

"B" - Distribution code for technical reports A+M on the measurement or calculation of A+M data, data evaluations, surveys and compilations and progress report. This group of recipients consists of the "A" distribution plus representations of all groups of A+M data users and producers (i.e. measurers, calculators and evaluators).

A list containing a "first approximation" "B" distribution was distributed to the subcommittee members, who were requested to review it and inform IAEA/NDS of any additions or deletions.

Appendix A

Progress Report on the IAEA Atomic and Molecular Data Programme

Prepared by the IAEA Nuclear Data Section

The programme on A+M data for fusion has been approved by the governing organs of the IAEA and is to be implemented for a trial period of two years (1977-1978).

Objective

The objective of the IAEA Atomic and Molecular Data programme is to review the requirements and co-ordinate the compilation, evaluation and dissemination of atomic and molecular data of importance to thermonuclear fusion research and technology.

The scope of this programme will be oriented towards meeting the important needs expressed by the fusion community. At present, data on injection systems, surface interactions, impurity effects and plasma diagnostics are needed. Bibliographic information and numerical atomic and selected molecular data will be compiled and disseminated in cooperation with national and regional data centres.

Current Status

In addition to preparing the first international meeting on atomic and molecular data, to be held in November 1976 at the Culham Laboratory, IAEA/NDS staff has established contact with key personnel at fusion research centres concerned with atomic processes.

To aid in establishing an efficient system for the collection and dissemination of A+M data information, IAEA/NDS has compiled a list of scientists engaged in atomic and molecular processes of direct pertinence to plasma research and fusion technology. This distribution list presently comprises the names and addresses of over 200 correspondents.

Staffing

Regarding the planned staffing of the A+M programme: three professionals, one P-4 physicist to head the programme, one P-3 physicist to assist in executing the programme and a P-3 programmer responsible for the programming needs, are planned to be hired for two years on special service agreements in 1977; one additional P-2 A+M physicist and a general service (GS) staff junior programmer are foreseen to be added at a later date. To assist in the execution of the A+M data programme, one data preparation clerk and one secretary have been approved for 1977 to be paid from temporary assistance funds.

Plans for 1977-78*

After an initial organizational phase during the current year (1976), work will be carried out for a trial period of two years, i.e. 1977-1978. During this period, the programme will be continuously reviewed by the joint subcommittee of the International Fusion Research Council and the International Nuclear Data Committee (INDC).

During the trial period, this programme will have the following aims:

- To start coordinating the systematic compilation and exchange of A+M data by existing centres and groups;
- To assemble all existing reference information on A+M data measurements and calculations and produce an international computerized index to the literature on A+M data;
- To identify existing atomic and molecular data and to coordinate their compilation to avoid duplication of effort;
- To formulate standardized computer input and output formats for the storage and retrieval of bibliographic and numerical atomic and molecular data;
- To establish an international system of data dissemination; and
- To develop guidelines for the publication of atomic and molecular data.

Plans for 1979-82

Provided that its continuation is recommended by the joint IFRC/INDC Subcommittee, the programme will have the following long-term objectives:

- To act as the central international data centre for A+M data and serve as a repository for bibliographic and numerical data collected from data centres specialized in atomic and molecular structure and collisions and in surface physics;
- To provide coverage of the world's report and conference literature, and make bibliographic and numerical data available to specialized data centres; and
- To initiate and support critical reviews by asking specialists throughout the world to write such reviews and to develop universal criteria for evaluating atomic and molecular data.

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* to be modified in accordance with the Subcommittee's recommendations outlined in 4D.

Agenda Items for next Subcommittee Meeting

1. Consider interaction between fusion and academic atomic physics community, and how IAEA/NDS can be functional in this. (Section 3.A.1.d)

2. Consider the establishment of a network of A+M data Liaison Officers (Section 3.A.1.e).

3. IAEA/NDS Programme, Assessment of Tasks:

   - Compilation of atomic wave functions (see action 4 and section 3.C.2)
   - Preparation of bibliographies on surface interaction data (see action 5 and section 3.D.1)
   - Compilation of numerical surface interaction data (see action 6 and section 3.D.2).
   - Index of A+M collision data (section 4.D.1)

4. A+M data publication (keywords included in journal publications, large sets of data to be send directly to data centres, etc.).

Summary of Actions resulting from the first Meeting of the Joint IFRC/INDC Subcommittee

1.	Braams/Schmidt	Write letter to CEC suggesting the establishment of a West European A+M data center (Section 3.A.1.c)
2.	Schmidt	To collect information on how IAEA can foster fusion/atomic physics interaction (for next meeting) (Section 3.A.1.d)
3.	Harrison	To check with the Belfast group if they compile atomic wave function in parametric form (Section 3.C.2)
4.	IAEA/NDS	Assess the extent of work involved in compiling atomic wave functions (Section 3.C.2) and present to next meeting.
5.	IAEA/NDS	Assess the extent of work involved in preparing bibliographies on surface interaction data for next meeting (Section 3.D.1)
6.	IAEA/NDS	Assess the extent of work involved in compiling numerical surface interaction data (Section 3.D.2) for next meeting.
7.	IAEA/NDS	Prepare the basic structure, scope and content of the Index of A+M collision data for next meeting (Section 4.D.1)
8.	IAEA/NDS	Write to US/ERDA and UK (Culham) to see if anyone could provide a review of dielectronic combination data (Section 4.E.2)
9.	IAEA/NDS	(See section 5.B.1)
10.	All members	To review the proposed "A" and "B" distribution lists and communicate changes and additions to IAEA/NDS (Section 6)