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INTERNATIONAL NUCLEAR DATA COMMITTEE

Minutes of the Fourth Meeting of the Joint IFRC/INDC
Subcommittee on Atomic and Molecular Data for Fusion

Vienna, 30 September 1978

Compiled by
A. Lorenz and R.E. Seamon
Nuclear Data Section
International Atomic Energy Agency

October 1978

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

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Agenda

1. Adoption of Agenda.
2. Review of Conclusions and Recommendations of 14 April 1978 Meeting.
3. Progress Report and Evaluation of Current Programme presented by the staff of Atomic and Molecular Data Unit:
 - (a) A+M Data Bulletin
 - (b) Atomic Collision Data Index.
4. Summary of IFRC Recommendation.
5. Review and discussion of the proposed future A+M Data programme.
6. Drafting of recommendations by the Joint Subcommittee.
7. Future Programme review procedures:
 - a) during evaluation year 1979
 - b) long term.
8. Next Meeting.

List of Meeting Participants

C.M. Braams	Subcommittee Chairman	FOM-Instituut voor Plasmafysica Rijnhuizen, Jutphaas, The Netherlands
W.G. Cross	INDC Chairman	Atomic Energy of Canada Limited Chalk River, Ontario KOJ 1J0, Canada
H.W. Drawin	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	Subcommittee Member	Nuclear Data Center Japan Atomic Energy Research Inst. Tokai-Mura, Naka-Gun Ibaraki-Ken 319-11 Japan
K. Katsonis	A+M Data Unit Staff Member	IAEA, Nuclear Data Section
A. Lorenz	Scientific Secretary	IAEA, Nuclear Data Section
M.K. Mehta	Subcommittee Member	Bhabha Atomic Research Centre Nuclear Physics Division Trombay, Bombay 400 085, India
H.T. Motz	INDC Executive Secretary	P Division Leader, MS 434 Los Alamos Scientific Laboratory Los Alamos, New Mexico 87545, USA
J.E. Phillips	Subcommittee Member	IAEA, Physics Section
J.J. Schmidt	Subcommittee Member	IAEA, Nuclear Data Section
R.E. Seamon	A+M Data Unit Staff Member	IAEA, Nuclear Data Section
J.F. Smith	Head A+M Data Unit	IAEA, Nuclear Data Section
P.M. Stone	Subcommittee Member	Division of Magnetic Fusion Energy U.S. Department of Energy Washington, D.C. 20545, USA

Progress Report of the Atomic and Molecular Data Unit

1. Introduction

A statement of progress of the Atomic and Molecular Data Unit of the Nuclear Data Section up to the beginning of July was given in Section II of the report "Proposal for the Future IAEA Programme on Atomic and Molecular Data for Fusion", which was sent to the members of the Joint IFRC/INDC Subcommittee on A+M Data for Fusion in a memorandum from Dr. Beaty and Dr. Schmidt dated 26 July 1978 (see Appendix I). The present report adds to this earlier statement, bringing it up-to-date.

2. Staff

The staff of the Unit consists of 3 professional staff and 2 temporary assistants. The three professional staff posts are currently filled as follows:

Professor F.J. Smith	Head of the Unit
Dr. K. Katsonis	Atomic physicist
Dr. R.E. Seamon	Programmer/physicist

Dr. E.C. Beaty, the previous head of the Unit, left the Unit on 31 July and was replaced by Prof. Smith on 1 September 1978.

Dr. R.E. Seamon will leave the Unit on 31 December 1978 and will be replaced by Dr. J. Rumble on 22 January 1979. It should be noted that they are both physicists; to maintain a high standard in the Unit this programmer post must continue to be filled by a physicist.

3. Bulletin on A+M Data

a) Numbers 5 and 6

The development of the Bulletin and its production has continued to take up a large part of the work of the Unit. Up to now there have been five issues, the last covering the period ending on 1 July 1978. Work on issue No. 6, including information collected up to the end of September 1978, is well advanced and should go to press in about one month's time. It will include references from the Soviet Union provided by the Kurchatov Institute, USSR, and a number of contributions from laboratories in other countries.

b) Scope

The scope of the Bulletin comprises mainly spectroscopic data, collision data and plasma-surface interaction data. The spectroscopic and collision data is limited to the atoms and molecules listed on Table I. The composition of this list was discussed during the Atomic and Molecular Data Centre Network Meeting in May 1977. Recently Dr. Drawin provided the Unit with a list of molecules of current interest to fusion which was included in Bulletin No. 5.

c) Survey

A questionnaire, distributed by Dr. Katsonis in Bulletin No. 3, received a very good response. As the statistics, shown in Table II, indicate, the Bulletin has been well received by the fusion and the atomic physics communities, suggesting that it already provides a service which the fusion community needs. The response to the questionnaire supports the continuing production and distribution of the Bulletin.

d) Surface Data

Efforts have been made to improve the section on Surface Interaction Data. As recommended at the last meeting a word or two defining the process or quantity in each data item has been added in Bulletin No. 5.

To improve the surface data bibliography contributions from different laboratories will be helpful. Initial approaches have been made to Oak Ridge and Garching.

e) Macroscopic Properties and Plasma Diagnostics

Little so far has been included in the Bulletin on "Macroscopic Properties and Plasma Diagnostics". This needs to be considered in the new year. Help from other laboratories will be welcomed.

4. Atomic Data Collision Index

A great deal of work has been carried out on the Index to atomic collision data since the last meeting in April 1978, and many difficulties have been found.

At the last meeting it was pointed out that the tasks to be completed for the preparation of the Index were as follows:

- a) Conversion of the information on each tape to a common coding system and its rearrangement to allow merging of the tapes;
- b) finding and resolving inconsistencies;
- c) elimination of material not relevant to fusion;
- d) preparation of the printout in final form for publication.

The programming of task a) was already nearly completed and these programmes had been designed to make easy the other tasks. However, when the Unit produced merged tapes from 2 sources and examined these in detail many problems were found. These were due to errors in the data on the original tapes, ill-defined data, missing data and the subjective indexing of data. These problems and the change in staff have put back the date on which an accurate and complete Index can be produced to June 1979 at the earliest.

5. Numerical Data

The maintenance of a high standard in the production of the Bulletin has had the highest priority in the Unit (and will continue to do so).

The production of the Index has also been given high priority because of the commitment to try to produce it by the end of 1978. Thus little time has been left to consider the sponsoring of future cooperation between data centres, the soliciting of reviews on specific topics and the proposed Atomic and Molecular Numerical Data Bank. Some initial work has been done on the design of a common format for the interchange of numerical data. In the new year more time must be given to these topics in preparation for the meeting of the Data Centre Network in May 1980 where such matters will probably be the main items of discussion.

Conclusions and Recommendations

The Subcommittee was briefed on the recommendations of the Agency's programme on A+M data for fusion which were made by the International Fusion Research Council at their last meeting (see Appendix II), reviewed the A+M programme proposal described in the memorandum by E.C. Beatty and J.J. Schmidt to the members of the Subcommittee dated 26 July 1978 (see Appendix I), and made recommendations on the following items:

1. International Bulletin on Atomic and Molecular Data for Fusion:
 - a) In context of the review of the overall programme of the Unit, the Subcommittee commended the Unit on its accomplishment, and felt that the Bulletin was its main achievement; it has received favourable response and constructive criticism from the fusion community.
 - b) Regarding the content of the Bulletin, decision as to what to include in the Bulletin should be guided by its usefulness to the plasma physics community - the users of the data - rather than to the atomic physics community - the generators of the data.
 - c) In view of the current budget situation, no attempt should be made to increase the present scope of the Bulletin.
 - d) The molecules about which information should be included in the Bulletin should be limited to those given in the list included in the contribution by Dr. H.W. Drawin on page 48 of Bulletin No. 5.
2. Scope and Activities of the Programme
 - a) The scope of the activities of the A+M Data Unit is directed towards both magnetic and inertial confinement; however, no steps will be taken to extend the coverage of data specifically pertaining to inertial confinement until specifically requested.
 - b) Work by the A+M Data Unit on the first edition of the Index to Atomic Collision Data must be completed by 1 July 1979, or as much earlier as necessary to avoid printing difficulties associated with the move of the Agency to the Donaupark in Summer 1979.
 - c) The Subcommittee noted that the second meeting of the A+M Data Centre Network has been postponed until Spring 1980, and that arrangements for its convening at Fontenay-aux-Roses at the time of the planned Advisory Group Meeting on A+M Data for Fusion will be made.

3. Proposed future A+M Data Programme

- a) With regard to the proposed personnel request, the Subcommittee found a staff complement of three professionals and two general service staff to be the appropriate level of effort at this time to regularize the programme;
- b) ~~In~~ considering the estimated annual cost of the programme (see Appendix I), the Subcommittee felt that specific funds should be allocated to enable members of the Unit to attend scientific meetings, visit laboratories, and to coordinate the international contributions to the programme.
- c) The Subcommittee approved the proposed overall budget of the regularized A+M Data Unit (see Appendix I), except for two minor modifications not affecting the suggested total cost:
 - (i) the line "Annual meeting of the A+M Data Centre Network ... 10,000", is to be replaced by "Meeting and Coordination of the A+M Data Centre Network ... 10,000", and
 - (ii) items listed under "Research Contracts" should be combined to read:

- Coordinated research programme	15,000.-
- Other research contracts	15,000.-

4. Review procedures and organization

- a) The Subcommittee notes that its mandate terminates at the end of 1978 and that the trial programme moves into a year of evaluation in 1979. Should the Agency wish to call on the Subcommittee during that period, the members would be willing to meet once more late in 1979.
- b) Concerning the future of the programme it was felt that the A+M Data Unit should have a position within the IAEA. An advisory Subcommittee should be appointed by the IFRC containing members who are knowledgeable about A+M data for fusion.

5. Final Recommendation

In concluding the review of the Agency's trial programme on Atomic and Molecular Data for Fusion, the Joint IFRC/INDC Subcommittee made the following final recommendation:

The Subcommittee has reviewed the progress which the IAEA programme on Atomic and Molecular (A+M) Data for Fusion made during the trial period (1977-1978), and discussed the future development of the programme as proposed in the 26 July 1978 memorandum submitted by E.C. Beaty and J.J. Schmidt of the IAEA Nuclear Data Section to the members of the Subcommittee.

On the basis of this review, and noting the strong endorsement by the International Fusion Research Council, the Subcommittee strongly recommends that the trial programme be continued in 1979 and regularized in 1980.

The Subcommittee concludes:

- the programme is proceeding according to its earlier recommendations, except that the Subcommittee accepts a delay of at most six months in the completion of the Index originally planned for the end of 1978;
- the future programme including the continuation of the International Bulletin on Atomic and Molecular Data for Fusion, the Index to Atomic Collision Data, the creation of an evaluated A+M Data File for Fusion, and the coordination of a network of data centres as described in the memorandum of 26 July 1978, is supported;
- the personnel request of three professional and two general service staff is found to be the appropriate level of effort at this time to regularize the programme;
- the proposed budget, with two minor modifications not affecting the total is considered adequate and is recommended to be accepted by the Agency.

It is the judgement of the Subcommittee that the response from the scientific fusion community has been very positive, that the programme is needed, and that the IAEA is uniquely qualified to implement this programme.

Table I

LIST OF ATOMS AND MOLECULES
USED IN PREPARATION OF
THE FULLETIN.

1 H	44 Ru	87 Fr	130 T ₃
2 He	45 Rh	88 Ra	131 H ₂ D
3 Li	46 Pd	89 Ac	132 D ₂ H
4 Be	47 Ag	90 Th	133 H ₂ T
5 B	48 Cd	91 Pa	134 T ₂ H
6 C	49 In	92 U	135 OH ₃
7 N	50 Sn	93 Np	136 D ₂ O
8 O	51 Sb	94 Pu	137 OD ₃
9 F	52 Te	95 Am	138 T ₂ O
10 Ne	53 I	96 Cm	139 OT
11 Na	54 Xe	97 Bk	140 OT ₃
12 Mg	55 Cs	98 Cf	141 CH
13 Al	56 Ba	99 Es	142 CH ₂
14 Si	57 La	100 Fm	143 CH ₃
15 P	58 Ce	101 Md	144 CD
16 S	59 Pr	102 No	145 CD ₂
17 Cl	60 Nd	103 D	146 CD ₃
18 Ar	61 Pm	104 T	147 CD ₄
19 K	62 Sm	105 hv	148 NH
20 Ca	63 Eu	106 e	149 NH ₂
21 Sc	64 Gd	107 p	150 NH ₃
22 Ti	65 Tb	108 H ₂	151 Ne ₂
23 V	66 Dy	109 D ₂	152 Ar ₂
24 Cr	67 Ho	110 T ₂	153 Kr ₂
25 Mn	68 Er	111 HD	154 Xe ₂
26 Fe	69 Tm	112 HT	155 Br ₂
27 Co	70 Yb	113 DT	156 Cl ₂
28 Ni	71 Lu	114 He ₂	157 Cs ₂
29 Cu	72 Hf	115 HeH	158 CT
30 Zn	73 Ta	116 CO	159 CT ₂
31 Ga	74 W	117 CO ₂	160 CT ₃
32 Ge	75 Re	118 O ₂	161 CT ₄
33 As	76 Os	119 N ₂	162 HDT
34 Se	77 Ir	120 H ₃	163 HDO
35 Br	78 Pt	121 H ₂ O	164 HTO
36 Kr	79 Au	122 CH ₄	165 DTO
37 Rb	80 Hg	123 NO	166 OHD ₂
38 Sr	81 Tl	124 NO ₂	167 OHT ₂
39 Y	82 Pb	125 N ₂ O	168 OD ₂ T
40 Zr	83 Bi	126 O ₃	169 OT ₂ D
41 Nb	84 Po	127 OD	170 OTH ₂
42 Mo	85 At	128 OH	171 ODH ₂
43 Tc	86 Rn	129 D ₃	

THE ATOMIC NUMBERS ABOVE 102
HAVE BEEN ARBITRARILY ASSIGNED.

Table II

Response to the Questionnaire Sent out in the
International Bulletin on Atomic and Molecular Data for Fusion No.3

The Questionnaire was sent out to 900 recipients of the Bulletin. Of these the A+M Data Unit received 350 replies. As a result of this questionnaire, the total number of copies distributed has been reduced from 1000 to 600. The tallies of answers to the individual questions are as follows:

1. Professional interest in the Bulletin
 - fusion research applications 135
 - generation of atomic and molecular data. 265
 - other. 30

2. Interest and Consultation of "Index to Data"
 - positive responses 270

3. Expectation to contribute to the "Work in Progress",
"Numerical Data" and "Data Requests" sections of the
Bulletin:
 - expected to contribute 210
 - perhaps. 28

4. Judgement on the scope of the Bulletin
 - too restricted 9
 - satisfactory 310
 - too broad. 1

MEMORANDUM

To: Members of the Joint IFRC/INDC
Subcommittee on Atomic and
Molecular Data for Fusion

26 July 1978

From: E.C. Beaty and J.J. Schmidt
IAEA Nuclear Data Section

E.C. Beaty
J.J. Schmidt (for J.J.S.)

Subject: Future IAEA programme on Atomic and Molecular Data for Fusion

Please find enclosed an outline of the possible future IAEA programme on atomic and molecular data for fusion as requested by the IFRC at its Ninth Meeting in Vienna, May 1978.

The Subcommittee's recommendations to IFRC and INDC will form the basis for the evaluation of the trial programme and any future action by the Agency's executive and policy-making organs.

Proposal for the future IAEA programme
on atomic and molecular data for fusion

I. Introduction

Upon the recommendation of the International Fusion Research Council (IFRC) of the IAEA at its 5th Meeting in Tokyo in 1974, the IAEA Nuclear Data Section started in the beginning of 1977 a trial programme for the years 1977 and 1978 for the collection and dissemination of atomic physics data needed in fusion research. Following a suggestion, to which IFRC agreed, by the International Nuclear Data Committee (INDC), which is the Agency's advisory committee on its nuclear data programme, the Director General appointed a Joint Subcommittee of IFRC and INDC on Atomic and Molecular (A+M) Data for Fusion (henceforth called the Subcommittee) with the mandate to review the atomic data activities of the Nuclear Data Section during the trial period 1977/78 and to advise him towards the end of the trial period whether and on what basis the programme should be continued.

This document is to provide the Subcommittee with the material needed for its review and final recommendation. It contains a report on activities during the trial period based on the Subcommittee's advice (chapter II), a brief Summary of the atomic physics data needs for fusion based essentially on the conclusions of the Advisory Group Meeting on Atomic Data for Fusion held by the IAEA at the Culham Laboratory in November 1976 (chapter III), an analysis of future strategies (chapter IV) and a proposal (chapter V) for the Agency's future A+M data programme. The report finishes with an estimate of the manpower required for this programme (chapter VI).

II. Report on the trial period 1977/78

The tasks which were undertaken by the A+M Data Unit of the Nuclear Data Section during the trial period 1977/78 were those suggested by the Subcommittee at its first meeting in November 1976. They are:

- 1) to publish quarterly a bulletin reporting new A+M data measurements;
- 2) to publish by the end of 1978 a computerized index of references to A+M collision data;
- 3) to convene a meeting of representatives of A+M data centres to develop plans for future co-operative activities in the exchange of bibliographic and numerical A+M data for fusion.

1. Bulletin

The development of the Bulletin has been a major part of the effort during the trial period, and up to now four issues of the Bulletin have been published. They include numerical data solicited from the data generating scientists, announcements of reports as they are called to our attention by contributors, and an index to data published in the recent literature; they include contributions received from the Soviet Union and Japan. The scope of the Bulletin comprises atomic spectroscopy, atomic collisions and plasma-surface interaction data.

The Bulletin has attracted a great deal of interest among atomic and fusion physicists in a number of countries and the mailing list was initially nearly 1000 copies. It is now being reduced to those who have recently confirmed their interest in a direct request to us and for issue no. 5 we expect to print between 500 and 600 copies.

We endeavour to improve the usefulness of the Bulletin in the near future by:

- 1) adding brief comments to each of the papers cited in the "Other Literature" section to indicate the scope of the paper and its particular relevance to fusion;
- 2) soliciting more contributions on fusion-related atomic physics data work in progress; and
- 3) soliciting contributions from scientists in fusion laboratories on specific data needs.

2. Index

The work on the Bulletin has required more time than expected with the result that the work on the cumulative index has received less attention than expected. Nevertheless it remains a reasonable prospect that work on this project can be completed by the end of 1978 as planned. Magnetic tapes have been received from three of the co-operating data centres: Oak Ridge National Laboratory (ORNL), the University of Paris/Orsay, and the Joint Institute for Laboratory Astrophysics, Boulder. The bibliographic data from these tapes have been reformatted into a uniform computer representation. In addition the data index and bibliographic portion of the Bulletin have been cast into the same format. Input from the Soviet Union and Japan comes so far through their contributions to the Bulletin. Programmes have been completed to print material from this combined computer file either in the form of the Bulletin or in the style of CINDA. The tasks remaining are essentially to correct the remaining errors and eliminate the material not relevant to fusion research.

Errors occur for three reasons:

- 1) the original data were in error;
- 2) our reformatting programmes did not properly anticipate the structure of the original data;
- 3) in view of the limited time available it was necessary for programme development and the reformatting work to proceed simultaneously resulting in some inconsistencies.

There is a limit to our ability to correct errors in the original data. However, the other problems are straightforward - just tedious. The current estimate of the size of the index is between 5000 and 10 000 references.

3. A+M data centre network

In May 1977 representatives from ten data centres (Japan (2), USSR(1), USA (3), Western Europe (3) and IAEA) met in Vienna to report on each others' work and to develop common future plans. This meeting provided the basis for the receipt of the tapes mentioned above. It also led to several contributions to the Bulletin including an indexed bibliography to appropriate Russian language literature. A second meeting of this network was planned but has been delayed because of the uncertainty about the regular continuation of the Agency's involvement in A+M data for fusion.

III. Atomic physics data needs in fusion

The review papers given at the 1976 Culham Meeting provided a good overview of how in fusion applications atomic physics data are used and, what is needed but not available. The considerations were largely concerned with applications to Tokamak devices. Other magnetic confinement devices can be expected to have similar needs. Inertial confinement devices are quite different with respect to atomic physics data needed; so far no consideration has been given to special data needs in this area.

In the following a brief account of the important A+M data needs in fusion is given.

A major problem encountered in the development of Tokamak devices is the large amount of energy radiated by ions of partially stripped heavy metals in the inner hot parts of the plasma. Data on ionisation and excitation cross sections for these impurity ions are needed to enable a realistic computer modeling of the plasma. Because of the high temperature all molecules are dissociated and light atoms are

fully stripped. This high temperature plasma is the focus of all current activity regarding magnetic confinement work - including the application of atomic physics data. However, lower temperature plasmas occur in Tokamak devices which require consideration and understanding:

- 1) The main Tokamak discharge starts in cool gas and it can be expected that some of the atomic and molecular processes occurring in the early stages will persist in the later development of the plasma.
- 2) That portion of the main plasma which is near the wall is relatively cool and loaded with impurities. A large number of atomic and molecular processes in this region has an impact on the higher temperature plasma. That portion of the plasma pulled out by magnetic divertors poses similar atomic data problems as the near-wall plasma.
- 3) Relatively low temperature plasmas are used as ion sources for the high-current heating beams.

The other principal application of atomic physics data is in atomic reactions occurring in the beam lines.

For some of these applications atomic physics data are incorporated into computer modeling codes. For this purpose it is most helpful to have the data prepared in machine-readable form. A view frequently expressed is that the plasma physicists do not so much need cross sections but rate coefficients, i.e. cross sections averaged over Maxwellian distributions. This process can be carried further and the rate coefficients be summed over the many excited states below each ionization level. Furthermore averages can be calculated over a coronal distribution of ionization states. The end result would be a power loss rate expressed as a function of plasma parameters such as plasma temperature and impurity concentration. To be most easily used in the plasma modeling codes the results need to be expressed in a compact mathematical form. In some future it can be expected that the effects of non-Maxwellian distributions will need to be examined in detail; then the cross sections will be needed as well.

Probably the most frequent uses of A+M data involve plasma diagnostics and system design without detailed computer modeling. The opinion expressed by most of the fusion scientists consulted has been that for this purpose up-to-date reports with tables and graphs provide a universal and adequate data source. Efficient preparation of such reports plus occasionally requested specific data retrievals require that the whole data bank be "computerized".

IV. Analysis

In this chapter we give a brief analysis of the strategies to be followed in a future IAEA programme on A+M data for fusion. The principal question to be answered is which services should and can the IAEA provide to the international fusion community.

An important decision concerns the continuation of the "International Bulletin on Atomic and Molecular Data for Fusion". In addition to serving as an up-to-date index to the most recent published literature on atomic structure and collision data and selected molecular data of importance to fusion, the Bulletin should in future provide more information on fusion-relevant A+M data work in progress and on current data needs for fusion. Then it would more and more fulfil the original intent to provide an informal international medium of communication between atomic and fusion scientists.

Further to the Bulletin we consider the continued build-up and provision of a cumulated "index-to-data" as an important service for the international fusion effort. An index-to-data allows a potential user of data, e.g. an evaluator, to quickly determine where to find specific items of data in a good library. Most of the atomic and molecular physics data considered here are or will be published and for many applications it is essential for the user to obtain not only the data themselves but the descriptive material published with the data. The publication of the comprehensive 1978 index will satisfy the need for consultation of the original literature for atomic collision data for the time being. The work on the Bulletin including the contributions from the co-operating data centres will provide a natural means to keep the bibliographic data file current and to allow a periodic publication of the updated index in a few years intervals as well as specific retrievals upon request. The master file should be kept at the IAEA and made available to the co-operating data centres in regular intervals.

The desired end result of a data-for-fusion programme is published tables of evaluated numerical data (or the equivalent in machine-readable form). While the index-to-data is an essential tool in collecting and evaluating numerical data, the user would almost always prefer appropriately certified evaluated data.

The question is what can the IAEA do to obtain and make evaluated data available to the fusion community. The following problems will have to be faced:

- 1) many of the data needed in fusion applications have not yet been measured; how can the IAEA stimulate required measurements?
- 2) many of the data measured and published have not been adequately evaluated; who should perform, co-ordinate and review the necessary evaluations?
- 3) many of the evaluated data which are available have not been re-packaged in a form suitable for fusion applications.

There are direct and indirect means by which the IAEA can help to solve the first problem. Activities such as the regular publication and dissemination of the Bulletin can be expected to stimulate data generation work in atomic physics laboratories. By means of research contracts or agreements to such laboratories the IAEA can promote and support the measurement and computation of particularly important data.

Data evaluation, the second problem, must in general be done as part of the work of atomic physics research groups and of the co-operating data centres; in both the measurement and the evaluation of required data also developing countries could make important contributions. Since data evaluation is very manpower-intensive and requires continuous contact with current research, it can and should not be done at the IAEA. The role of the IAEA should be predominantly that of co-ordinating and supporting the data evaluation work performed externally. In this context the IAEA should make sure that common evaluation rules are being developed and that data evaluations are appropriately reviewed before their dissemination. In future it will be necessary to extend the scope to selected atomic spectroscopic and plasma-surface interaction data.

The third problem can effectively be tackled by the IAEA. The first step would be to build up gradually a master file of evaluated atomic collision data of relevance to fusion from input provided by atomic physics research groups and by the A+M data centre network, and to develop the necessary data handling and processing programmes for data retrieval and for conversion of the microscopic collision data into the rate coefficients required for fusion. The master file should be made available in appropriate intervals to the data centre network. The dissemination of the evaluated data to interested fusion laboratories will be mostly in the form of reports with tables and graphs, but also in the form of magnetic tapes or listings to fulfil specific requests. The Agency might consider to temporarily employ outstanding scientists as fellows or consultants to review the reliability and adequacy for fusion of the content of the evaluated data master file.

V. Possible future IAEA programme on A+M data for fusion

On the basis of the foregoing analysis the following future programme of the IAEA in A+M data for fusion is suggested:

1. Continue to review the A+M data requirements for fusion and the status and availability of the required data by specialist meetings to be convened at appropriate intervals of two or more years. Support the generation of required important data through research contracts and agreements with pertinent atomic physics research groups with due consideration of the possible contributions by developing countries.
2. Continue to publish the International Bulletin on Atomic and Molecular Data for Fusion in quarterly intervals. Increase its effectiveness as a current communication medium between atomic and fusion scientists. Agree on common indexing rules and regular input from the co-operating data centres.

3. Maintain the computer master file of the bibliographic index on atomic collision data for fusion. Future issues of the index should be published as required in intervals of a few years. As an additional service the master file should be distributed in machine-readable form to interested fusion laboratories and co-operating data centres as needed. Since accuracy and completeness of this data index are very important a continuing effort would be required to control and check the input with other bibliographic data sources.
4. Establish a data bank of numerical evaluated atomic collision data and reaction rate coefficients 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 would be solicited from the co-operating data centres as well as from research groups with pertinent experience in those A+M data required for fusion. Data evaluation should be performed mainly by several experienced research groups in atomic physics co-operating in a coordinated research programme of the IAEA. The participants in this programme should be convened in annual meetings to report and compare the results of their evaluations, to review the quality of the data in the evaluated data file and to work out strategies for improving it. The data in the master file would be subjected to the scrutiny of independent experts as regards their reliability and adequacy for fusion applications, and the full file would be made available in appropriate intervals to the data centre network. The data would be disseminated to interested fusion laboratories in the form of reports, computer listings or magnetic tapes.

Tasks 2 and 3 are related in that the Bulletin provides the means to keep the bibliographic index current. Tasks 3 and 4 are related in that the index provides the means to determine the availability of data which should be evaluated and incorporated into the numerical data bank. All four tasks can be performed efficiently only in continuous international communication and co-operation. Assistance would be required of the co-operating A+M data centres for all four tasks. Approximately annually, representatives of the data centres should meet to coordinate their work and future plans.

VI. Manpower requirements

The size of the manpower needed for the future A+M data programme of the IAEA depends critically upon whether the efforts in numerical data would be restricted to coordination or would comprise also evaluation. Assuming that data evaluation is done only outside the IAEA, the programme as proposed in chapter V can be expected to require three professional staff supported by one data preparation clerk and one secretary.

The size of this manpower would thus be the same as that which was available as consultants on special service agreements (three professional staff) and on temporary assistance (two general service staff) to carry out the Agency's A+M data programme during the trial period 1977/78. The regularization of this programme with the tasks described above would

thus require and entail the regularization of the presently available staff equivalent. In fact, the experience during the trial period showed that this level of effort was capable of forming an effective and productive unit. The detailed staff requirements would be as follows.

With computer file maintenance and error corrections by fully trained personnel, a smoothly working system and some assistance from the co-operating data centres, the continuous quarterly publication of the Bulletin and the additional work to maintain the bibliographic data index would require approximately one professional full-time equivalent (FTE), with a substantial amount of clerical and data entry assistance. The foregoing assumptions are probably correct for the time after 1978.

The establishment of the evaluated data file, the data exchange and dissemination, the coordinated research programme on data evaluation and scientific contracts for data measurements and computations should require altogether 1.5 FTE; this assumes a limitation of the scope to atomic collision data as first priority data requirement for the development of magnetic confinement devices. In the first few years after 1978 the work would consist mainly in developing the evaluated data file and the associated computer programmes and organizing the input from the co-operating research groups and data centres. Later on the emphasis would turn to corrections to the evaluated data and to data dissemination.

Administrative matters and supervision of the work of the A+M Data Unit and the organization of meetings, and secretarial and organizational work for an Advisory Committee to the programme would require an additional 0.5 FTE approximately. The breakdown of professional work given in the table below in terms of physics and programming work adds up to three FTE altogether, entailing somewhat more than two full physicists and somewhat less than one full programmer analyst. It would thus be required that on the programmer analyst position also some of the physics work be carried out, so that the programmer analyst position should preferably be filled by an atomic physicist with extensive computer and data handling experience.

Breakdown of professional manpower requirements

Item	FTE	Type of Professional
Administrative matters and supervision of A+M Data Unit	0.2	physicist
Meetings	0.3	physicist
Co-ordinated research programme and scientific contracts	0.5	physicist
Bulletin plus index/physics	0.7	physicist
Bulletin plus index/programming	0.3	programmer analyst
Evaluated data/physics	0.5	physicist
Evaluated data/programming	0.5	programmer analyst
Total	<u>3.0</u>	professional FTE

VII. Estimated Annual Cost

Based on the programme and manpower requirement outlined in chapters IV and V above, the approximate cost of a possible IAEA programme on atomic and molecular data for fusion, based on current programme costs, is estimated at US \$ 250.000,-.

The breakdown of this estimated cost is given in the Table below.

Approximate costs of a possible future IAEA A+M Data Programme

(all figures in US \$ per annum unless indicated otherwise)

- Three professional posts (at 3500 \$/month)	126.000
- Two general service posts	25.000
- One advisory group meeting every 3 or 4 years (at 15.000 - 20.000 per-meeting)	5.000
- Annual meeting of Advisory Committee	4.000
- Annual meeting of A+M Data centre network	10.000
- Research contracts	
- Coordinated research programme	
- annual meeting	5.000
- associated research contracts	10.000
- Other research contracts	15.000
- Publications, printing, etc.	20.000
- Computer use	30.000

Estimated total yearly cost: \$ 250.000
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Excerpt from the draft minutes of the 10th Meeting of the International Fusion Research Council (IFRC), held at Innsbruck, Austria, 21-22 August 1978

IFRC Recommendations on the Agency's programme on Atomic and Molecular Data for Fusion:

The IFRC reviewed the Agency's proposal for its future A+M data programme (memorandum by E.C. Beaty and J.J. Schmidt dated 26 July 1978) which was reported by Braams and Schmidt. The Council

- thanked the Agency for initiating the A+M data programme and commented positively on the achievements during the trial period 1977/78;
- strongly supported this programme, which is putting order in this very important field and meets an important requirement of the fusion community;
- strongly supported the budgetary requirements for this programme.