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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Technical Meeting:

13th MEETING OF THE IFRC SUBCOMMITTEE ON ATOMIC AND MOLECULAR DATA FOR FUSION

24-25 June, 2002, IAEA Headquarters
Vienna, Austria

SUMMARY REPORT

Prepared by:

R.E.H. Clark
N. J. Peacock

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Abstract

This report briefly describes the proceedings, conclusions and recommendations of the 13th Meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council held on 24-25 June, 2002 at the IAEA Headquarters in Vienna, Austria. The report includes an Executive Summary of the Subcommittee from this Meeting.

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1. INTRODUCTION

The 13th Technical Meeting of the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council was held on 24-25 June, 2002 at the Agency Headquarters in Vienna. The main objectives of the Meeting were to review and assess the Agency activities in the area of atomic and molecular data and plasma-surface interaction data for fusion for the period May 2000 – May 2002 and to provide recommendations to the Agency regarding its programme for the years 2004-2005.

The Meeting was attended by seven Subcommittee members (see Appendix 1). Dr. N. Peacock served as the chairman of the meeting. Dr. R. Clark, Head of the Atomic and Molecular Data Unit of the IAEA served as the Scientific Secretary of the Meeting. Prof. D. Reiter from Jülich, Germany, attended as an observer and to provide information on the facilities available for the Technical Meeting to be held in Jülich, Germany on 28-31 October, 2002.

2. BRIEF MEETING PROCEEDINGS

A. Activity Report of the A+M Data Unit

The meeting was opened by the Scientific Secretary, R. Clark, who welcomed the participants and introduced Dr. D. Sood, Director of the Division of Physics and Chemistry. Dr. Sood welcomed the participants and stressed the importance of the advice the Subcommittee offers to the Agency. Dr. Sood pointed out the high probability of agreeing on a site for ITER in the next six months to a year. That strong possibility is likely to increase the activity in fusion related research, in particular in the atomic, molecular and plasma-surface interaction areas. Dr. Sood also pointed out that the recognized increased importance of fusion research has led to positive actions in the Agency and that the activity has a strong record of success.

Following the address of Dr. Sood, the agenda was reviewed and adopted by the Subcommittee (see Appendix 2).

During the first session R. Clark outlined the main activities of the Unit during the period of May 2000 – May 2002 (see Appendix 4). The main topics covered included the Data Centre Network, the Program Performance Assessment System (PPAS), Co-ordinated Research Projects (CRP), the International Centre for Theoretical Physics workshop to be held in 2003, database management issues, Unit publications and staffing issues for the Unit. These topics generated useful discussions among the Subcommittee members and resulted in several recommendations, as detailed in the following paragraphs.

R. Clark reported that the Data Centre Network (DCN) held its biennial meeting on 10-11 September, 2001. Each Data Centre presented a progress report at that time. A complete review of the list of data needs and priorities was undertaken and the revised list was included in the Summary Report of the meeting (INDC(NDS)-430), a copy of which was distributed to the A+M Subcommittee members. It was emphasized by Clark that the DCN is a major source of both numerical and bibliographic data for the Unit databases. Discussion then focused on the possible need to add new members to the DCN. The recommendation was made that new Data Centres be considered as long as there is evidence of: 1) a strong

connection to fusion, 2) there is evidence of a useful database 3) the database is preferably in electronic form and accessible through the Internet, or soon to be in such a condition 4) the database description is in the English language. It was recommended that some potential data producers, groups in Brazil and Mexico for example, might be encouraged to participate in some other A+M Unit activities to see if there is sufficient fusion related activity to warrant their inclusion in the DCN.

The next topic was a review of the PPAS that took place in 2001 with a Panel meeting on 13-17 November, 2001. The A+M Unit was included in that review process along with the fusion activities of the Physics Section, due to the main emphasis of the A+M Unit on data for fusion. Extensive background papers were prepared for the Panel meeting and there was a comprehensive review of materials by the Panel members. During the course of the meeting the Panel explored the fusion activities in detail, listening to presentations and asking numerous clarifying questions. The final report from the Panel indicated that the staff in the fusion related areas were accomplishing more that should be expected in view of the available resources. The Panel recommended that the Agency attempt to add more resources to fusion activities and to make fusion research a more visible element of the Agency programs. The A+M Subcommittee also recommended that an effort be made to inform officials from Member States represented by the Subcommittee members of the importance of fusion activities and the important role played by the IAEA in these activities.

The next topic covered in the review of the Unit activities was CRPs. Three CRPs have been concluded recently. Each completed CRP resulted in a new edition of the journal series, *Atomic and Plasma-material Interaction Data for Fusion* (APID): the CRP on "Atomic and Plasma-wall Interaction Data for Fusion Reactor Divertor Modelling" contributed to Volume 9, the CRP on Charge Exchange Cross Section Data for Fusion Plasma Studies" resulted in Volume 10 (in press), and the CRP on "Plasma-interaction Data for Mixed Materials" was published in volume 12 (in preparation). Results from these CRPs are being added to the Unit electronic databases as they are collected and assessed, a process that will continue over the next reporting period. The A+M Subcommittee expressed satisfaction with the outcomes of these successful CRPs and encouraged the continuing effort at adding the new data to the electronic databases. The Subcommittee noted that this work has been somewhat delayed pending the arrival of a new professional staff member. It was then reported that two new CRPs, "Data for Molecular Processes in Edge Plasmas" and "Atomic and Molecular Data for Fusion Plasma Diagnostics" have started and each has held the first Research Coordination Meeting (RCM) in 2001. A third new CRP on "Tritium Inventory in Fusion Reactors" has been approved and is scheduled to hold its first RCM in 2002. The subcommittee noted that this fulfils the recommendation that the Unit sponsor three CRPs if at all possible and expressed satisfaction that the new Section Head supported the A+M Unit in this aim. Future CRPs were discussed in a later session.

R. Clark next reported on a proposal for an International Centre for Theoretical Physics (ICTP) workshop. A proposal has been submitted for a Workshop on "Atomic and Molecular Data for Fusion Energy Research". With strong support from the Section Head and the Division Director, the proposal was approved and scheduled for September 2003. IAEA-ICTP will provide funding for approximately fifteen students and five lecturers. The Subcommittee expressed strong support for this effort and viewed it as a very good start on what they recommend be a series of workshops. The Subcommittee recommended that the Unit follow up this workshop with a proposal for another in 2005 involving an increase in

number of students and a length of two weeks. It was also recommended that the follow up workshop focus on a specific area, such as plasma-material interactions.

The current status of the electronic databases of the Unit was then reviewed. R. Clark noted that during the past two-year interval, the databases have doubled in total number of entries and total amount of data. It was noted that K. Sheikh has reviewed all records in the database during the review period to ensure that each record gives meaningful results within the valid energy range and does not allow extrapolations outside the range of validity. Several records that did not comply were identified and rectified. The databases experience approximately 10,000 significant usages (sessions of duration of up to 30 minutes) per year. It was noted that a survey undertaken in connection with the PPAS emphasized the user appreciation for assessment of the data before entering it into the databases. It was recommended that careful assessment of data continue to be a priority of the A+M Unit. Clark summarized several new features of the Unit web page, including links to other databases, the addition of the capability to run cross-section calculations on the web server through the Internet and a new bibliographic search capability. These topics were discussed in more detail in a later session.

As had been detailed under the topic of CRPs, the Unit has completed or is in the process of completing five issues of the APID. Volumes 7B and 9 have been distributed. Volumes 10 and 11 are in press, with Volume 11 containing extensive data from calculations of ionisation balance and radiated power from fusion related materials. Volume 12 is undergoing a final editorial process. In addition the Unit has continued to publish the *International Bulletin on Atomic and Molecular Data for Fusion* (the Bulletin) every six months, the latest being Number 61, published in December, 2001. It was mentioned that due to the departure of J. Stephens and the time lag of a replacement, it is likely that Number 62 will be combined with Number 63 and will be published in December, 2002. The Subcommittee agreed that publication of the Bulletin is still valuable to fusion researchers. Although information can now be found electronically, it is still important to have the printed copy available. Over 800 copies are distributed at each printing. It was recommended that the Unit add a newsletter at the front of the Bulletin to draw attention to new activities of the Unit, such as new data additions and new features on the Unit web page.

R. Clark then summarized some other activities the Unit participated in, mainly representing the Unit at scientific conferences. These included a workshop on "Topics on atomic and molecular processes in fusion plasmas" in Madrid, Spain 13-15 September, 2000, a visit to the GAPHYOR Data Centre in October 2000, attendance of the International Conference on the Physics of Electronic and Atomic Collisions in Santa Fe in 2001, attending the ADAS workshop in 2001, attending the Symposium on Atomic and Surface Physics in Going, Austria in 2002, and attending and serving on the program committee of the International Conference on Atomic Data and Their Applications in 2002. In addition, the Unit continues to maintain the extra-budgetary project on properties of irradiated nuclear graphite and hosts the yearly meetings of the steering committee of that database.

The final topic in the Unit review was the issue of staffing. It was pointed out that J. Stephens left the Agency in December 2001 to return to his home country. As soon as the official notification of the vacancy was received, advertisement was made for the position. Even with the fastest possible action on the hiring procedure, the successful applicant, D. Humbert of the GAPHYOR database in France, will not arrive at the Unit before the middle of September 2002. Due to this time delay, it is inevitable that the Unit will not be able to

complete all tasks in the desired time scale. It was further pointed out that the Unit does have a need for more professional staff in view of the amount of work being carried out. The Subcommittee noted that although the overall fusion budget in not increasing, the larger and faster computers as well as increased network capabilities make it possible to carry out numerical simulations of increasing complexity and to carry out simulations in more detail than ever before. This gives rise for the need of much larger data sets and higher accuracy of data. This, in turn, puts increasing pressure on the Unit to add more assessed data to the electronic databases. This led to a recommendation that the Unit explore all possible avenues of increasing the professional staff support for the Unit.

B. Review of CRPs

The status of existing CRPs was reviewed during the activity report of the Unit. During the next session discussion took place on recommendations for new CRPs. Many topics were proposed. The Subcommittee recognized the limit of the number of new CRPs and recommended that some of the proposed topics be combined in existing CRPs, while noting that this also leads to a recommendation to extend those existing CRPs. Such new topics included spectroscopic characteristics of impurities for tile erosion, high frequency spectral characteristics in transient plasmas, e.g. ELMS, analysis of dust effects on fusion machines, for example size, origin, disappearance and arcing and data for X-ray spectroscopy. It was recommended that some of these topics be also considered as meriting separate specialist meetings if possible.

It was recommended that two new CRPs be initiated by the Unit, one in 2004 and one in 2005. The new CRP in 2004 should be on the topic of "Establishment of recommended A+M databases for plasma edge modelling" and should include some representatives of major modelling effort as well as data generators. A second CRP on "Data for surface composition dynamics relevant to erosion processes" should be initiated in 2005. The Subcommittee strongly recommended that these two CRPs be initiated in light of the needs of such data for next generation devices such as ITER.

C. Technical Committee Meeting in Jülich

The proposed Technical Meeting in Jülich in October 2002 was discussed. The Agency has approved this meeting and approval from the German Mission is expected shortly. Prof. Reiter from the Institut fur Plasmaphysik, which has offered facilities for this meeting, presented a review of the facilities. A preliminary agenda was discussed in detail. A number of modifications were proposed and accepted. Potential topics for all invited speakers were discussed and finalized. A list of potential participants was completed. The concept of forming three working groups was discussed and recommended. It was recommended that members of the Subcommittee be co-chairmen of those working groups. It was also recommended that the Subcommittee meet after the adjournment of the Technical Meeting to summarize the recommendations and conclusions of the Meeting.

D. Internet Related Activities

During the session on Internet related activities, L. Costello, Unit Head for Computer Operations in the Nuclear Data Section was invited to attend as an observer. Several new capabilities of the Unit electronic database server were demonstrated. First, the means of performing searches of remote databases and returning data found on remote sites was

demonstrated. It was pointed out that the databases to be searched were added to the search engine and that the search was restricted to those databases. The Subcommittee expressed strong approval for this activity and applauded the efforts of the Unit in this area. The Subcommittee strongly recommended that the Unit continue the development with the eventual goal of using this device to link all the databases in the DCN. Next, a set of atomic physics codes from J. Peek, who brought these codes to the Agency as a Consultant, was demonstrated. These codes are accessible through the web page of the Unit and allow the calculation of atomic structure and electron impact cross sections for arbitrary ion stages of elements. The Subcommittee was favourably impressed by this capability and strongly encouraged more work in this area. Some discussion took place of the possibility of forming a Computer Code Network similar in nature to the DCN. Exploration of this was encouraged with a recommendation that an experts meeting on this topic be held in 2005. A further demonstration took place to show a new method of access of bibliographic entries. The subcommittee had a strong positive reaction to this. The Subcommittee expressed the feeling that these developments are significant new capabilities and that they are very useful to the fusion community. There was a strong recommendation to publicize these capabilities. Two specific recommendations were to add a newsletter section to the Bulletin and to compose an email list method of informing potential users of these new developments. The Subcommittee also recommended that in view of the increasing and heavy use of the web page, that the Unit upgrade the hardware at the earliest possible time and attempt to undertake the hardware upgrades often.

3. RECOMMENDATIONS AND CONCLUSIONS

The final session of the meeting was devoted to formulating the list of recommendations. The areas that had been covered during the course of the meeting were reviewed and a final list of recommendations was formulated. The final list of recommendations follow:

Two specialist meetings should be held: 1. On the subject of characterization of dust and its role on retention of tritium and on edge plasma behaviour. 2. To prepare and coordinate a meeting to establish an A+M computer code network.

Extend the two existing CRPs on “Data for molecular processes in edge plasmas” and Atomic and molecular data for fusion plasma diagnostics”. There are several reasons to call for these extensions, such as the need for more information on spectroscopic characteristics of impurities for tile erosion and high frequency (about 100 kHz) spectral characteristics in transient plasmas, e.g. ELMS. These extra topics could also justify separate Technical Meetings if it is possible to hold them.

Establish a new CRP on “Establishment of recommended A+M databases for plasma edge modelling” This CRP should include the establishment of as complete as possible database to be recommended for use in computer codes modelling edge plasmas and should start in 2004.

Establish a new CRP on “Data for surface composition dynamics relevant to erosion processes”. This CRP should include data collection of solid state diffusion of components of refractory metals and metal multi-layers of elements such as Be, B, C, Cu, and W and should start in 2005

In view of the importance of CRPs to respond to the increasing data needs in new plasma scenarios and new materials issues, the simultaneous organization of 3 CRPs is endorsed and may need to be increased to 4 in the future.

Continued development of the search engine should take place with the goal being to access to all DCN member databases

Publication of the Bulletin is still valuable work in this field. It is recommended that the addition of a newsletter style section at the front of the Bulletin to publicize new features of the electronic databases be considered.

DCN should consider expansion in new geographic areas. New members should work toward having electronic databases online, using the English language and have databases relevant for fusion.

There should be more publicity for the excellent progress being made on the data network. In addition to a newsletter section in the Bulletin, the Unit should consider establishment of an email list to distribute information on new features of the databases as they become available. In view of the number of hits on the network, there should be a major upgrade of computer facilities.

In light of the importance placed on assessment of data by users of the Unit databases, it is recommended that such careful assessment continue to be the standard for additional entries to the database.

The ICAMDATA is held on alternate years from DCN. Informal meetings of DCN representatives should be encouraged at the ICAMDATA meetings.

The Unit should plan to follow up the ICTP workshop of 2003 with a further one in 2005 of two weeks on a focused topic, e.g. plasma-material interactions, and larger number of attendees, with similar format.

In general the concept of a code network was endorsed. The recommendation is that codes linked to the A+M Unit should have a level of quality consistent with that of the DCN. Increasing data needs and the increasing networking of computers has led to greatly increased needs for large amounts of high quality data, which puts increasing demands on the A+M Unit. It is strongly recommended that additional professional staff support be made available for the Unit, in particular in the area of plasma-surface interaction physics. All possibilities should be explored.

In order to make fusion more visible as an important topic for the IAEA, it is recommended that each Subcommittee member consider informing his/her Member State representative to the IAEA of the importance of this topic.

To balance expertise on the Subcommittee, there should be an additional member added in the area of plasma-surface interactions.

In view of the fact that from time to time some Subcommittee members are unable to attend due to financial constraints, it is recommended that means of offering some travel assistance be investigated.

4. EXECUTIVE SUMMARY (Prepared by N.J. Peacock)

The IFRC Subcommittee on Atomic and Molecular Data for Fusion held their biennial meeting at the IAEA Headquarters in Vienna on 24-25th June, 2002. Seven members of the Subcommittee were in attendance, including J. Roth (IPP), E. Menapace (ENEA), T. Kato (NIFS), R. Janev (Macedonian Acad. of Sciences), N. Peacock (UKAEA), M. Crisp (DoE), W. P. West (GA) and D. Reiter (KFA: in capacity of observer). Apologies for absence were received from T. Shirai (JAERI), R. Guirlet (Centre Etudes Nucleaires de Cadarache) and Yu. V. Martynenko (Kurchatov Inst.). The purpose of the Meeting was to review the activities of the A+M Data Unit of the IAEA since the last Subcommittee Meeting in May 2000 and to make recommendations to the Office of the Director General concerning the work of the Unit over the next two years budget cycle. The A+M Data Unit was represented by Dr. D.D. Sood (Director, Division of Physical & Chemical Sciences, NAPC) and Dr R. E. H. Clark (Head of the A & M data Unit). A short meeting was arranged between Drs Peacock and Clark and Dr Burkart, the Deputy Director General (Nuclear Data Section) to appraise him of the efforts of the Subcommittee.

Dr. D. Sood opened the meeting with a strong endorsement of the work of the Subcommittee and emphasised the importance of their recommendations to the agenda of the A+M data Unit and of their advisory role to the IFRC. He noted the long-term need for A+M Data with the trend to large, internationally managed, fusion devices. There is a strong possibility of a site selection for the ITER project in the next year and this will have a continuing, positive impact on fusion research.

The Subcommittee received from Dr Clark a detailed presentation of the activities of the A+M Data Unit. The Subcommittee recognizes the excellent effort of the Unit over the past two years and was gratified to learn of the favourable outcome of the Nov. 2000, Performance Assessment (PPAS) examination by an appointed international Committee. The work of Dr J. Stephens, who has now left the Unit, was acknowledged while the arrival of his replacement, Dr Denis Humbert (GAPHYOR) with his past experience in Codes, is keenly anticipated. Of particular note are the advances in the services offered through the Internet. It was noted that there is now a usable electronic link to several members of the Data Centre Network (DCN) through a search engine. In addition there are now some computational capabilities available as well as greatly improved access to bibliographic databases. The size of the database has grown by approximately a factor of two over the past two-year period and has a high level of access by users. The Unit is to be commended for these advances and it is recommended that this direction continue to be a priority for the Unit's activities.

The Subcommittee noted with satisfaction that the Unit has two current CRPs already in progress with a third to start this year, bringing the total to three, a minimum of three being a strong recommendation as the core projects of the Unit at the previous meeting of the Subcommittee.

The Subcommittee endorses the continued publication of the journal series *Atomic and Plasma-Material Interaction Data for Fusion* which has seen two new volumes (Vol.s 7b, 9) printed and three additional volumes (Vol.s 10,11,12) in press. In addition the Subcommittee strongly commends the Unit in the continued publication of the *International Bulletin on Atomic and Molecular Data for Fusion* which is widely circulated and used by many researchers in the community.

The above activities are seen to be the core priorities of the A+M Data Unit.

The continuous updating of the "International Database on Irradiated Nuclear Graphite Properties", an extra-budgetary item funded by a small consortium of nuclear power agencies, was noted with satisfaction.

Apart from the core activities (above), the Subcommittee recognises the invaluable catalytic effect on international collaboration on the A+M database for fusion. A good example is item: Meetings (iii), below.

After careful review and discussion of all aspects of the Unit activities, the Subcommittee made a number of specific recommendations to the A+M Data Unit for the 2004-2005 budget cycle. These recommendations are:

On the subject of Co-ordinated Research Projects:

(i) In view of the responsiveness of CRPs to the increasing data needs for new plasma scenarios and new materials issues, the simultaneous organisation of 3 CRPs is endorsed and this may need to be increased to 4 in the future.

(ii) Extend the two existing CRPs on "Data for Molecular Processes in Edge Plasmas" and "Atomic and Molecular Data for Fusion Plasma Diagnostics". There are several reasons to call for these extensions, such as the need for more information on spectroscopic characteristics of impurities for tile erosion and high frequency (about 100Khz) spectral characteristics in transient plasmas, e.g. ELMS. These extra topics could also justify separate Technical Meetings if it is possible to hold them.

(iii) Establish a new CRP on "Establishment of recommended A+M databases for plasma edge modelling" This CRP should include the establishment of databases which are as complete as possible and which can be recommended for use in computer codes modelling edge plasmas. This CRP should start in 2004 and could include a request for improved data on K- and M-shell dielectronic recombination rates in low Z- atoms.

(iv) Establish a new CRP on "Data for surface composition dynamics relevant to erosion processes". This CRP should include data collection of solid state diffusion of components of refractory metals and metal multi-layers of elements such as Be, B, C, Cu, and W and should start in 2005.

On the subject of Sponsored, Co-ordinated or Co-hosted Meetings:

The Subcommittee recommends that,

(i) The Subcommittee approves of the overall programme and working group topics at the upcoming IAEA Technical Meeting on Plasma – Material Interactions to be held on 28-31 Oct. 2002 at Jülich. The agenda has been discussed in detail with Drs. Roth and Reiter, members of the local organising Committee.

(ii) Two Advisory Group, Specialist meetings should be held:

1) On the subject of characterization of dust and its role on retention of tritium and on edge plasma behaviour. This topic could lead to a new CRP or may be incorporated later into an existing CRP.

2) On the preparation and co-ordination required to establish an A+M computer code network.

The Subcommittee endorses the efforts of the A+M Data Unit in co-hosting a one week Workshop/Summer School (2003 ICTP-IAEA) at Trieste on the Uses of Atomic and Molecular Data for Fusion Research, the cost to be borne largely by the IAEA. The projects, involving about 15 students and 5 lecturers, will concentrate on edge processes and use appropriate numerical codes. In anticipation of the success of this meeting, the Unit should plan to follow up the 2003 ICTP workshop with another Meeting. The duration of this 2005 workshop could be extended to two weeks on a focused topic, e.g. plasma-material interactions and could involve a larger number of attendees, but using a similar format.

The ICAMDATA Meetings are wide ranging and of interest to astrophysicists and fusion scientists alike. They are held on alternate years to the Data Center Network (DCN) meetings, see below. The Subcommittee recommends that informal meetings of DCN representatives should be encouraged at the ICAMDATA meetings.

On the subject of Data Center Network (DCN),

The Subcommittee recommends that,

(i) Continued development of the search engine should take place with the goal being to access eventually all DCN member databases. A good start has been made with links to several of the Data Centres.

(ii) In light of the importance placed on assessment of data by users of the Unit databases, it is recommended that such careful assessment continue to be the standard for additional entries to the database.

(iii) DCN should consider expansion into new geographic areas. Any new members should work toward having electronic databases online, using the English language and have databases relevant for fusion.

(iv) In general the concept of a code network is endorsed. The recommendation is that codes linked to the A+M Unit should have a level of quality consistent with that of the DCN.

(v) There should be more publicity for the excellent progress being made on the data network. In addition to a newsletter section in the Bulletin, the Unit should consider establishment of an email list to distribute information on new features of the databases as they become available. In view of the number of hits on the network, there should be a major upgrade of computer facilities.

On the subject of publications and publicity:

The Subcommittee acknowledges that,

(i) Publication of the Bulletin is still valuable work in this field. It is recommended that the addition of a newsletter style section be considered at the front of the Bulletin to publicize new features of the electronic databases.
(ii) In order to make fusion more visible as an important topic for the IAEA, it is recommended that each Subcommittee member consider informing his/her Member State representative to the IAEA of the importance of this topic.

On the subject of Staff:

The Subcommittee recommends that,

(i) Increasing data needs and the increasing networking of computers has led to greatly increased needs for large amounts of high quality data, which puts increasing demands on the A+M Unit. It is strongly recommended that additional professional staff support be made available for the Unit, in particular in the area of plasma-surface interaction physics. All possibilities should be explored.

On the subject of Subcommittee business:

The Subcommittee recommends that,

(i) In order to balance existing expertise on the Subcommittee, there should be an additional member added in the area of plasma-surface interactions.

(ii) In view of the fact that from time to time some Subcommittee members are unable to attend due to financial constraints, it is recommended that means of offering some travel assistance be investigated

(iii) Prof. N. Peacock was present as chairman of the Subcommittee, the second meeting in which he has held this role. In that event, in accordance with the Terms of Reference for the Subcommittee (see Appendix 3), Prof. Peacock indicated his intention to step down as the chairman when his term comes to an end. Therefore, it will be necessary for a new chairman to be selected at the next meeting of the Subcommittee in 2004.

Respectfully submitted on behalf of the Subcommittee,

Nicol J. Peacock
Chairman

Appendix 1

IAEA Technical Committee Meeting: 13th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

24-25 June 2002, IAEA Headquarters, Vienna

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Appendix 2

IAEA Technical Committee Meeting: 13th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

24-25 June 2002, IAEA Headquarters, Vienna

MEETING AGENDA

Monday, June 24 **Meeting Room: F 01-25**

09:30 - 10:00	Opening. Welcome to Subcommittee members. Adoption of Agenda
Session 1:	*General Report on Activities since May 2000*
10:00 - 10:40	Report on the activities of A+M Data Unit 2000-2001
10:40 - 11:00	Discussion of aspects of the report.
11:00 - 11:30	*Coffee break*
Session 2:	*Data Centre Network and Workshop activities*
11:30 - 12:30	Review of DCN status. Review of outcomes from ICAMDATA 2002. Proposed ICTP Workshop.
12:30 - 14:00	*Lunch*
Session 3:	*Review of Current and planned CRPs*
14:00 - 15:30	Currently running CRPs. New CRPs to start in 2002-2005 period
15:30 - 16:00	*Coffee break*
Session 4:	*2002-IAEA Technical Meeting on Atomic and Molecular Interaction Data for Fusion Reactor Technology*
16:00 - 17:30	Discussion of the Meeting - Objectives, programme, participants. Report from the TM hosting organization (FZ-Jülich; Prof. Reiter)

Tuesday, June 25 **Meeting Room: F 01-25**

Session 5: *Internet related activities*

09:00 - 10:30 Status of database.. Search engines. Codes on the Internet. Possibility of Code Network.

10:30 - 11:00 C*offee break*

Session 6: *Business Matters*

11:00 - 12:30 Outcome of Programme Performance Assessment System (PPAS). Staffing matters. Budgets.

12:30 - 14:00 *Lunch*

Session 7: *Meeting Conclusions and Recommendations for Activities during the next budget cycle*

14:00 - 13:30 Formulation of meeting conclusions, recommendations, and Executive Summary of the Meeting

15:30-16:00 *Coffee Break*

16:00 – 17:30 Meeting summary continued, meeting adjournment.

Appendix 3

TERMS OF REFERENCE

IFRC Subcommittee on Atomic and Plasma-Material Interaction Data for Fusion

The International Fusion Research Council (IFRC) Subcommittee on Atomic and Plasma Material Interaction Data for Fusion will serve as a continuing Subcommittee within the framework of the International Atomic Energy Agency. Its function will be to review periodically the planning and execution of the Agency's Atomic and Plasma-Material Interaction Data Programme for Fusion and to advise the Director General on its direction in accordance with the needs of fusion research and reactor design.

Composition: the Subcommittee shall be composed of fusion and atomic scientists nominated by IFRC.

Methods of Work: the Subcommittee shall determine its own methods of work. The IAEA Nuclear Data Section shall provide the secretariat services to the Subcommittee.

Meetings: the Subcommittee shall be convened at a frequency not exceeding two years, and shall normally meet at the IAEA Headquarters. The cost of participation of Subcommittee Members will be born by the Government or sponsoring institute of the member. No interpretation will be required.

METHODS OF WORK

IFRC Subcommittee on Atomic and Plasma-Material Interaction Data for Fusion

Under the Terms of Reference of the IFRC Subcommittee on Atomic and Plasma-Material Interaction Data for Fusion (hereinafter referred to as the Subcommittee), as approved by the IAEA Administration on ……1993, the Subcommittee is authorized to determine its own Methods of Work.

I. Scope and Responsibilities

In addition to the general functions of the Subcommittee, stated in the Terms of Reference, the Subcommittee shall

- periodically review the IAEA programme on A + PMI for Fusion,
- review A + PMI data needs and recommend their priorities,
- assist in specifying and planning topical data meetings and coordinated research programmes,
- assist in maintaining contacts between the IAEA A + PMI Data Unit and the fusion community,
- assist in the coordination of data centres.

II. Organization

1. Chairman: the Chairman shall be a member of the Subcommittee and shall serve for 2 meetings. The Chairman may be renominated by the Subcommittee. The responsibility of the Chairman shall remain in effect between meetings, until the following meeting, and he shall be kept informed by the Subcommittee members and the Scientific Secretary of relevant activities and developments.

2. Scientific Secretary: the Scientific Secretary shall be the Head of the A + PMI Data Unit of the IAEA Nuclear Data Section, and shall serve as a member of the Subcommittee.

3. Membership: should it become necessary for a Subcommittee member to be relieved of his membership, it shall be his responsibility to arrange for his replacement in collaboration with the pertinent IFRC member, and to inform the Chairman and the Scientific Secretary of the Subcommittee of the membership change in writing.

III. Meetings

1. Preparation: the preparation of the meetings shall be done timely by the Scientific Secretary of the Subcommittee in collaboration with the incoming and outgoing Chairman.

2. Frequency: the time between meetings of the Subcommittee shall be determined by progress in the field of fusion research and technology pertinent to A + PMI data and development within the IAEA, but shall not exceed two years.

3. Proceedings: the proceedings of the meetings shall be written by the Scientific Secretary, and shall be issued as an IAEA report after having been approved by all Subcommittee members. The proceedings of every meeting shall be distributed to the IFRC and INDC committees, the A + PMI data centres and to the directors of all major fusion laboratories in member states.

4. Observers: all meetings of the Subcommittee shall be open to observers.

Appendix 4

Atomic and Molecular Data Unit Activities
(Period: May 2000 - May 2002)

1. Introduction

The mission of the Atomic and Molecular (A+M) Data Unit is to establish and maintain databases in support of magnetic fusion energy (MFE) and other nuclear energy applications. This encompasses a very large number of processes in atomic, molecular, and plasma-material interaction physics. Data for these processes are supplied by research centers around the world participating in activities such as the Data Centre Network, CRPs, and various other technical meetings. The resulting data are incorporated into the databases maintained at the A+M Data Unit. The Unit develops and maintains interfaces to these databases, which are accessible to all Member States through the Internet.

2. Data Center Network

The Data Centre Network (DCN) reviews progress in A+M data related activities in the twelve established Data Centres. It sets priorities among the data activities perceived by its different members, reviews the methods and procedures applied in the data processing and exchange, and co-ordinates work plans among the Data Centres. The DCN meets biennially with the last meeting held on September 10-11, 2001.

At the latest meeting progress reports were presented by each of the Data Centres. Included were specific reports on generation, compilation, and dissemination of data in printed and electronic form, as well as status of the Data Centre programmes and plans for future work. The conclusion was that the Data Centres are effectively following the recommendations from the previous meeting and from the IFRC A+M Subcommittee, and that there is good co-operation among the Data Centres.

A lengthy review of the priorities in data generation and compilation took place during the last meeting. Each item on the previous list was discussed and evaluated in terms of how well the needs have been filled and the urgency of each need on the list. The result was a revised and very comprehensive list of priorities for generation, evaluation and compilation of data in support of fusion energy research. The complete list of the priorities formulated in the meeting is available in the summary report (INDC(NDS)-430).

An additional and extremely valuable activity of the DCN is the provision of bibliographic data for the A+M Unit publication, the *International Bulletin on Atomic and Molecular Data for Fusion*, published biannually. Several Data Centres supply the bibliographic data to the A+M Data Unit, which then combines the data into the finished publication, which is distributed to Member States.

3. Atomic and Molecular Data Subcommittee of the International Fusion Research Council

The A+M Subcommittee of the International Fusion Research Council (IFRC) gives advice and recommendations to the A+M Data Unit. The IFRC Subcommittee is made up of eleven members, and it meets biennially, with the last meeting in May 2000. The Subcommittee reviews the past activities of the Unit and recommends future directions. In the May 2000 meeting the Subcommittee strongly recommended the initiation of three new CRPs. The Subcommittee also recommended holding several other meetings to assess the current status of several types of data relevant to fusion reactors. The review of the activities of the A+M Data Unit indicated that the Unit is doing an excellent job in meeting data needs.

4. Programme Performance Assessment System

A formal review of fusion activities was undertaken in a Programme Performance Assessment System (PPAS) during 2000. This review processes made a detailed assessment of aspects of fusion related activities of the IAEA. The A+M Data Unit was included in this assessment due to the focus of the Unit on data needs for fusion energy research. An independent outside panel was convened during the period 13-17 November, 2000. A large amount of background material was provided to the panel and oral presentations were made. The panel asked for clarification of a number of issues from IAEA management and asked for additional presentations from several support organizations to outline the background of the current status of fusion research activities. The panel concluded that the main improvement in fusion activities at the IAEA would be for more resources to be devoted to it. The panel emphasized that fusion is close to becoming a realistic alternative to other methods of power generation and should have broader support. The panel concluded that the staff working on fusion topics was doing an excellent job with the available resources.

5. Co-ordinated Research Projects

The CRPs represent the main method of generating new data needed by the fusion energy research community. Data from these projects are reviewed and published in the journal *Atomic and Plasma-Material Interaction Data for Fusion* (the APID series). During the period 2000-2001, three CRPs completed their formal activities while two new ones were initiated.

The CRP on the topic “Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling” gave rise to a wealth of data on interactions relevant to the divertor region of fusion machines. A very comprehensive compilation of critically assessed data is now available as volume 9 of the APID series. Much of the new data has been carefully evaluated and where found to be of high quality, entered into the A+M online databases.

The CRP on “Plasma-interaction Data for Mixed Materials” resulted in a large amount of information on the effect that mixing of materials has on interactions of those materials with components of the plasma. Mixing of materials is being considered for use in different parts of the fusion reactor, and can form *in situ* during reactor operation as well. As an example, carbon used in tiles will be eroded by the plasma and later deposited on metals used in other parts of the machine. The resulting mixed material interacts with the plasma in a much different manner that either pure material. This CRP held its final RCM in October 2000. The participants have been finalizing their results that have now been gathered. These

manuscripts will be published as a new volume of the APID series. Plans are also being made to review the data produced and add it the online databases.

The CRP on "Charge Exchange Cross Section Data for Fusion Plasma Studies" held its final RCM in September 2000. The participants produced a large amount of experimental and theoretical results for cross sections for charge exchange processes for atomic and molecular targets, including state-to-state processes. This is extremely useful in analyzing spectra obtained from neutral beam injection in these plasmas where electrons from the neutral species are captured by the ions in the plasma. Good data on the cross sections allows an analysis of the resulting emitted radiation as the transferred electron cascades down in the ion. Manuscripts from the participants are in the final editorial phase for publication in the APID series.

In 2001 a new CRP was initiated on the topic of "Data for Molecular Processes in Edge Plasmas" with its first RCM held on 18-19 October 2001. The IFRC Subcommittee recommended this CRP at its meeting in May, 2000. It is known that in the edge regions of fusion plasmas the temperature is low enough to support the existence of molecules in the plasma. This has a number of effects on the plasma and can have a significant impact on modeling the plasma behavior in the edge region. Of special concern is the formation of molecules containing tritium, especially hydrocarbons. Formation of tritium containing molecules depletes fuel from the fusion reaction and also increases the total inventory of tritium in the machine, which is a safety concern. This CRP brings together a large number of experts in molecular physics with the purpose of increasing the amount of data available for processes related to the formation and destruction of such molecules in conditions relevant to fusion reactors. At the first RCM a very effective work plan was developed and adopted.

A second new CRP, also recommended by the IFRC Subcommittee, on the topic of "Atomic and Molecular Data for Fusion Plasma Diagnostics" was initiated with an RCM held on 12-13 November, 2001. The focus of this CRP is to gather and generate more data relevant to the diagnostics of fusion plasmas. There are a number of areas in diagnostics work that need more data, mainly cross sections for excitation, charge exchange, and other processes which can be used to analyze spectra produced in a plasma. At the RCM there was much discussion of the types of data that are most urgently needed and which members of the group would be able to work on the most urgent needs. A comprehensive list of needs was drawn up. Each participant indicated an area where significant work could be accomplished.

6. Database Management

During the period 2000-2001 the size of the electronic databases has grown by over a factor of two. Large amounts of new data have been assessed and added to the databases. In a user survey taken in connection with the PPAS process, it was noted that the assessment of the data is a very high priority with the users. Much of the assessment work is carried out in the course of the CRPs and also through the use of consultants.

During recent years a number of other databases have become available through Internet interfaces. At several conferences the possibility of linking databases has been discussed. As a result of such discussions, the A+M Unit has facilitated collaborative work on an interface that allows a user to pass one request to a number of completely independent databases and to gather the results of those requests. This interface was installed on the web server of the

A+M Unit in December 2001 after having been developed over the year by Y. Ralchenko of the Weizmann Institute, Israel and D. Humbert of GAPHYOR, France.

The bibliographic database maintained by the A+M Unit has been accessible only through a Telnet interface. This is no longer a viable method to access a public database. During the past year preliminary work has been undertaken to prepare the database for use with a more modern interface, similar to the database management system used for the numerical data. These efforts have prepared the way for a new web based interface to be developed in the near future.

The extra-budgetary project on "International Database on Irradiated Nuclear Graphite Properties" has continued. The Steering Committee met in September 2000 at Oak Ridge National Laboratory (USA), and in September 2001 at IAEA Headquarters in Vienna. Each year an updated version of the complete database was compiled and distributed to all members. At each Steering Committee meeting, priorities have been set and the previous year activities reviewed. The Unit has carried out several consulting agreements to fulfill the needs in developing the database.

Atomic and Molecular Data Unit
Meetings, Consultancies, Publications
(2000 – 2001)

Meetings:
2000

1) *Technical Committee Meeting:* 12th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion
8-9 May 2000, IAEA Headquarters, Vienna, Austria

2) *Consultants' Meeting:* CRPs on Plasma Diagnostics and Molecular Processes
19-20 June 2000, IAEA Headquarters, Vienna, Austria

3) *Consultants' Meeting:* 2nd Meeting of the Technical Steering Committee for the International Database on Irradiated Nuclear Graphite Properties
7-8 September 2000, Oak Ridge National Laboratory, Oak Ridge, U.S.A.

4) *Consultants' Meeting:* Programme Performance Assessment System (PPAS) Evaluation of Fusion Research Activities
14-18 November 2000, IAEA Headquarters, Vienna, Austria

5) *Research Coordination Meeting:* Charge Exchange Cross Section Data for Plasma Studies
25-26 September 2000, IAEA Headquarters, Vienna, Austria

6) *Research Coordination Meeting:* Plasma Material Interaction Data for Mixed Plasma Facing Materials in Fusion Reactors
16-17 October 2000, IAEA Headquarters, Vienna, Austria

2001

1) *Advisory Group Meeting:* Assessment of New Data for tritium Retention in Fusion Reactor Materials
2-3 July 2001, IAEA Headquarters, Vienna, Austria

2) *Advisory Group Meeting:* Technical Aspects of Atomic and Molecular Data Processing and Exchange (16th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)
10-11 September 2001, IAEA Headquarters, Vienna, Austria

3) *Consultants' Meeting:* 3rd Meeting of the Technical Steering Committee for the International Database on Irradiated Nuclear Graphite Properties
27-28 September 2001, IAEA Headquarters, Vienna, Austria

4) *Research Coordination Meeting:* Data for Molecular Processes in Edge Plasmas
18-19 October 2001, IAEA Headquarters, Vienna, Austria

5) *Research Coordination Meeting:* Atomic and Molecular Data for Fusion Plasma Diagnostics
12-13 November 2001, IAEA Headquarters, Vienna, Austria

Consultancies:
2000

1) Advise the IAEA on "Several Topics Related to A+M Data Unit Activities"
8-12 May 2000, IAEA Headquarters, Vienna, Austria
Consultant: Dr. Ratko K. Janev (Skopje, Macedonia)

2) Advise the IAEA on "Physical Sputtering Database"
14-25 August 2000, IAEA Headquarters, Vienna, Austria
Consultant: Dr. Wolfgang Eckstein (Garching, Germany)

3) Advise the IAEA on "Planning of Centralized Database Search Capabilities within the A+M Data Centre Network.
4-8 December 2000, IAEA Headquarters, Vienna, Austria
Consultant: Dr. Yuri Ralchenko (Rehovot, Israel)

2001

1) Advise the IAEA on "A+M on-line System Development and Enhancement of Technical Base of AMDIS and ALADDIN"
12-14 September 2001, IAEA Headquarters, Vienna, Austria
Consultants: Drs. Denis Humbert (Orsay Cedex, France) and Yuri Ralchenko (Rehovot, Israel)

2) Advise the IAEA on "Matters Arising from the Issue of the APID Series on the Topic of Charge Exchange"
14-16 November 2001, IAEA Headquarters, Vienna, Austria
Consultant: Dr. Ratko K. Janev (Skopje, Macedonia)

Publications:
2000

1) International Bulletin on Atomic and Molecular Data for Fusion
Issue # 58 (June 2000)

2) International Bulletin on Atomic and Molecular Data for Fusion
Issue # 59 (December 2000)

3) IAEA International Database on Irradiated Nuclear Graphite Properties
Report: INDC(NDS)-413 (February 2000)

4) IAEA Technical Committee Meeting: 12th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion
8-9 May 2000, IAEA Headquarters, Vienna, Austria
Summary Report: INDC(NDS)-420 (December 2000)

2001

1) International Bulletin on Atomic and Molecular Data for Fusion
Issue # 60 (June 2001)

2) International Bulletin on Atomic and Molecular Data for Fusion
Issue # 61 (December 2001)

3) Atomic and Plasma-Material Interaction Data for Fusion
(Volume 7 Part B), 2001

4) Atomic and Plasma-Material Interaction Data for Fusion
(Volume 9), 2001

5) 2nd (Final) IAEA Research Co-ordination Meeting on "Charge Exchange Cross Section Data for Fusion Plasma Studies"
25-26 September 2000, IAEA Headquarters, Vienna
Summary Report: INDC(NDS)-426 (November 2001)

6) 2nd (Final) IAEA Research Co-ordination Meeting on "Plasma-material Interaction Data for Mixed Plasma Facing Materials in Fusion Reactors"
16-17 October 2000, IAEA Headquarters, Vienna
Summary Report: INDC(NDS)-429 (November 2001)

7) IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (16th Meeting of the A+M Data Centres and ALADDIN Network)
10-11 September 2001, IAEA Headquarters, Vienna
Summary Report: INDC(NDS)-430 (December 2001)

Appendix 5

CRP on "Data for Molecular Processes in Edge Plasmas"

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