

INDC International Nuclear Data Committee

17th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

27-28 April 2010

Prepared by

B. J. Braams

June 2012

IAEA Nuclear Data Section, Vienna International Centre, A-1400 Vienna, Austria

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Printed by the IAEA in Austria

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Abstract

The 17th meeting of the Subcommittee on Atomic and Molecular Data of the International Fusion Research Council (IFRC) was held on 27-28 April 2010 at IAEA Headquarters in Vienna, Austria. Activities of the Atomic and Molecular Data Unit for the period 2006-2008 were reviewed, and recommendations were made for the 2010-2011 budget cycle. The proceedings, conclusions and recommendations of the Subcommittee meeting are briefly described in this report. Specific recommendations of the Subcommittee from this meeting, as well as the report on the activities of the IAEA Atomic and Molecular Data Unit for the period May 2006 – March 2008, are also included.

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Executive Summary and Recommendations

Prepared by M. Crisp with B. J. Braams

1 Introduction

The IFRC subcommittee on atomic and molecular data is very pleased with the work that has been carried out by the Atomic and Molecular Data Unit during the past two years, May 2008 – April 2010. The professional staff of the unit turned over near the end of 2009 with the replacement of Dr Bob Clark by Dr Bas Braams and of Mr Denis Humbert by Dr Hyun-Kyung Chung. The subcommittee thanks the previous professional staff of the Unit for their service to the development and dissemination of atomic, molecular and plasma-material interaction data and welcomes the new staff. The subcommittee appreciated the presentations by the new staff at the meeting in April 2010 and is confident of a successful continuation of the work of the Unit. The valuable continued support by Mr Khalid Sheikh is noted.

Specific recommendations by the subcommittee for the work of the Unit in the years 2010-2012 follow.

2 Databases

With respect to ALADDIN and other numerical datasets the subcommittee considers that quality control and the provision of unique recommended data are issues of ongoing concern. Possible actions:

- Have CM/TM or consultant visits to evaluate data, or at least to identify datasets that are ripe for evaluation (different from assembling a CRP for new data).
- Focussed question for CM or individual consultant: What should be done to upgrade APID 7A/7B on erosion? For one thing, it needs physics-based fits rather than splines.

Concerning development of the bibliographical database AMBDAS the subcommittee appreciates the addition of the DOI-based hyperlinks.

The subcommittee notes that AMBDAS is in recent years based exclusively on compilations done at NIST for spectroscopic data and at CFADC (Oak Ridge) for collisional data. Apparently this data compilation work at CFADC is under review. The subcommittee wishes to stress the unique and very valuable role of the CFADC in maintaining and updating these bibliographical data.

The subcommittee notes that the Bulletin appears most useful in electronic form, searchable through AMBDAS with full-text links through the DOI. Still, the subcommittee endorses continued publication of the paper bulletin for the next few years. It is noted that the printed distribution was much reduced recently, from about 800 to about 200.

GENIE provides a valuable interface to multiple datasets. It should be maintained and possibly expanded to access additional databases.

The subcommittee recognizes the recent initiative to develop a wiki-style Knowledge Base as interesting and potentially very valuable. The Knowledge Base can serve for dialog about data, data needs and data quality. It may serve also for background scientific information on methods and context of data. It will be necessary to find people to contribute to the Knowledge Base.

3 Data and Code Centre Networks

The Unit should continue its role of coordinating the data centre network activities through the biennial DCN meetings. Quality control of data and the provision of recommended data remain most important issues.

With regard to Code Centre Network the subcommittee recognizes the value of making codes for the production of A+M and PMI data available through a convenient on-line interface. Several suggestions:

- Documentation of the codes should clarify weaknesses, appropriate use, etc.
- Plasma-material interaction codes are also appropriate for CCN, e.g., TRIM-SP.
- The interface at the Agency should allow to execute a code or it should point to an official code home; it should not be a repository for downloading a code.
- The Code Center Network should encourage code comparison efforts.
- The access to the codes through our web pages also serves to demonstrate code capabilities.

4 Coordinated Research Projects

For the recently concluded CRPs the final APID reports need to be published without undue delay. (For more on APID see below.)

The subcommittee recommends that the ongoing CRPs on surface composition dynamics and on characterization of dust both be continued to a 3rd RCM.

The subcommittee is pleased with the start of the CRP on light elements and with the approval of the CRP on tungsten in plasma.

Concerning future CRPs the subcommittee recommends the following working titles:

- 2011-2015: Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma. There should be a CM/TM later in 2010 to identify the most pressing gaps in the data and potential participants in the CRP.
- 2012-2016: Erosion and tritium retention for beryllium plasma-facing materials. There should be a CM/TM in 2011 to define this CRP further.
- 2013-2017: Plasma-wall interaction of irradiated tungsten and tungsten alloys in fusion devices. (Details to be reviewed at the next IFRC subcommittee meeting.)

If there is a possibility to start a further CRP then the subcommittee endorses:

• (2013-2017): Data for processes of hydrocarbon ions in fusion plasma.

It is understood that it is not so likely that there will be funds to start a third CRP in the 2012-2013 biennium. Priority for that biennium goes to CRPs on beryllium and tungsten surfaces.

5 Publications

The review and publications procedures of APID need to be streamlined.

It is very desirable that APID be published electronically in addition to paper; and past issues should be electronically accessible if IAEA publications policy allows it.

If APID were again a Supplement to Nuclear Fusion then that would much increase its stature, but this will be difficult to achieve. Consider the possibility for summaries in Nuclear Fusion.

Alternative publication routes should be pursued, as exemplified by the joint focussed review article following the Tritium Inventory CRP.

AMDU Newsletter would be valuable (at conclusion of a CRP, or other occasions)

6 Workshops and Other Meetings

The subcommittee finds the ICTP workshops (2003, 2006 and 2009) to be valuable and supports the effort to hold another such workshop in 2012, or earlier if the budget allows it. It is suggested to track the participants to estimate better the impact.

The subcommittee is very interested in the NLTE code comparison workshops and strongly supports the proposal for the Unit to be the local host for NLTE-7 in 2011.

The subcommittee notes with pleasure the Unit's involvement in the organization of a Technical Meeting on ITER materials in connection with the Monaco Fusion Energy Days.

7 Unit Participation in Other Meetings

With regard to participation of the Unit in international meetings the subcommittee assigns highest priority to ICAMDATA, ICPEAC and PSI. However, there are many other valuable meetings including EGAS/ECAMP, the ADAS meetings, European Fusion Task Force meetings, EFDA events, Atomic Processes in Plasmas and others. The IAEA Fusion Energy Conference should also be considered. Geography and schedule must be taken into account.

The subcommittee notes that there does not exist a true Fusion Atomic Data meeting on par with PSI as the Fusion PMI meeting. This is a role for the infrequent large A+M data meeting last organized in Juelich in 2002.

8 Development of XSAMS

The subcommittee is pleased with the release of v.0.1 and with the pilot implementations of XSAMS. The use of XSAMS within the Virtual Atomic and Molecular Data Centre looks very promising.

The subcommittee echoes its earlier recommendation for the Unit to maintain a strong role in coordination of development of XSAMS and in encouraging its implementation, but not to take a leading role due to limited Unit resources.

The subcommittee recommends to look at possible coordination of XSAMS development and implementation with work by the Integrated Tokamak Modelling task-force.

Other Activities

The subcommittee took note of the move of the graphite properties database project to NE. It was worthwhile for the Unit to host the graphite properties database and the Unit can be open to a future extra budgetary project if the occasion arises.

1. Introduction

The 17th Technical Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion was held on 27-28 April 2010 at the IAEA headquarters in Vienna, Austria. Eleven members of the Subcommittee attended: J.W. Davis (University of Toronto), R. Guirlet (CEA, Cadarache), J. Roth (Max Planck IPP, Garching), G. Mazzitelli (ENEA, Frascati), D. Kato (NIFS), R.K. Janev (Macedonian Academy of Sciences), I. Mazul (Efremov Institute), M. Crisp (Department of Energy, USA), N. Hawkes (representing K.-D. Zastrow, CCFE, UK) and B.J. Braams (IAEA), as well as H.-K. Chung (IAEA A+M Data Unit) (see Appendix 1). T. Nakano (JAEA), Yu. Martynenko (Kurchatov Institute) and newest member D.R. Schultz (ORNL) were not able to attend.

The purpose of the Subcommittee meetings is to review the activities of the A&M Data Unit over the two years prior to each meeting, and to make recommendations to the IFRC committee and the Agency on the direction that the atomic and molecular data programme should take over the next two-year budget cycle to meet the needs of the international fusion community. The agenda of the meeting is provided in Appendix 2.

The meeting was opened by Dr G. Mank, head of the Physics Section within the Division of Physical and Chemical Sciences. On behalf also of Division Director Dr N. Ramamoorthy and Nuclear Data Section Head Dr R. A. Forrest Dr Mank welcomed the participants to Vienna. He described the interest of the Physics Section in nuclear fusion. The International Fusion Research Council (IFRC), currently chaired by Dr T. S. Lee of Korea, advises the Agency in this regard. Dr Mank noted the IAEA-ITER agreement under which ITER is represented at the IFRC meetings and IAEA is represented at ITER Council meetings. Dr Mank also noted the biennial Fusion Energy Conference for which the Physics Section is responsible and recommended to the IFRC subcommittee to seek to be represented at a future instance of that conference. The Physics Section is also responsible for the Nuclear Fusion journal. Dr Mank noted two current activities: the production of a book "50 years of fusion" edited in the Physics Section and an upcoming Technical Meeting on Analysis of ITER Materials and Technologies in Monaco in November 2010; the A+M Data Unit is also involved in the organization of this meeting.

In discussion following the Welcome it was remarked that the activities in the Nuclear Energy (NE) department on fusion materials have been reduced. On the other hand, the Physics section is expanding its work on irradiated materials.

The election of a Chair was deferred to after lunch at which time Dr M. Crisp was nominated and elected by acclamation.

The agenda included the following presentations by unit staff:

- 1. General Report on Unit activities since April 2008 by B.J. Braams.
- 2. Review of the Data Centre Network (DCN) activities and computer issues by H.-K. Chung.
- 3. Review of coordinated research projects by B.J. Braams.
- 4. Review of other unit activities by B.J. Braams
- 5. Presentation of web interfaces and publications by H.-K. Chung.

Each presentation had a generous allotment of time so that the discussions were interspersed with the presentations.

The full report of the A+M Data Unit activities is included as Appendix 3. A summary of the presentations and discussions is provided in Section 2. The recommendations from the subcommittee are assembled together in Section 3. Concluding remarks are in Section 4.

2. Meeting Proceedings

2.1. General Report on Unit Activities since April 2008

B. J. Braams presented an overview of activities of the Unit with reference to recommendations from the previous IFRC subcommittee meeting in April 2008.

Staff Changes

There has been a change of personnel. Dr Robin Forrest became the new Section Head of the Nuclear Data Section in July 2009 replacing Dr Alan Nichols (retired). Dr Forrest is a nuclear data physicist and nuclear data evaluator with a PhD in experimental atomic physics. He came to the Agency from Culham Laboratory (CCFE) where he worked on nuclear data and development of activation codes of special relevance to fusion. Dr Bastiaan (Bas) Braams came to the Agency at the end of August 2009 as the new Unit Head, replacing Dr Bob Clark (retired). Bas Braams did his PhD in plasma physics and has worked in computational plasma physics and molecular modelling. Dr Hyun-Kyung Chung came to the Agency at the end of September 2009 as physicist in the Unit replacing Denis Humbert (rotation policy). Her PhD is in nuclear engineering and engineering physics and her primary recent work is in numerical modelling of atomic processes in dense matter related to nuclear fusion. The Unit's database clerk, Mr Khalid Sheikh, provides a stable connection almost to the start of the Unit in 1977-1978. Mr Sheikh came to the Agency and to this Unit in 1982.

Recommendations and Actions from the 2008 Subcommittee Meeting

The CRP "Tritium inventory in Fusion reactors" should be brought to a close in 2008 with the preparation and issue of APID Volume 15.

ACTION: A major report based on this CRP was published [Skinner et al., Fusion Science and Technology, 2008]. Contributions for APID Vol 15 were collected, refereed and revised; the volume is in copy-editing.

The CRP on "Atomic and molecular data for plasma modelling" should hold the final RCM in 2008, and be brought to a close in 2009. A new volume of the APID series should be produced from the work of this CRP.

ACTION: The CRP held its 3rd and final RCM 17-19 November 2009. Summary report was published. Articles for APID were produced and refereed. The volume (APID Vol. 16) is in copyediting.

The CRP on "Atomic data for high Z element impurities in fusion reactors" should hold its final RCM in 2009. A new volume of the APID series should result from this work in 2010.

ACTION: The CRP held its 3rd and final RCM 4-6 March 2009. Summary report was published. Articles for APID have been produced and refereed. The Volume (APID Vol. 17) is to be published in 2010.

The CRP on "Data for surface composition dynamics relevant to erosion processes" should continue through 2010. Progress of this CRP will be reviewed at the next meeting of the Subcommittee.

ACTION: The 2nd RCM was held 11-13 March 2009 and the final RCM is scheduled for 13-15 Sep 2010. Articles for APID Vol. 18 then for publication in 2011.

The initiation of a CRP on dust was previously proposed for 2007 and the Subcommittee reinforced the recommendation to pursue a new CRP on "Data requirements for the characterization of size, composition and origins of dust in Tokamaks."

ACTION: This CRP was approved and held its 1st RCM 10-12 December 2008; 2nd RCM due 21-23 June 2010. Participants from Garching, Bochum, Frascati, NIFS, Kurchatov, Culham, INEL and PPPL.

A new CRP on data for light ions in cold, recombining divertor plasmas should be initiated in 2009. New data on two- and three-body recombination and multi-step recombination processes involving H2+, H3+, He+ and Be ions are needed for a full definition of the ITER divertor.

ACTION: The CRP was initiated, focus broadened to H, He, Li, Be, B, C, N and O and their hydrides. First RCM was held 18-20 November 2009; 11 participating institutes. Summary report is available. The second meeting is expected in Q2 2011.

A new CRP on tungsten should be initiated in 2010 as a follow-on to the existing CRP on high Z elements, but with focus strictly on tungsten data for plasma modelling and diagnostic interpretation.

ACTION: The detailed proposal for CRP "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" was approved in Feb 2010. CRP is now being assembled (due by June 2010); first meeting in Q4 2010.

Should budgetary constraints allow, another CRP should be initiated during the 2010-2011 timeframe to focus on data requirements for the diagnosis of the isotopes of hydrogen and light fusion products such as 4He and 3He in the core of a burning plasma. A Technical Meeting may be useful to recommend specific well-focused goals for this CRP.

ACTION: CRP with tentative title "Isotopic Ratio Diagnostics and Control in Burning Plasmas" is in the Programme and Budget to start in 2011. Plans to be reviewed and perhaps revised at this subcommittee meeting and at a TM in Fall 2010.

The Unit should continue close collaborations with other A+M data centres of the Data Centre Network. Development of unified web access, greatly strengthened by the new XML schema, will benefit all plasma modelling and spectroscopic interpretation efforts.

ACTION: DCN Meeting was held 7-9 Sep 2009; summary report and new Data Needs document are published. Unit has organized 4 XSAMS meetings since last IFRC, most recently 24-26 March 2010 at NIFS. Version 0.1 of XSAMS was released in Sep 2009.

Inclusion of the ADAS database through the development of "OPEN-ADAS" should also be encouraged.

ACTION: A contract with H. Summers resulted in the release of OPEN-ADAS. This includes ADAS data for charge exchange, electron impact ionization, radiative and dielectronic recombination, photon emissivity, and other.

The Unit should continue active participation in the ICAMDATA and ICPEAC meetings.

ACTION: Bob Clark and Denis Humbert attended ICAMDATA 2008 in Beijing; Bob for the Program Committee and an invited talk; Denis for posters on XSAMS and on our databases, plus XSAMS working meeting. Bas is invited speaker at ICAMDATA 2010; possibly Hyun will also travel there. ICPEAC was July 2009, not attended due to transition. Next ICPEAC is July 2011. Other important meetings: EGAS/ECAMP, ADAS, PSI.

Through the ICAMDATA meetings and the DCN, the Unit should continue to encourage the development and application of evaluation criteria to define the accuracy of data contained in each database.

ACTION: This is a difficult issue, raised again at Sep 2009 DCN meeting. NIST successfully addressed it for spectroscopy. In general, it is open for further action.

Further Activities and Summary

Subsequent presentations at this meeting expand upon the work of the Data Centres Network, our database and computing activities, coordinated research projects and other activities.

A detailed report on activities of the Unit in the period April 2008 - March 2010 is provided in Appendix 3.

Bas Braams concluded with the observation that recommendations of the Subcommittee have been closely followed during the past two years and have helped the Unit accomplish good progress. These recommendations are very important to the Unit and considerable weight is given by Agency to the advice of the IFRC subcommittee, especially in the approval of meetings and coordinated research projects.

2.2 Data Centre Network (DCN) and Database Activities and Computing Issues

Hyun-Kyung Chung presented a review of the core database and computing activities of the Unit and of the most recent Data Centres Network meeting. Please see Appendix 3 for the detailed report on past activities.

Web Home and Database Access

The Unit's home page is <u>http://www-amdis.iaea.org</u>. Please see this page for access to the databases, Knowledge Base, Unit reports, meeting announcements and other materials. The web page was revised in early 2010 to provide a more uniform view to all the Section's pages.

Database access to the numerical database ALADDIN, bibliographical database AMBDAS and search engine GENIE has been slowly increasing since 2004, but essentially flat over 2008-2009. The Wiki pages are very new; it is too early to offer meaningful statistics.

The AMBDAS Bibliographical Database continues to be maintained through contributions from the Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge for collision data and from National Institute of Standards and Technology (NIST) for spectroscopy. The database contains about 50,000 entries in 2010. Recently we obtained a contract with the CrossRef registry and have added their digital object identifier (DOI) links to the database entries.

It was raised at the subcommittee meeting that the future of the CFADC is uncertain. The subcommittee is very concerned about the possible loss of the contributions of CFADC to AMBDAS and more generally about the loss of such an important national A+M+PMI data centre.

The ALADDIN numerical database contains data on atomic and molecular collision processes and (more recent) plasma-material interaction processes. The data mainly come from IAEA Coordinated Research Projects and consultancies. In discussion it was noted that ALADDIN data are recommended data at the time of their production, but ALADDIN cannot at present be viewed as the library of international standard recommended data. In general the international effort on data evaluation needs to be revisited.

The GENIE search engine for numerical databases searches at this time 8 databases for radiative properties and 4 databases for atomic collision processes. The subcommittee considers that GENIE provides a valuable and convenient interface to multiple databases and recommends to consider expanding the collection of databases that are accessed by GENIE. The first priority should go to Open-ADAS and to Spectr-W3. The priority after that is for access to molecular databases, but the subcommittee is aware that this requires a non-trivial extension to the interface.

The Unit has started to develop a wiki-style Knowledge Base for atomic, molecular and plasmamaterial interaction data to complement the numerical and bibliographical databases. The inspiration for this comes from several sources: the success of the global Wikipedia, but also the experience with the data needs document at DCN and the experience with the Knowledge Base being developed as successor to the graphite properties database (see below). The knowledge base should provide information about atomic, molecular and plasma-material interaction processes and data, plus context. The knowledge base is addressed to fusion and plasma scientists and to A+M+PMI scientists. We hope to engage many contributors, but we do not envisage a wiki that is open to the world for editing. The basic layout is shown at the present meeting, but there are many gaps.

The subcommittee appreciates the knowledge base initiative for the reasons given. The main risk and uncertainty is the extent to which the community will be willing to contribute. The development of this Knowledge Base should not overwhelm Unit resources, so it is important to find people willing to contribute.

Data Centre Network

The Data Centre Network (DCN) held its 20th meeting in September 2009. B. Braams had just started at the Agency and H.-K. Chung attended as a consultant; she joined the Agency at the end of September. D. Humbert was scientific secretary. A meeting report is available and is summarized in Appendix 3. We note especially the historical review that was given by Dr W. Wiese of NIST who attended all 20 meetings.

The Terms of Reference of the DCN specify that its domain is atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties data for fusion and other applications. Participating centres must have an established programme in the collection, dissemination, critical assessment (evaluation) and generation of A+M+PSI data. The DCN activities are coordinated by the IAEA A+M Data Unit and reviewed by the IFRC subcommittee. The Data Centre Network represents one of the main instruments by which the international fusion related A+M/PMI data collection and evaluation programmes are implemented.

At the 20th DCN meeting in 2009 data centres presented progress reports on their activities in data compilation, evaluation and generation, web interfaces and publications. There were also presentations and discussions on data needs for ITER, on the new Code Centres Network and on the XML Schema for Atoms, Molecules and Solids, XSAMS.

One of the outputs of a DCN meeting is an update of a "data needs" document for long-term priorities in A+M and PMI data for fusion energy research. The document was updated, but our participation in the process provided motivation to look for different ways to handle this process in the future. We think that the Knowledge Base can provide a much more effective mechanism for the community to maintain a "data needs" document together with pointers to relevant literature and data collections. The DCN document is maintained here: <u>http://www-amdis.iaea.org/DCN/fusion_data.php</u>. Coordinated research projects are in place to address the key data needs.

Another important and topic of discussion at the DCN meeting, and we return to it at this subcommittee meeting, is the importance of data evaluation to assign uncertainties to the data and, ultimately, to provide internationally recommended data. The DCN recognizes that coordinated

research projects are less suitable for this task and in general the manpower that is available for data evaluation has declined.

2.3 Review of Coordinated Research Projects

Presentation

Bas Braams presented a review of recent and ongoing CRPs of the Unit. They are:

- 2002-2006: Tritium Inventory in Fusion Reactors
- 2004-2008: Atomic and Molecular Data for Plasma Modelling
- 2005-2009: Atomic Data for Heavy Element Impurities in Fusion Reactors
- 2007-2011: Data for Surface Composition Dynamics Relevant to Erosion Processes
- 2008-2012: Characterization of Size, Composition and Origins of Dust in Fusion Devices
- 2009-2013: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions
- 2010-2014: Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV

Please see Appendix 3, Activities of the Unit, for a description of these CRPs.

With respect to future CRPs it is noted that establishing a CRP is a two-stage process extending over several years. Sometime in the summer of an even-numbered year the CRP (title and brief description) is submitted for the Programme and Budget (P+B) for the next biennium (2010-2011 and 2012-2013 are relevant). Later, closer to the desired start of the CRP, a detailed proposal is prepared for review by the Committee on Coordinated Research Activities (CCRA). It is allowed for the detailed proposal to CCRA to deviate from the brief description in the P+B and it is also possible to propose an unplanned CRP to CCRA if funds are available, but we try to look ahead with care and not deviate much from the topic or topics that are in the P+B.

In the P+B for 2010-2011 the Unit has tentative CRPs on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" and on "Isotopic Ratio Diagnostics and Control in Burning Plasma" as was recommended by the IFRC subcommittee in 2008. A detailed proposal for the Tungsten CRP was prepared and was approved by CCRA in Feb 2010 to start later in 2010. The second CRP would start in 2011 and it is appropriate to review the plans at this meeting. Furthermore we wish to review at this meeting plans for CRPs to be entered into the Programme and Budget for the 2012-2013 biennium.

Discussion

The discussion concerned general principles for our CRPs and possible topics for future CRPs.

The committee emphasized the importance of the CRP mechanism for the production of recommended and evaluated data, that being the primary mission of the A+M Data Unit.

The publication mechanism at conclusion of a CRP needs to be improved. The "Greenbook" publication in the series Atomic and Plasma Material Interaction Data for Fusion (APID) has often been delayed. Until Vol 6 (1995) the series was published as a supplement to Nuclear Fusion, but this was discontinued.

At the conclusion of a CRP an effort should be made to publish a semi-review based on the CRP in the primary journal literature, as was done for the CRP on tritium inventory [C. H. Skinner et al., Fusion Science and Technology Vol 54, 891-945, 2008]. This needs to be established with participants at the start of the CRP. Also a newsletter or other form of communication can be valuable to let the community know about our CRPs.

Proposed Future CRP on H and He and Their Isotopes

In addition to the tungsten CRP that is starting in 2010 a second CRP is named in the Programme and Budget for 2010-2011: "Isotopic ratio diagnostics and control in burning plasma". A detailed proposal for this CRP has not yet been prepared in April 2010; the schedule calls for a proposal to CCRA by late 2010 or early 2011 so that the CRP may start later in 2011. However, the Unit wished to discuss with the IFRC subcommittee a change of title and emphasis of this CRP. For isotope diagnostics in the core plasma the favoured methods rely on plasma waves and on neutron emission due to a modulated beam, so methods that do not involve A+M data. Isotope effects are primarily an issue for molecular data. That makes the isotope effects most important for the edge plasma, but then in conjunction with a larger body of questions about atomic and molecular processes. Therefore it is suggested to choose a broader title for this CRP: "Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma". (The word "kinetic" was later changed to "state-resolved"; it refers to molecular excited states.)

The subcommittee reviewed the plan for this CRP. It was agreed that a focus on edge plasma molecular processes rather than core plasma isotope diagnostics is appropriate. Also beam-plasma interaction and issues of negative ion beams can be part of the CRP.

ITER will have a non-nuclear initial phase of operation during which only the ¹H isotope and He will be used (no D or T) and because of that there is interest in data for the molecular ions He2+ and HeH+ that haven't been much considered to-date. The CRP would then be considered with state-resolved and isotope-resolved data for processes of H, H+, H2, H2+, H3+, He, He+, He2+, HeH+, He2+, H-, H2-. The objective should be to establish an as near as possible complete and compressive database for collisional processes of these particles relevant to fusion plasma. It was noted that wall reflection properties and production of molecules on walls are important processes as well; it is to be assessed still to what extent processes on surfaces should be included in this CRP. The subcommittee recommends to organize a CM or TM in Fall 2010 to prepare detailed work plan and proposal for the CRP for consideration by CCRA. Upon approval the CRP could have its first meeting in Q3 2011.

Possible CRPs to Start in 2012 and Beyond

The Unit and Section have to prepare their plans for the Programme and Budget for 2012-2013 in the summer of 2010 in time for discussion at the IAEA General Conference that takes place in September. Therefore, this is the correct time to discuss those plans. In his presentation Bas Braams suggested as first priority a CRP on plasma interaction with tungsten surfaces and as the next priority one on hydrocarbon molecular data. Other possibilities that were suggested are a CRP on beryllium surfaces (JET will have data), one on diagnostics mirror surfaces (damage and cleaning), one on metallic surfaces in general (W, Be, steel) as an umbrella topic, or possibly one on multispecies plasma interaction with materials.

The topic gave rise to a lively discussion in the subcommittee about priorities. There was more or less immediate consensus that the next CRP, and probably the next two CRPs, should be concerned with plasma-material interaction that is relevant for ITER and for a reactor. Further the subcommittee recommended to focus the CRP or CRPs on specific materials rather than have an umbrella project. For tungsten the subcommittee assessed that the primary need for new data is in the area of its behaviour in a reactor environment, so properties of irradiated tungsten and tungsten alloys.

A consensus developed then that the highest priority should be a CRP on beryllium surfaces. The experimental database on beryllium is rather sparse due to its toxicity, but JET will start operation with a beryllium main wall in the second half of 2011. There will be copious new data produced in the 2012-2015 timeframe during which this new CRP would be active. There is still much uncertainty about tritium retention properties of beryllium and about the lifetime of a beryllium wall. Therefore the subcommittee strongly advised the Unit that the first CRP to start in the 2012-2013 biennium should be concerned with erosion and tritium retention in beryllium plasma-facing materials. The CRP should take in the new experimental data from JET and should help to prepare for ITER operation with a beryllium main wall. It was briefly considered if the CRP should also consider plasma interaction with lithium, but the subcommittee recommended against this dilution of the focus. Working title of the proposed CRP: "Erosion and tritium retention in beryllium plasma-facing materials".

The discussion then moved to the next priority in new research and data development and the subcommittee agreed that the next CRP to start should be concerned with plasma interaction with tungsten surfaces. This CRP should look beyond ITER and support the design efforts for a DEMO or other next step fusion experiment that are going on around the world. The CRP should focus on irradiated tungsten and on tungsten alloys, for which very few data are available at present. Multispecies plasma issues are important including He, N, O, Ne, Ar, W. As a suitable working title for that CRP the committee recommended "Plasma-wall interaction for irradiated tungsten and tungsten alloys in fusion devices".

It is unlikely that there would be room in the budget to start a 3rd CRP in the 2012-2013 biennium. The subcommittee recommended that plans for a CRP on hydrocarbon molecules should be kept in reserve. Carbon-based wall material is important in present experiments but is unlikely to have a role in a reactor and uncertain still even for ITER.

Conclusion with Regard to New CRPs

The subcommittee is pleased with the approval for the CRP on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" that is expected to have its first meeting later in 2010. With regard to the 2nd new CRP that is in the 2010-2011 budget the subcommittee proposes the working title "Atomic and Molecular Data for [Kinetic / State-Resolved] Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma". Isotope effects in relevant atomic and molecular processes should be of special concern for this CRP.

For the next biennium, 2012-2013, the subcommittee strongly recommends to give highest priority to two CRPs on plasma-wall interaction involving beryllium and tungsten. Because of the schedule of operation of JET with ITER-Like wall the first of these two to start should be concerned with beryllium. Working title: "Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials". The tungsten CRP should be the second to start and it should be concerned with use of tungsten in DEMO and in a reactor. Working title: "Plasma-wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices".

The subcommittee also considered a possible CRP focussed on data for hydrocarbon ions in fusion plasma. The subcommittee recommends to keep plans for such a CRP in reserve in case funds are available. Projects on beryllium and tungsten walls have first priority.

2.4. Review of Other Unit Activities

XSAMS: XML Schema for Atoms, Molecules and Solids

As described in Appendix 3 the Unit continued to support and coordinate the development of the XML Schema for Atoms, Molecules and Solids (XSAMS). Version 0.1 of the schema was released in September 2009 following the Data Centres Network meeting. Pilot implementations have been

carried out for four databases including ALADDIN. The schema is well developed for atomic processes (radiative processes and electron-atom collisions, "atom" being understood to include all charge states). The development is more limited for molecular processes and it is only a skeleton for particle-surface interaction processes. Also there is no real supporting infrastructure yet that would make XSAMS attractive for plasma modellers and other users of the A+M data.

The contact with the astrophysics community is providing a boost for development and implementation of XSAMS through the Virtual Atomic and Molecular Data Centre (VAMDC) project; a European Union Framework 7 infrastructure project. VAMDC, coordinated by M.-L. Dubernet, aims to provide interoperability among some 25 A+M databases used by the astrophysics community and XSAMS is the leading candidate to be adopted as the basis for data exchange. A decision is to be reached in mid-2010.

The subcommittee discussed the continued coordinating role of the Unit for XSAMS. Development of standards for data exchange is a task that is particularly suited to the IAEA and the subcommittee is pleased with the release of XSAMS version 0.1 and with its tentative adoption by VAMDC. The subcommittee echoes its advice of 2008 that the Unit continue to take a strong supporting role in the development and dissemination of XSAMS, but not to take a dominant role due to limited Unit resources.

Graphite Properties Database

The final meeting of the steering committee for the "International Database on Irradiated Nuclear Graphite Properties" was held 12-13 November 2009 and the project now moves from our Department to the Nuclear Energy Department as the "International Knowledge Base on Irradiated Nuclear Graphite Properties". Some of the history of the project and the Unit's involvement since 1999 is described in Appendix 3.

The A+M Unit and Nuclear Data Section had been pleased to host the project on irradiated graphite and we somewhat regret to see them leave NA. The meeting in November 2009 was interesting for us for their discussions on quality assurance and on the organization of the new Knowledge Base project. Some good pilot web design work (by KorteQ, Ltd, in the UK) was shown towards the Knowledge Base phase of the project and this reinforced our desire to create our own knowledge base for A+M+PMI data for fusion.

The subcommittee took note of the move of the graphite properties database project to NE and they concur with the view expressed by the unit. It was worthwhile for the unit to host the graphite properties database as an extra budgetary project. The project might have remained with us in the next phase, but the move to NE is rational too. The unit can be open to a future extra budgetary project if the occasion arises.

Our Meetings and Workshops

Please see Appendix 3 for a list of meetings organized by the Unit in the period April 2008 - April 2010. In brief they are Research Coordination Meetings (RCM) of the various CRPs, Technical Meetings (TM) of the Data Centre Network, the Code Centre Network and the IFRC Subcommittee, and Consultancy Meetings (CM) related to XSAMS and to the International Graphite Properties project.

In addition, as described in Appendix 3 a workshop on atomic and molecular data for fusion was held at ICTP in April 2009, following similar workshops in 2006 and 2003.

Except for the termination of the Graphite project the Unit expects a similar schedule of meetings and workshops in the 2010-2012 period, with one substantial addition. The Unit would like to raise with

the subcommittee the idea to cooperate in 2011 in the organization of the 7th Non-local Thermodynamic Equilibrium (NLTE) code comparison workshop.

The NLTE sequence of workshops brings together authors of codes that compute population distributions and radiative properties for finite temperature matter by solving rate equations using collisional and radiative rates. Generally the densities of interest for NLTE are higher than those in fusion plasma, but not so high that opacity effects dominate. The nature of these workshops, in which H.-K. Chung has participated since the start, is that problems are specified about 6 months in advance, participants submit their calculations before the workshop, and detailed comparisons are then made at the meeting. The NLTE7 workshop would play a complimentary role to the Tungsten CRP. The workshop attracts 20-30 participants and we would seek to support a small number of them.

The subcommittee found the concept of the code comparison workshop very interesting and strongly supports the proposal to cooperate in the organization of NLTE7 in Vienna in 2011. To some degree this workshop serves as an outreach to atomic physicists and data producers outside the fusion atomic data community and this will be valuable. An effort should be made to include test cases relevant to fusion energy, such as tungsten in plasma.

With regard to the ICTP workshop the Unit has submitted a proposal to hold one again in 2011 and if it fails for 2011 then the Unit intends to try again for 2012. The previous workshops were much appreciated by students and lecturers and they have been valuable for introducing new researchers to the large variety of A+M data needed for understanding fusion plasma modelling efforts.

The subcommittee also strongly supports the continuation of the series of IAEA-ICTP workshops on atomic, molecular and plasma-material interaction data for fusion energy. The ICTP is very well known for its meetings and workshops and cooperation with ICTP is very valuable for attracting participants from less developed countries.

As was mentioned by Dr Mank in his welcome the Physics Section has taken the initiative to organize an ITER-IAEA Technical Meeting on Analysis of ITER Materials and Technologies in connection with the Monaco ITER International Fusion Energy Days in November 2010. The A+M Unit was asked to share in the scientific secretary duties. The subcommittee supports the Unit's participation in the organization of this meeting.

The subcommittee considered other incidental meetings that would be valuable for the Unit. In this discussion especially the area of data for plasma-material interaction was considered. The planned CRPs on beryllium and tungsten surfaces are some distance in the future still and there is a need to revisit some of the basic data on erosion and particle reflection on the most common wall materials. This data was assembled in APID Vols 7A (chemical erosion) and 7B (mainly physical sputtering) in 1998 and 2001 respectively. These data should be revisited even in quite mundane ways such as reconsideration of the form of various fit-functions. Consultancies, a consultant meeting or a small technical meeting are suitable mechanisms and the subcommittee strongly recommends to the Unit to organize an activity to update the basic sputtering and reflection data of APID Vols 7A/B.

3. Concluding Remarks

Following the change of personnel in 2009 including the Section Head, Unit Head and Unit physicist the subcommittee appreciates the continuity in the work of the Unit. The subcommittee hopes that the recommendations about database management, data and code centres coordination, coordinated research projects, publications and further meetings and activities will guide the unit to a fruitful next biennium.

Appendix 1

List of Participants

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Agenda

Tuesday 27 April

09:30 – 10:00 Opening. Welcome to Subcommittee members. Adoption of Agenda, selection of a Chair

Session 1: General Report on Activities since April 2008

- 10:00 11:00 General report on activities, *B. Braams*
- 11:00 11:30 *Coffee break*

Session 2: Data Centre Network, Database Activities and Computer Issues

- 11:30 12:30 Review of DCN, databases and computing issues, *H.-K. Chung*
- 12:30 14:00 Lunch

Session 3: Review of Current and Planned CRPs

- 14:00 15:30 Results from recent CRPs, review of current CRPs and new CRPs to start in 2010-2011 period and beyond, *B. Braams*
- 15:30 16:00 *Coffee break*
- 16:00 17:30 <u>Session 3 (continued)</u>
- Wednesday 28 April

Session 4: Review of Additional Unit Activities

- 09:00 10:30 Review of activities, *B. Braams*
- 10:30 11:00 Coffee break

Session 5: Code Interfaces and Publications

- 11:00 12:30 Status of interfaces to codes on the Internet and Unit publications, *B. Braams and H.-K. Chung*
- 12:30 14:00 Lunch

Session 6: Review of Unit Status

14:00 – 14:45 Review of status of A+M Unit, *Subcommittee members*

Session 7: Recommendations for New Projects, Setting of Priorities

- 14:45 15:30 Recommendations for any new projects as well as setting priorities for Unit activities, *Subcommittee members*
- 15:30 16:00 *Coffee Break*

Session 8: Subcommittee Business and Formulation of Meeting Conclusions

- 16:00 17:30 Membership issues, other business, meeting conclusions, *Subcommittee members*
- 17:30 Adjournment of Meeting

Activities of the Unit (April 2008 - March 2010)

A3.1. Data Centres Network, Databases and Computing Issues

Web Home and Web Access Statistics

The web services and the databases of the A+M Data Unit are reached through the web address <u>http://www-amdis.iaea.org/</u>. The appearance of this page was revised early in 2010 to bring it in line with that of the Nuclear Data Services home page at <u>http://www-nds.iaea.org/</u>. Behind the amdis web address is a server called amdu1 and behind the nds address is a server called nds. Since 2006 amdu1 and nds are actually the same hardware. The server was upgraded in 2009; it is now a 64-bit Compaq with 2 quad-core Intel Xeon processors, 16 GB memory and 584 GB hard disk with RAID5. The system runs Redhat Enterprise Linux.

The presentation at the subcommittee meeting shows access statistics in graphical form. There has been steady slow growth in accesses since 2004, essentially flat between 2008 and 2009. ALADDIN receives the most accesses, about 35000 in 2009. For GENIE the number is about 10000 and for the bibliographical database AMBDAS it is about 3000.

Data Centre Network Activities

The International Network of Atomic and Molecular Data Centres (DCN) brings together 12 national centres that have a programme in collection, dissemination, evaluation and generation of atomic, molecular and plasma-material (A+M+PMI) data (and to some extent material properties data) for applications in fusion energy research and other fields. The history of the A+M Data Unit is strongly tied to that of the DCN; this Unit developed out of the work of the national data centres and from the start in 1977-1978 one of the roles of the Unit has been to facilitate exchange of data among the data centres and to help coordinate the work in the member centres. The activities of the DCN are reviewed by the IFRC subcommittee on atomic and molecular data. The DCN meets biennially in the odd years.

The 20th meeting of the International Network of Atomic and Molecular Data Centres was held in September 2009 with D. Humbert as scientific secretary. B. Braams had just started at the Agency and H.-K. Chung was present as a consultant; she started at the Agency at the end of September. The following data centres were represented: CFADC and NIST (USA), JAEA and NIFS (Japan), CRAAMD (China), KAERI (Korea), Kurchatov Institute (Russia), IPP Garching (Germany), GAPHYOR (France), ADAS (UK) and IAEA. ITER was represented as the most important customer. ENEA (Italy) was not represented at this meeting, but sent in a report. R. Clark (UT San Antonio) was present as a consultant to discuss code centre issues and Yu. Ralchenko (NIST) was present in connection with XML/XSAMS.

Dr Wolfgang Wiese of NIST (USA) who attended all 20 meetings presented a brief history of the DCN. The priorities of the DCN and the A+M Unit remain valid since 1977 :

- To compile and publish international computerized indices to the literature on A+M collision, structure and surface interaction data pertinent to fusion research
- To compile and disseminate in a quarterly bulletin newly measured and/or calculated A+M data and associated information
- To devise common formats for the exchange of bibliographic and numerical A+M data among the centre network
- To develop standardized computer input and output formats for the systematic compilation and the dissemination of bibliographic and numerical A+M data

All data centres presented progress reports on their activities in A+M data for fusion in the period October 2007 – August 2009. In addition, M. Shimada (ITER) described requirements for modelling ITER and the main new data needs, R. Clark described the IAEA Code Centre Network and Yu. Ralchenko led a discussion on the XML Schema for Atoms, Molecules and Solids (XSAMS).

The DCN supports the development of XSAMS (XML Schema for Atoms, Molecules and Solids) as a reliable and convenient tool for AM/PMI data exchange. Many of the data centres are ready to use XSAMS.

GENIE continually evolves to search new available databases on the web. The DCN recommends to enlarge the scope of GENIE to more processes and to molecular data.

The DCN also discussed data evaluation (accuracy, uncertainties) and traceability. It is recognized as being important and also difficult. Data evaluation work is still rather isolated.

A recurring task of the Data Centre Network meeting is to review priorities in A+M+PMI data compilation, evaluation, generation and exchange for fusion and to update a document on those data needs, on the web at <u>http://www-amdis.iaea.org/DCN/fusion_data.php</u>. The discussion looked in turn at atomic and molecular data (spectroscopic data, collisional data for edge plasma and neutral beam heating, impurity atomic processes in core and edge), plasma-material interaction data (erosion, hydrogen reflection, retention and release, surface evolution) and material properties. Many of the key needs are addressed in coordinated research projects. An updated version of the data needs document was produced at the meeting.

Database status

The principal numerical database ALADDIN was upgraded to version 3.2 in July 2009. This was a major upgrade for the part of the database that concerns plasma-surface interaction. At the same time the PSI database has been reviewed and a large amount of new data (3508 entries) has been added. Both web interfaces, for collisional and PSI data, now present the same interface, which was developed by P. Krstic and Yu. Ralchenko in August 2005 for A+M collisions and by P. Krstic, F. Meyer and D. Humbert in June 2007 for PSI data. Searches are performed efficiently using a combination of search criteria. A filtering function provides for successive refinement of the search query. All requested data are displayed in the same units as far as possible. A unit conversion tool is available. All results can be displayed in tabular and graphic modes.

The bibliographical database AMBDAS was upgraded to version 3.1 in April 2010. In this version DOI (Digital Object Identifier) numbers are included with the bibliographic data. In April 2010, out of 46878 reference data in the AMBDAS database 34420 data are linked to the full text of the electronic journal and 5115 data are linked to the abstract by the DOI link. Users can access the on-line source by clicking on the DOI number of an article. This facility required an agreement with the CrossRef DOI registry and we obtained an agreement for passive use of their database; i.e., we can query CrossRef, but not add data to it.

OPEN-ADAS was launched at the end of July 2008 based on a contract with IAEA. The Atomic Data and Analysis Structure (ADAS) project provides to its subscribers an interconnected set of computer codes and data collections for fusion plasma modelling. OPEN-ADAS provides free web access to the basic ADAS data, but not the higher-level modelling codes. Registration is required (in 2010) for access to OPEN-ADAS, but it is cost free. According to the presentation by A. Whiteford to the Data Centres Network meeting in September 2009 there are 124 registered users (89 from non-ADAS sites) as of August 2009.

OPEN-ADAS, like ADAS, is concerned with collisional and radiating properties of ions and atoms in plasma for use in fusion and in astrophysics. The datasets included in OPEN-ADAS are ADF01 Charge exchange cross sections, ADF04 Resolved specific ion data collections, ADF07 Electron impact ionisation coefficients, ADF08 Radiative recombination coefficients, ADF09 Dielectronic recombination coefficients, ADF11 Iso-nuclear master files, ADF12 Charge exchange emission

coefficients, ADF13 Ionisation per photon coefficients, ADF15 Photon emissivity coefficients, ADF21 Effective beam stopping coefficients and ADF22 Effective beam emission coefficients.

The GENIE search engine for atomic data is at version 2.3 since September 2007. It searches 8 databases for radiative properties and 4 databases for collisional properties. Log statistics are generated each month and are sent to DCN and IFRC members. Priorities for development of GENIE are to add Open-ADAS and Spectr-W3 to the searched databases and subsequently to extend the search to additional processes and molecular data. Also a link to bibliographical data should be provided if it is available.

Code Centre Network Activities

The Code Centres Network developed out of informal conversations and a technical meeting in 2005 to bring together potential centres and discuss ways to share codes and related expertise. A further exploratory meeting (the 1st TM of the CCN) was held in December 2008. The 2nd TM of the International Code Centre Network is scheduled for September 2010.

At the meeting in December 2008 the 12 participating centres summarized their expertise and plans. The centres and their representatives are:

- CCC & RCCC, Curtin University, Australia, Igor Bray
- CR Model, Kitasato University, Japan, F. Koike
- MELDF*-TCAM, QUAN, EIKON, CTMC, Universidad Autonoma de Madrid, Spain, Ismanuel Rabadan
- CDW and VPN, University P. & M. Curie, France, Alain Dubois; Centro Atomico Bariloche CNEA, Argentina, P.D. Fainstein
- Molecular cross Sections, SI calculations, University of Bari, Italy, Mario Capitelli
- CR Models, Kurchatov Institute, Russian Federation, Alexander Kukushkin
- ATOM, ATOM-AKM, GKU, Lebedev Institute, Russian Federation, L. Vainshtein
- HYDKIN, Forschungszentrum Juelich, Germany, Detlev Reiter
- MCHF, GRASP2K, FLYCHK, NOMAD,, National Institure for Standards and Technology, USA, Yuri Ralchenko
- DEGAS databases, Princeton Plasma Physics Laboratory, USA, D. Stotler
- LANL Codes, Los Alamos National Laboratory, USA, J. Abdallah, Jr.
- AMD Services, International Atomic Energy Agency, H. Chung

This first meeting of the new code centres network led to the following agreements.

- An IAEA web page is created to include basic information from summaries of the current code capabilities and links directly to the centre web pages. (The centres maintain their home pages with updates as capabilities change.)
- The group should begin utilizing the XSAMS format for data transmission/exchange.
- Code authors will attempt to assess the accuracy of the calculations in a similar manner to the numerical database estimate.
- The Network will meet biennially at IAEA headquarters to monitor progress and identify future needs.
- The Network will constitute an informal federation to permit flexible membership.
- The Network should make the broader fusion community aware of the capabilities represented by this group (presentations at fusion-oriented conferences).

The centres agree that the Network is at least initially an informal arrangement. Membership and functions of the network should evolve.

The next meeting of the code centre network is scheduled for September 2010 and the Unit wishes to discuss at the present meeting with the subcommittee how the CCN should evolve.

IAEA Online calculation capabilities

In connection with the work of the code centres network the A+M Data Unit web page offers several online calculation capabilities. A code by J. Peek, AAEXCITE, uses the Average Approximation to calculate electron impact excitation of ions. For heavy particle collisions the code HEAVY by A. Dubois, J. P. Hansen and P. Vainstein calculates cross sections for excitation, ionization and charge exchange for one-electron systems (bare nucleus on hydrogenic target). The LANL (Cowan) modelling codes are an important part of the CCN but these codes could not be run locally at IAEA. Instead, results from collisional radiative calculations of the LANL codes are available. Level population distributions and radiative power loss rates are provided.

The Unit provides an interface to run several Los Alamos atomic physics codes to calculate atomic structure and electron impact excitation and ionization cross sections (fine structure levels and configuration average). Also complete data sets calculated by the LANL codes for collisional radiative modelling of argon, chlorine and silicon are provided; these datasets were produced as part of the CRP on atomic data for heavy element impurities in fusion reactors. The data include level energies and statistical weights of fine-structure levels of the ground and excited configurations, oscillator strengths and electron-impact excitation cross-sections, and photo-ionization and electron-impact ionization cross-sections.

The most recent addition to the online capabilities is an interface to the FLYCHK code at NIST. FLYCHK, developed by H.-K. Chung, is a collisional-radiative modelling code based on a hydrogenic model. It can be used to calculate ionization distributions and spectral properties of elements from hydrogen to gold (Z=79). In addition to the interface tabulated outputs are provided for elements from H to Au in the range of plasma conditions of $0.5 \text{ eV} \le \text{Te} \le 100 \text{ keV}$ and $1012 \text{ cm}-3 \le \text{Ne} \le 1024 \text{cm}-3$.

Wiki Knowledge Base Development

The numerical and bibliographic databases have some limitations for data collection and dissemination. They are not well suited for heterogeneous and often qualitative data such as are associated with surface composition dynamics or formation of dust. They do not offer an intrinsic data description. In general a numerical database needs an extensive environment in which the data sources and limitations of the data are described.

The success of Wikipedia inspired us to start a wiki-style Knowledge Base on atomic, molecular and plasma-surface interaction data for fusion, <u>http://www-amdis.iaea.org/w/</u>. These pages are addressed to scientists in fusion plasma modelling or data analysis and in the relevant areas of atomic, molecular and plasma-material interaction (A+M+PMI) physics. We aim to provide information about data in fusion energy research and related fields, sources of A+M+PMI data, data collections, data producers, data- and code-oriented conferences and workshops and much else. The wiki format makes it possible to organize much more information than could fit in our established numerical and bibliographical databases.

This work was started early in 2010 within the Unit and at the present time the information is almost all drawn from our own meeting reports and from published volumes of the IAEA Atomic and Plasma-Material Interaction Data for Fusion (APID) series. The wiki is public on the web, but editing is restricted to those that have obtained a password. However, we intend to make passwords liberally available to participants of our meetings and CRPs. The A+M Data Unit expects to have a coordinator role while the wiki pages are contributed and peer-reviewed by our community of data producers and data users.

A3.2. Review of Coordinated Research Projects

Coordinated Research Projects (CRPs) are the principal mechanism by which the Unit encourages new research and data development. A CRP brings together researchers from about 10 to (at most) 15 institutes world-wide for coordinated research to achieve certain well defined goals related to data generation, compilation and evaluation for a class of A+M collision or plasma-material interaction processes. The participants of a CRP normally meet three times with intervals of about 18 months for

a Research Coordination Meeting (RCM). After the 3rd RCM a final report is produced. Thus the total duration of a CRP is 4-5 years. During the past 10 years the IAEA A+M Data Unit has been running about 3-4 active CRPs each year, and effort has been made to start one new CRP each year if the budget allows it.

CRP descriptions, RCM summary reports and in some cases participants' meeting presentations are available on the NDS Atomic and Molecular Data Unit web pages via <u>http://www-amdis.iaea.org/CRP/</u>. Meeting reports and CRP final reports (APID) have also been used in the preparation of our Knowledge Base wiki pages.

CRP on Tritium Inventory in Fusion Reactors (2002-2006)

This CRP was concerned with data on erosion and tritium retention in the candidate wall materials for ITER: Be, C, W and mixed materials. Research coordination meetings (RCM) were held in Nov 2002, Oct 2004 and Sep 2006 and summarized in INDC(NDS) reports Nrs. 442, 495 and 516. Following the final RCM the participants produced a substantial journal publication as a record of the work of the CRP [C. H. Skinner, A. A. Haasz, V. Kh. Alimov, N. Bekris, R. A. Causey, R. E. H. Clark, J. P. Coad, J. W. Davis, R. P. Doerner, M. Mayer, A. Pisarev, J. Roth, T. Tanabe, "Recent Advances on Hydrogen Retention in ITER's Plasma-Facing Materials: Beryllium, Carbon, and Tungsten", Fusion Science and Technology **54** (2008) 891-945].

The principal conclusion of the CRP, amply documented in the CRP reports, is that of the proposed ITER wall materials tungsten demonstrates the lowest tritium-inventory risk, carbon presents the greatest risk and demands tritium removal techniques, while beryllium presents major risk through codeposits in the presence of oxygen so that tritium removal techniques need also to be developed and applied for Be.

CRP on Atomic and Molecular Data for Plasma Modelling (2004-2008)

This CRP was created to provide data for atomic and molecular processes that take place in the low-temperature, near-wall region of fusion plasma experiments, where molecules and molecular ions are present in addition to neutral hydrogen, neutral atoms and low-charged impurity ions, and the main plasma hydrogen ions. The CRP brought together researchers from 14 different institutes. Research Coordination Meetings were held on 26-28 September 2005, 18-20 June 2007, and 17-19 November 2008 and summary reports of these meetings have appeared in the INDC(NDS) series of reports as Nrs. 482, 515 and 544. These summary reports and the participant presentations are available on the NDS Atomic and Molecular Data Unit web pages via http://www-amdis.iaea.org/CRP/.

The participants have produced a large number of scientific articles connected to the subject matter of the CRP. In addition the participants have submitted manuscripts based on the CRP for publication in Atomic and Plasma-Material Interaction Data for Fusion; the manuscripts have been refereed and the journal issue is in preparation. One database output of the CRP is a major upgrade of the Hydride Kinetics (HYDKIN) database that is maintained in the Institute for Plasma Physics at the Forschungszentrum Jülich.

CRP on Atomic Data for Heavy Element Impurities (2005-2009)

The CRP was created in order to gather and assess data and to generate new data for collisional and radiative processes of heavy elements likely to be found in a fusion reactor or in ITER. Key elements are argon and krypton as deliberately introduced radiating impurity, tungsten as wall material, and other heavy elements that may be introduced via doping of carbon tiles for diagnostic purposes.

The CRP has brought together researchers from 10 different institutes. Research Coordination Meetings were held on 14-15 November 2005, 26-28 September 2007, and 4-6 March 2009, and Summary Reports of these meetings have appeared. (INDC(NDS) reports 487, 521, and 552.)

The participants have produced a large number of scientific articles connected to the subject matter of the CRP. In addition the participants have submitted manuscripts based on the CRP for publication in the IAEA journal Atomic and Plasma-Material Interaction Data for Fusion; the manuscripts have been referred and the journal issue is in preparation. Much of the work in this CRP was focussed on the

noble gases Ar, Kr, and Xe, on the likely wall material W, and on other possible impurities Fe, Cl, and Si.

Two datasets were added to the ALADDIN numerical database as a result of this CRP and one further extremely large dataset received its own separate home among our numerical databases. One new dataset, by V. K. Nikulin and N. A. Guschina, provides cross-sections for charge transfer and excitation in collisions between He or He2+ and a heavy ion: selected charge states of C, O, Si, Ti, Cr, Fe, Ni, Cu, Mo, and W. The other new dataset, by M. B. Trzhaskovskaya, V. K. Nikulin and R. E. H. Clark, provides cross-sections for photoionization from selected charge states of Si, Cl, Ar, Ti, Cr, Fe, Ni, Cu, Kr, Mo, Xe, and W. These photoionization data are resolved with respect to final state, making this a very large dataset. The third dataset, by J. Colgan, H. L. Zhang et al., provides detailed state-to-state radiative and collisional transition rate coefficients for all ionization stages of argon, chlorine and silicon. With this highly detailed data set it is possible to establish a population kinetics model to obtain excited level populations within one ionization stage. The level of detail of these data is beyond the scope of ALADDIN and they received a separate home.

CRP on Data for Surface Composition Dynamics Relevant to Erosion Processes (2007-2011)

This CRP was organized to increase understanding of erosion processes for mixed materials, especially the Be-C-W mix foreseen for ITER.

The CRP participants are Alain Allouche (CNRS / Universite de Provence, France), Russell Doerner (University of California at San Diego, USA), James Davis (University of Toronto, Canada), Junglin Chen / Guangnan Luo (Chinese Academy of Sciences, China), Rinad Zalavutdinov (Russian Academy of Sciences, Russia), Yury Martynenko (RRC Kurchatov Institute, Russia), Predrag Krstic (Oak Ridge National Laboratory, USA), Karl Krieger (IPP Garching, Germany), Kai Nordlund (University of Helsinki, Finland) and Daiji Kato (National Institute for Fusion Science, Japan). Research coordination meetings were held in October 2007, March 2009. The final RCM is scheduled for September 2010.

CRP on Characterization of Size, Composition and Origins of Dust in Fusion Devices (2008-2012)

In a long-pulse device such as ITER it is conceivable that hundreds of kg of dust are produced over the course of a campaign. Tritium may be aborbed in the dust and there is an explosion hazard, making dust and measurement of dust and of absorbed tritium a major concern. Therefore, there is a need for information on properties of dust, such as particle size distribution (physical and aerodynamic mass median diameter), composition (elemental and chemical) and their origins in fusion machines. The primary goal of this CRP is to address these data needs.

The participants in the CRP are Christian Grisolia, Volker Rohde (IPP Garching, Germany), Jorg Winter (Ruhr University Bochum, Germany), Carmine Castaldo, Naoko Ashikawa, Anna Widdowson (CCFE, UK), Phil Sharpe / Paul Humrickhouse (INL, USA), Charles Skinner (PPPL, USA) and Suk-Ho Hong (NFRI, Korea). The first Research Coordination Meetings was held in December 2008 and the second one is scheduled for June 2010.

CRP on Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions (2009-2013)

The purpose of this CRP is to generate new data on processes including excitation, ionization, recombination and heavy particle collisions for ions of hydrogen, helium, lithium, beryllium, boron, carbon, nitrogen and oxygen and molecules of these atoms.

The participants and consultants in this CRP are Pierre Defrance (Université Catholique de Louvain, Belgium), Igor Bray / Dmitry Fursa (Curtin University of Technology, Perth, Australia), Ratko Janev (Macedonian Academy of Sciences and Arts, Skopje, Republic of Macedonia), Luis Mendez (Universidad Autónoma de Madrid; Madrid, Spain), James Brian Mitchell (University of Rennes I, Rennes, France), Teck Lee / Michael Pindzola (Auburn University, Alabama, USA), David Schultz

(Oak Ridge National Laboratory, Tennessee, USA), Hidekazu Takagi (Kitasato University, Sagamihara, Japan), Jianguo Wang / Ling Liu (Institute of Applied Physics and Computational Mathematics, Beijing, China), Baoren Wei (Fudan University, Shangai, China), Mats Larsson, Asa Larson (Department of Physics, Stockholm University, Sweden), Ioan Schneider (Department of Physics, University of Le Havre, France), Viorica Stancalie (National Institute of Laser, Plasma and Radiation Physics, Bucharest, Romania), John Curry / Joseph Reader (Atomic Physics Division, National Institue of Standards and Technology, USA). The first Research Coordination Meetings was held in November 2009; the second would take place in Q2 2011.

CRP on Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV (New, 2010-2014)

Based on a recommendation of the IFRC subcommittee at their meeting in 2008 a proposal for a CRP on "Spectroscopic and Collisional Data for Tungsten from 1 eV to 20 keV" had been included in the Programme and Budget for 2010-2011 with intended start year 2010. Inclusion in the P+B is one step towards establishing the CRP; a detailed proposal must be prepared for consideration by the Committee on Coordinated Research Activities (CCRA) and if the CRP is approved by CCRA then the participants can be selected.

The detailed proposal for the CRP on tungsten in plasma was submitted to CCRA for their meeting in February 2010 and it was approved. According to the proposal to CCRA the CRP "... will bring together experts in experimental and theoretical atomic physics to address data needs for tungsten as an impurity in fusion plasma. It will cover the data needs over the whole range of relevant plasma conditions, ranging from the cool, high-density near-wall plasma to the fusion core, and it will cover all the principal collision and radiative processes. Excitation and ionization by electron impact, including multi-stage ionization, auto-ionization, and radiative and dielectronic recombination, together with photon-induced and radiative excitation and de-excitation, are the principal processes that determine the balance of ionization stages in the plasma. Line radiation is the principal energy loss mechanism, and all radiative processes have their distinct spectral properties that are important for interpretation of experimental data. Proton impact processes are relevant in the high density edge plasma, and charge exchange collisions are important in connection with neutral beam plasma heating. The relevant data include cross-sections for kinetic modelling, integrated rate coefficients for macroscopic modelling, and spectroscopic signatures for direct experimental simulations. The output of the CRP will support the interpretation of spectroscopic measurements on current and future fusion experiments, the modelling of tungsten in fusion plasma, and the design and optimization of fusion reactor experiments, and will advance the fusion energy research efforts."

At the time of the IFRC subcommittee meeting in April 2010 the participants were being selected with the objective to have the first RCM in Q4 2010.

A3.3. Review of Additional Unit Activities

XML Schema for Atoms, Molecules and Solids, XSAMS

The development of XSAMS goes back to the 17th meeting of the International Atomic and Molecular Data Centres Network (DCN), in October 2003, where a working group composed of Yu. Ralchenko, D. Humbert, D. R. Schultz, T. Kato and Y.-J. Rhee was formed to create a new format for the exchange of A+M data for fusion. The objective of the working group was to develop a proposal for an "Atomic and Molecular Data Markup Language" (AMDML) for presentation and discussion at the 2004 ICAMDATA meeting in Toki, Japan. This AMDML format, later renamed XSAMS, should encode as much as possible all essential information for the description of A+M collision processes, and ultimately particle-surface interaction processes too. In parallel the International Virtual Observatory Alliance (IVOA) developed a Simple Line Access Protocol (SLAP) and Simple Spectra Line Data Model (SSLDM) for XML encoding of spectroscopic data.

During the course of the 2004 ICAMDATA meeting development of AMDML was discussed further including now also people from the astrophysics community. In the years 2004-2009 the XML schema

was developed by a group consisting of Yu. Ralchenko of the National Institute of Standards and Technology (USA), D. R. Schultz of Oak Ridge National Laboratory (USA), M.-L. Dubernet of Universit'e Pierre et Marie Curie (France), N. Moreau and E. Roueff of the Observatoire Paris-Meudon (France), D. Humbert and R. E. H. Clark of the International Atomic Energy Agency (Austria), and joined in 2008 by P. Loboda and S. Gagarin of the All-Russian Institute of Technical Physics, Russia.

An outline of XSAMS was presented at the 2008 ICAMDATA meeting in Beijing in an invited talk (Yu. Ralchenko) and a detailed poster (D. Humbert et al.), and XSAMS version 0.1 was released in September 2009 following the 20th meeting of the Data Centres Network. At that time exploratory implementations had been carried out for the Atomic Spectra Database at NIST, ALADDIN at IAEA, Spectr-W3 at VNIITF and BASECOL at the Observatoire de Paris.

Development of XSAMS was strongly supported and coordinated by our Unit with endorsement by the IFRC subcommittee at their meetings in 2004, 2006 and 2008. According to the report of the 2008 subcommittee meeting: "The Subcommittee notes that the Unit is following previous advice to maintain a strong role in these activities, but not to take a dominant role due to limited Unit resources". We organize Consultants' Meetings to bring the principal XSAMS authors together; in the past two years such meetings were held 15-16 May 2008 in Vienna, 26-27 August 2008 in Vienna, 27 October 2008 in Beijing (in conjunction with ICAMDATA), 10-11 September 2009 in Vienna and 24-26 March 2010 at NIFS in Japan.

At release 0.1 in September 2009 XSAMS is well developed for atomic processes (radiative processes and electron-atom collisions, "atom" being understood to include all charge states). The development is more limited for molecular processes and it is only a skeleton for particle-surface interaction processes.

Graphite Properties Database

The "International Database on Irradiated Nuclear Graphite Properties" has been hosted by the A+M Data Unit since 1999 as an extra-budgetary project funded by Member States and by Graphite Database Members. The project aims to preserve and expand the existing scientific information on physical, chemical, mechanical and other properties of irradiated graphite relevant for nuclear power, nuclear safety and other nuclear science and technology applications, and to create a comprehensive international source for such information, including reference data. In 1999 the initial project members were the United Kingdom, Japan, the United States, and the Forschungszentrum Juelich, Germany. Meetings were held approximately annually and were hosted by our Unit at IAEA. The first version of the database was provided to members and sponsors of the project on CD-ROM in April 2006. The 11th meeting of the "Technical Steering Committee for the International Database on Irradiated Nuclear Graphite Properties" was held 25-26 March 2009 and the 12th meeting was held 12-13 November 2009, both at IAEA Headquarters. Participants in the 12th meeting came from the UK, China, Germany, Japan, Korea, the USA, France, South Africa, the Ukraine and the IAEA. Throughout the years the driving force and very effective Chairman of the project was Mr Tony Wickham, UK.

The meeting 12-13 November 2009 was the final meeting of the Graphite Properties Database project hosted by the A+M Data Unit in the Department of Nuclear Applications. As of 2010 the project continues in a new form in the Department of Nuclear Energy as the IAEA International Knowledge Base on Irradiated Nuclear Graphite Properties: <u>http://www.iaea.org/NuclearPower/Graphite/</u>. This move of the project from the NA to the NE department was made in connection with the start of a CRP within NE on "Improved Understanding of the Irradiation Creep Behaviour of Nuclear Graphite". The final instance of the "IAEA International Database on Irradiated Nuclear Graphite Properties" was released to members and sponsors of the project in August 2009. We retain a set of web pages for the concluded project as an archive: <u>http://www-amdis.iaea.org/graphite/</u>.

Meetings Organized by the Unit

The Unit organized the following meetings during the period April 2008 - April 2010.

TM of the "16th IFRC Sub-committee on Atomic and Molecular Data for Fusion Research" (17-18 April 2008)

CM on "XML Schema for Atomic and Molecular Data" (15-16 May 2008)

CM on "XML Schema for Atomic and Molecular Data" (26-27 August 2008)

CM on "XML Schema for Atomic and Molecular Data" (27 October 2008, Beijing, China)

Third and final RCM of the CRP on "Atomic and molecular data for plasma modelling" (17-19 November 2008)

TM on "International Code Centres Network" (2-3 December 2008)

First RCM of the CRP on "Characterization of size, composition and origins of dust in fusion devices" (8-10 December 2008)

Final RCM of the CRP on "Atomic Data for Heavy Element Impurities in Fusion Reactors" (4-6 March 2009)

Second RCM of the CRP on "Data for Surface Composition Dynamics Relevant to Erosion Processes" (11-13 March 2009)

CM of the "11th Technical Steering Committee for the International Database on Irradiated Nuclear Graphite Properties" (25-26 March 2009)

TM on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (20th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)" (7-9 September 2009)

CM on "XML Schema for Atomic and Molecular Data" (10-11 September 2009)

CM of the "12th Technical Steering Committee for the International Database on Irradiated Nuclear Graphite Properties" (12-13 November 2009)

First RCM of the CRP on "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" (18-20 November 2009)

CM on "XML Schema for Atomic and Molecular Data" (24-26 March 2010, NIFS)

TM of the 17th IFRC Sub-committee on Atomic and Molecular Data for Fusion Research (27-28 April 2010)

Workshops

A workshop on "Atomic and Molecular Data for Fusion Energy Research" was held at the International Centre for Theoretical Physics (ICTP) 20 - 30 April 2009 with R. Clark as Director. This workshop had the goal of introducing participants to the role of atomic and molecular (A+M) data in nuclear fusion energy research and to give the participants the opportunity to use actual data in some simple but realistic exercises. Earlier similar workshops were held in 2006 (2 weeks) and 2003 (1 week).

Lecturers Alain Dubois, Robert E. H. Clark, Joseph Abdallah Jr., Denis Humbert, Tilmann Maerk, Thomas Schwarz-Selinger, Detlev Reiter and James W. Davis gave presentations on data in the areas of molecular processes, heavy particle collisions, electron impact collisions, collisional radiative modelling, plasma-material interaction and co-deposition of materials in fusion devices. The lecture materials have been made available through the ICTP and the A+M Data Unit web pages. Lecturers also had time to interact and discuss their continuing research. In addition the lecturers made themselves available to the students at every opportunity resulting in many fruitful discussions.

The workshop was attended by twenty-two students and three ICTP associates, representing ten Member states. The students came from a variety of backgrounds, including plasma-material interaction, molecular physics, heavy particle interactions and plasma modelling. The students gave brief presentations of their work and gave poster presentations one afternoon of the workshop.

Attendance at International Conferences

Fifth International Conference on Physics of Dusty Plasmas, 18-23 May 2008, Azores, Ponta Delgada, Portugal; R. E. H. Clark.

Annual ADAS workshop, 29 Sep – 2 Oct 2008, Juelich, Germany; R. E. H. Clark and D. P. Humbert.

6th ICAMDATA meeting, 27-31 Oct 2008, Beijing, China; R. E. H. Clark and D. P. Humbert.

Joint ICTP-IAEA workshop on Atomic and Molecular Data for Fusion Energy Research, 20-30 Apr 2009, Trieste, Italy; R. E. H. Clark and D. P. Humbert.

Annual ADAS workshop, 4-7 Oct 2009, Schloss Ringberg, Tegernsee, Germany; B. J. Braams.

17th European Fusion Physics Workshop, 7-9 Dec 2009, Velence, Hungary; B. J. Braams.

6th NLTE Code Comparison Workshop, 7-11 Dec 2009, Athens, Greece; H.-K. Chung.

A3.4. Publications

R. E. H. Clark and D. Humbert: "Atomic, Molecular and Plasma- Surface Interaction Data for Fusion Energy Research", in "ICAMDATA- 2008: 6th International Conference on Molecular Data and Their Applications", AIP Conf. Proc. 1125, pp. 197-206.

Yu. Ralchenko, R. E. H. Clark, M.- L. Dubernet, S. Gagarin, D. Humbert, P. A. Loboda, N. Moreau, E. Roueff, and D. R. Schultz: "Development of new standards for exchange of atomic and molecular data", in "ICAMDATA- 2008: 6th International Conference on Molecular Data and Their Applications", AIP Conf. Proc. 1125, pp. 207-216.

INDC(NDS)-0566: IAEA International Database on Irradiated Nuclear Graphite Properties, Summary Report of the 12th Meeting of the Technical Steering Committee, IAEA Headquarters, Vienna, Austria 12-13 November 2009. Prepared by H. K.Chung and A. J. Wickham

INDC(NDS)-0564: Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions, Summary Report of the First Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 18-20 November 2009. Prepared by B. J. Braams (January 2010)

INDC(NDS)-0563 Technical Aspects of Atomic and Molecular Data Processing and Exchange, Summary Report of the 20th Meeting of the A+M Data Centre Network, IAEA Headquarters, Vienna, Austria 7-9 September 2009. Prepared by D. Humbert and B. J. Braams (January 2010)

INDC(NDS)-0562 XSAMS: XML Schema for Atomic and Molecular Data, Summary Report of Consultants Meeting, IAEA Headquarters, Vienna, Austria 10-11 September 2009. Prepared by D. Humbert and B. J. Braams (January 2010)

INDC(NDS)-0556 IAEA International Database on Irradiated Nuclear Graphite Properties, Summary Report of the 11th Meeting of the Technical Steering Committee, IAEA Headquarters, Vienna, Austria 25-26 March 2009. Prepared by D. Humbert and A.J. Wickham

INDC(NDS)-0553 Data for Surface Composition Dynamics Relevant to Erosion Processes , Summary Report of the Second Research Coordination Meeting , IAEA Headquarters, Vienna, Austria 11-13 March 2009. Prepared by R.E.H. Clark (April 2009)

INDC(NDS)-0552 Atomic Data for Heavy Element Impurities in Fusion Reactors, Summary Report of the final Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 4-6 March 2009. Prepared by R.E.H. Clark (April 2009)

INDC(NDS)-0550 Characterization of Size, Composition and Origins of Dust in Fusion Devices, Summary Report of the First Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 10-12 December 2008. Prepared by R.E.H. Clark (March 2009)

INDC(NDS)-0549 XSAMS: XML Schema for Atomic and Molecular Data and Particle Solid Interactions, Summary Report of an IAEA Consultants' Meeting, Beijing Friendship Hotel, China, 27 October 2008. Prepared by D. Humbert (February 2009)

INDC(NDS)-0548 International Code Centres Network, Summary Report of an IAEA Technical Meeting International Code Centres Network, IAEA Headquarters, Vienna, Austria, 2-3 December 2008. Prepared by R.E.H. Clark (February 2009)

INDC(NDS)-0544 Atomic and Molecular Data for Plasma Modelling, Summary Report of the final Research Coordination Meeting, IAEA Headquarters, Vienna, Austria, 17-19 November 2008. Prepared by D. Humbert (February 2009)

INDC(NDS)-0538 16th Meeting of the IFRC Subcommittee on Atomic and Molecular Data for Fusion, Summary Report, IAEA Headquarters, Vienna, Austria 17-18 April 2008. Prepared by R.E.H. Clark and W.P. West (November 2008)

INDC(NDS)-0537 XSAMS: XML Schema for Atomic and Molecular Data, Summary Report of Consultants' Meeting, IAEA Headquarters, Vienna, Austria 26-27 August 2008. Prepared by D. Humbert (October 2008)

INDC(NDS)-0532 XML Schema for Atomic and Molecular Data, Summary Report of Consultants' Meeting, IAEA Headquarters, Vienna, Austria, 15-16 May 2008. Prepared by D. Humbert (August 2008)

INDC(NDS)-0531 IAEA International Database on Irradiated Nuclear Graphite Properties, Summary Report of the 10th Meeting of the Technical Steering Committee, IAEA Headquarters, Vienna, Austria, 26-27 March 2008 . Prepared by D. Humbert and A.J. Wickham (June 2008)

INDC(NDS)-0565 XSAMS: XML Schema for Atomic and Molecular Data, Summary Report of Consultants Meeting, IAEA Headquarters, Vienna, Austria 6-7 December 2007. Prepared by D. Humbert (April 2008)

INDC(NDS)-0527 Technical Aspects of Atomic and Molecular Data Processing and Exchange, Summary Report of the 19th Meeting of the A+M Data Centre Network, IAEA Headquarters, Vienna, Austria, 3-5 October 2007. Prepared by Denis Humbert (May 2008)

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