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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 19th Meeting of the A+M Data Centres and ALADDIN Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

3 – 5 October 2007

Prepared by

Denis Humbert

May 2008

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Abstract

The proceedings of the IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (19th Meeting of A+M Data Centres and ALADDIN Network), held on 3-5 October, 2007 in Vienna, Austria, are briefly described. Conclusions and recommendations are presented concerning various proposed projects and their priorities involving A+M data compilation and evaluation and technical aspects of data processing, exchange, and distribution.

May 2008

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1. Introduction

A meeting on Technical Aspects of Atomic and Molecular Data Exchange and Processing (19th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network) was held on 3-5 October 2007 at IAEA Headquarters, Vienna, Austria. The objectives were to review progress in A+M data activities in the data centres, the methods and procedures applied in data processing and exchange, and to coordinate the working plans for the next two years.

All Data Centre members were represented, and seventeen participants attended the meeting. The Network welcomed three new Data Centre representatives: Dr. Nakano from JAEA in place of Dr. Kubo (promoted to the JAEA Policy Planning and Administration Department); Dr. Mazzitelli from ENEA (in place of Dr. Menapace who retired); and Dr K. Katsonis from GAPHYOR (in place of Dr. Bretagne who had also retired).

Representatives of two data centres were invited as observers: Dr. A. Whiteford from Strathclyde University, UK, represented ADAS; and Dr. L. Machado from Universidade Federal de São Carlos, Brazil, representing BRAMPDAC, a Brazilian data centre handling atomic and molecular data for fusion (unfortunately, Dr. Machado was unable to attend the meeting).

Dr. Yuri Ralchenko from NIST, USA, specialist in data exchange and web databases tools was invited to attend for his expertise on XML. ITER was officially represented by Dr. D. Kato from NIFS, while the IAEA was represented by Drs. A.L. Nichols, R.E.H. Clark and D. Humbert.

The full list of participants and related data centres is available in Appendix 2.

The Meeting was opened by Dr. A.L. Nichols (Head, Nuclear Data Section, Division of Physical and Chemical Sciences), R.E.H. Clark (Head, A+M Data Unit, Nuclear Data Section), and D. Humbert (Physicist, A+M Data Unit, Nuclear Data Section). They welcomed all participants and stressed the usefulness of this TM to the Data Centres Network, and noted new developments in this field that had occurred since the 18th Meeting held in October 2005. The agenda was adopted (see Appendix 2).

The meeting covered the following topics:

- Current activities of the A+M Data Centres and invited talks
- Data issues: XML for AM/PSI data, priorities in data compilation for fusion, data evaluation
- Membership status
- Interfaces and web tools
- Meeting conclusions and recommendations

2. Proceedings of the Meeting

2.1 Current Activities of the A+M Data Centres

During the first session, representatives from all data centres presented their progress reports on activities for the period October 2005 – September 2007. The main focus was Atomic and Molecular Data related to fusion, including data compilations, evaluations and generation, WWW developments, Data Centre publications produced during the reporting period, and the status of ongoing Data Centre programmes and their plans for future work. The presentations in this session indicate that Data Centre activities have closely followed the recommendations of the previous meeting, both in terms of content and mutual cooperation. The presentations are available on the A+M Data Unit web site: http://www-amdis.iaea.org/

W. Eckstein, Max-Planck Institut fur Plasmaphysik, Garching, Germany

Dr. Eckstein presented a comparison of experimental and theoretical sputtering yields. Energy and angular dependences were studied, as well as other effects such as surface temperature. Results have been published by Behrisch and Eckstein in a book entitled "Sputtering by Particle Bombardment" (publisher: Springer). He reported on new reflection coefficients, and new fit formula which need fewer fitting parameters than in work done by Thomas et al. These data provide a more accurate presentation than the previous work due to the larger calculated database.

Yu. V. Martynenko, Kurchatov Institute, Russian Federation

Dr. Martynenko presented the activities on A+M data at the Kurchatov Institute regarding A+M/PSI data generation (experiment, theory, codes) and the development of modelling codes for tokamak plasma processes. The "Data Access System (DAS)" project was described as a web resource for use in controlled fusion energy research (http://t10.fusion.ru), providing a database of measurements of various controlled nuclear fusion devices as well as graphics and calculation tools.

Giuseppe Mazzitelli, ENEA, Italy

Dr. Mazzitelli presented work done at ENEA on data for ionization balance evaluations of atoms and ions (Mattioli, Mazzitelli et al). Ionization data have been reviewed, compiled and evaluated for elements from H to Ge covering most ionization stages. Further work is in progress on Kr and Mb, to respond to the needs of fusion energy research. A full data set is available, including ionization as well as both Radiative and Dielectronic Recombination (Bryans et al.). Dr. Mazzetilli pointed out the strong need for data to analyze the FTU tungsten spectra – these data are crucial to simulate the W impurity transport in ITER and in many other devices (JET, ASDEX-U, FTU).

D. Kato, NIFS, Japan

Significant amounts of atomic data for Fe ions have been produced, compiled and evaluated to develop a non-equilibrium ionization model for fusion and solar plasmas. Measured spectra from the NIFS fusion device LHD were used to analyze and validate the model, which has been applied to solar spectra measured by the Hinode satellite for a better understanding of the coronal heating mechanism.

Dr. Kato presented results from different experiments and calculations on plasma surface interactions (PSI) at NIFS. Studies were carried out on hydrogen recycling at refractory metal surfaces, as well as on hydrogen retention in non-occluder metals.

NIFS has forged strong international collaborations through the DCN to produce, compile and evaluate A+M/PSI data for fusion energy research. Dr. Kato reviewed this collaboration and presented the new data inputs and new service developments on the NIFS web site (http://dbshino.nifs.ac.jp/).

D. Humbert, IAEA

Primary objectives of the Atomic and Molecular (A+M) Data Unit are to establish and maintain atomic and molecular databases relevant to controlled fusion research and related applications. These goals are fulfilled through Co-ordinated Research Projects (CRP), technical meetings (TM), consultancies and direct staff efforts. Data are disseminated through the A+M Data Unit web site (http://www-amdis.iaea.org) by means of database interfaces, search engines (GENIE), and on-line numerical codes.

Three CRPs are in their final phase of completion, with two APID volumes in press (CRP on "Data for molecular processes in edge plasmas" and "Atomic and molecular data for fusion diagnostics") and one in preparation (CRP on "Tritium inventory in fusion reactors"). Two CRPs were initiated in 2005: "Atomic and molecular data for plasma modelling" and "Atomic data for high-Z element impurities in fusion reactors". A first CRP meeting on "Data for surface composition dynamics relevant to erosion processes" will be held in October 2007.

Major improvements in the development of web tools and databases have taken place. The joint-project for OPEN-ADAS, initiated in September 2005, will allow free web access to most of the basic ADAS cross-section data. A first version of OPEN-ADAS is planned for release in 2008. GENIE is the web search engine for atomic data, and has recently been updated with the inclusion of the NIST database on "Electron impact cross sections for ionization and excitation". As well as excitation and ionization by electron impact, searches can now be requested for dielectronic recombination. New data are regularly added to the ALADDIN and AMBDAS databases, and the collisional data interface in ALADDIN underwent a major upgrade in 2006. The same upgrade is in progress for particle-surface interactions. A first version of the XML schema for atomic and molecular data (AMDML) is planned for June 2008. The calculation tools available from the A+M Data Unit web site have also been improved. Ionisation has been added to the cross-section calculational tool for heavy-particle collisions (http://ww-amdis.iaea.org/HEAVY/). The online LANL codes now include calculation of cross sections for ionisation processes (http://aphysics2.lanl.gov/tempweb/lanl/).

A. Whiteford, ADAS, UK

Dr. Whiteford reviewed of the Atomic Data and Analysis Structure (ADAS), highlighting interactive ADAS, callable ADAS, extended ADAS and offline ADAS. His talk subsequently focused on the ADAS database which underpins all of the other ADAS functionality. The size, scope and general structure of the database were discussed, and the distinction between fundamental and derived data in relation to ADAS was explained, along with examples of such data.

OPEN-ADAS is a web-based extension of ADAS, designed to allow free access to a large part of the ADAS database. Precise details of implementation were presented along with the proposed coverage. OPEN-ADAS will be launched in 2008, and the DCN made suggestions as to how this system might be improved in the run up to the launch.

Y. Rhee, KAERI, Republic of Korea

After a brief introduction to studies on atomic spectroscopy, Dr. Rhee reported on the results of applying the MCDF computer code to the calculation of dipole transition probabilities for tungsten ions with charge states ranging from +33 to +37, and to the calculation of electron impact ionization cross sections of W and W^+ (as well as Mo and Mo^+). Orbital parameters such as binding energies and occupation numbers were presented, along with transition probabilities between energy levels. These data are of high interest in fusion energy research. Atoms in high-temperature plasmas may be stripped from many electrons to become highly-charged. The spectroscopic characteristics of highly charged ions are not well known because elaborate relativistic theories of interacting electrons and nuclei are required and level-by-level transitions are difficult to study experimentally. Furthermore, the generation of high-temperature experimental environments to obtain highly-charged ions of a specific ionization stage is not easy in laboratories. High-temperature plasmas require devices such as nuclear fusion systems or EBIT machines. Tungsten has recently been regarded as a good candidate for a plasma-facing material in magnetic fusion devices, and more applications are planned in many facilities such as the ASDEX, ITER despite the strong radiative losses.

D. R. Shultz, CFADC, ORNL, USA

After giving an overview of the present organization of the Controlled Fusion Atomic Data Center (CFADC, http://www-cfadc.phy.ornl.gov/), Dr. Schultz described the important role of the CFADC in collecting, producing and disseminating data relevant to fusion energy research. The CFADC approach is to target and focus data production on the fusion research needs by answering fusion community requests (e.g. participation in IAEA CRPs, SciDAC projects). Dr. Schultz also mentioned the upgraded MIRF experimental facility which is used to address volume molecular processes in the cool/dense edge and divertor plasmas (hydrocarbon ions atom interactions, electronic collisions) as well as plasma-material interaction, wall erosion and tritium retention. The work of the SciDAC CPES (Center for Plasma Edge Simulation) was outlined.

K. Katsonis, GAPHYOR, LPGP, France

Collisional-Radiative (C-R) models are essential for optical diagnostics of plasmas which cannot be assumed to be in Local Thermodynamic Equilibrium (LTE). The principal activities of the GAPHYOR Data Centre are related to the calculation and evaluation of the atomic data necessary to apply these models to argon and xenon plasmas of various devices such as the WEGA Stellarator and SPT-50 prototype plasma thrusters. Dr Katsonis presented the results of his CR model, with special focus on atomic data calculations and evaluations. These data pertain to radiative and collision processes involving rare gas species, with emphasis placed on the study of low-ionized Ar and Xe species (I to IX). Benchmark data characterize the behaviour of the impurities encountered mainly in the plasma edge region (where the conditions may be comparable to those encountered in plasma thrusters), and occasionally in the core regions of fusion reactors. This work is the result of a collaborative effort with GAPHYOR, the IAEA AMD Unit and the LUTH Laboratory of the Observatory of Paris, and is part of the IAEA CRP on "Atomic data for heavy element impurities in fusion reactors".

W. Wiese, NIST, USA

During the course of 2006 to 2007, the NIST Atomic Spectroscopy Data Center (http://physics.nist.gov/PhysRefData/) completed a number of critical data compilations and initiated several new ones. Tabulations of energy levels and wavelengths have been completed for Be II, Ne II, III, VII, VIII, Ga, Rb, Xe, Ba I, II, W and Kr. Tabulations and critical assessments of transition probabilities were completed for all spectra of Na, Mg, Al, Si, Cl I, Ne II-IV, Fe I-II, C I-II and N I-II. These data have been incorporated into the Atomic Spectra Database (ASD) which is now defined as version 3.1.3. Major data compilations are in press or nearing completion. A new unified bibliographic database is available for wavelengths, energy levels, transition probabilities and line shapes.

T. Nakano, JAEA, Japan

JAEA (Japan Atomic Energy Agency) staff have been producing, collecting and compiling cross-section data for atomic and molecular collisions and spectral data relevant to fusion research. Electron capture and the electron loss cross-section data of singly-ionized tungsten by collision with H_2, He, Ne, Ar and Kr were measured at collision energies of 40.8 and 54.3 eV/amu. Relative cross-section data of the X-ray emission from Ne-like tungsten (W^{64+}) through di-electronic recombination have been measured in an electron beam ion trap (EBIT) [1]. The state selective charge transfer cross-section data of Be^{3+} and C^{6+} by collision with H* (n = 1, 2) in the collision energy range between 62 eV/amu and 6.2 keV/amu have been calculated with a molecular-bases close-coupling method. Cross-section data for 47 collision processes of He, He^+ and He^{2+} with H, H_2, He, He^+ and Li have been complied. Recommended cross-section data are represented by analytic functions to facilitate the practical use of the data. Compiled data are in preparation for the web at URL http://www-jt60.naka.jaea.go.jp/engish/JEAMDL/. Charge transfer data published in 2005 and 2006 have been collected, and the database for the chemical sputtering yield data of graphite materials with hydrogen isotope collisions has been established.

The atomic and molecular data activities in JAEA are pursued in collaboration with NIST, Japanese universities, and another department of JAEA.

Reference

[1] Watanabe H., Nakamura N., *et al*., *Plasma Fusion Res*., **2** 027 (2007).
The Japan Atomic Energy Agency (JAEA) and Japan Nuclear Cycle Development Institute (JNC) – have been merged into a new independent agency named the Japan Atomic Energy

Jun Yan, CRAAMD, China

Dr. Jun Yan presented the activities of the China Research Association of Atomic and Molecular Data (CRAAMD) over the previous two years. Activities include data collection, calculations and measurements. Dr. Yan detailed experimental results on heavy-particle collisions, as well as inner

shell ionization by electron impacts. Molecular ionization potential and vibrational ionization energies have been calculated for a wide range of molecules and their ions. Energy levels, oscillator strengths and electron impact collision strengths have been determined for Ni-like ions (Gd, Ta, and W). Dr. Jun Yan also mentioned the next ICAMDATA conference which will be held in Beijing, China, on 28-31 October 2008.

2.2 Specialized Presentations of General Interest for Controlled Fusion Energy Research

During a meeting in October 2003, the DCN committee recommended the inclusion of presentations of general interest for controlled fusion energy research. Thus, a presentation on molecular data needs in fusion energy research was made in 2005. This year an ITER representative was invited to participate, and a presentation was also made on the new developments of the XML schema for AM/PSI data.

D. Kato: "AM/PSI Data Needs for ITER"

Dr. Kato presented two joint talks prepared by the ITER international team: "Atomic, Molecular and Surface Data Needs for ITER Modelling" and "Atomic and Molecular Processes in ITER". There is a strong need for AM/PSI data, with a special focus on tungsten, in order to attain a better understanding of the plasma behaviour in the core and divertor region. Data for plasma edge modelling requires special attention, and dust formation is expected in the ITER vessel. Dust characterization and formation mechanisms, in which AM/PSI processes play an important role, need to be better understood.

Yuri Ralchenko: "XML and AM/PSI Data Exchange"

Dr. Ralchenko was invited to present the new developments of the XML scheme for Atomic and Molecular data (AMDML). The development of AMDML is based on the eXtensible Markup Language (XML). This work was initiated by the DCN during a meeting in October 2003, and is supported by the IAEA, NIST, ORNL, JAEA, KAERI and Observatoire de Paris-Meudon. Dr. Ralchenko pointed out the advantages of using XML as a new standard for exchanging atomic and molecular data. A special session was organized on this topic at the last ICAMDATA, October 2005, in Paris. AMDML needs to be opened to a larger audience in order to be successful. Contribution from the Data Centres, such as adding AMDML to the DCN databases, would be welcome. The next step is to release the first version of the XML schema by the end of June 2008. A special session will be devoted to XML at the next ICAMDATA in China, October 2008.

3. Data Issues

3.1 Priorities in A+M Data Compilation, Evaluation and Exchange for Fusion

A new agreed list of A+M data priorities was generated by removing data needs that have been fulfilled, keeping those that require more work and adding new data requirements. Some merging and splitting of collision categories took place, along with the elimination of previous needs now deemed to be redundant or irrelevant. The adjusted and updated data priorities are summarized in Annex 3, and are available on the A+M Data Unit web site (http://www-amdis.iaea.org/DCN/fusion_data.php). The DCN recognizes a need for more expertise in molecular data, and recommends inviting specialists in this field to future meetings. Agreement was made to add the word "exchange" to the wording of the title.

3.2 Data Evaluation

The topic of data evaluation was addressed. Only NIST is strongly active in data evaluation, which has been a difficult task to perform due to the increase of available data and important emerging data needs. Evaluation is very time consuming activity, for which most of data centres lack resources.

A further recommendation would be to provide estimated accuracy (uncertainties, and error bars) when possible. Traceability of the data should also be mandatory.

3.3 Data for the International Bulletin on Atomic and Molecular Data for Fusion

The list of contributors to the International Bulletin on Atomic and Molecular Data for Fusion has been reviewed.

4. DCN Membership

The topic of membership in the DCN was thoroughly discussed. At the present time no reference exists regarding the specific roles and activities that a data centre should fulfill as a member of the DCN. No decision was taken regarding the "Terms of Reference for the AM/PSI DCN", as proposed during the last meeting. Members agreed to evaluate their contribution to fusion energy research, and to focus their talk for the next meeting on data activities relevant to fusion.

A number of Member States that are not represented in the DCN have significant interest in AM/PSI data related to fusion. ADAS was invited to attend this year, and is foreseen to be a new member contributing by means of OPEN-ADAS. Dr. Whiteford will raise the matter at the next ADAS steering committee meeting. Other Member States should be identified and invited to DCN meetings as observers for mutual benefit. A lack of molecular expertise has also been noted.

Brazil membership was not discussed due to the absence of Dr. Machado.

Term of reference for the AM/PSI DCN

Domain: Atomic and molecular physics and particle surface interactions (AM/PSI). Data should be strongly relevant to fusion.

Established programs:

- Collection of data
- Dissemination of data
- Calculation and/or measurement of data
- Assessment/evaluation of data, with the description of the process used

5. Data Centres – WWW and Software Presentations

This session gave the opportunity for participants to demonstrate new tools, interfaces or databases developed by the data centres available on the web.

ENEA, Dr. Mazzitelli

Dr. Mazzitelli presented details of new data (ionization, radiative recombination and ielectronic recombination rates) available online from the CHIANTI database (http://hea-www.harvard.edu).

CRAAMD, Dr. Jun Yan

Dr. Jun Yan presented developments on the CRAAMD web site (http://www.camdb.ac.cn/e/). He focused specially on the new electron-molecule collision database. Data available include elastic and inelastic differential cross-sections, optical oscillator strength and generalized oscillator strength.

ADAS, Dr. Whiteford

Dr. Whiteford presented a test version of OPEN-ADAS, which is a web-based extension of ADAS designed to allow free access to a large part of the ADAS database.

NIST, Dr. Ralchenko

NIST provides several online computational tools in conjunction with a large numbers of databases (http://physics.nist.gov/PhysRefData/). Dr. Ralchenko presented the plasma kinetics SAHA (NLTE3) and NLTE4 databases which contain benchmark results for the simulation of plasma population kinetics and emission spectra, as obtained from contribution of participants in the Non-LTE Code Comparison Workshops. FLYCHK was demonstrated which constitutes an online collisional radiative model where steady state and time dependent calculations for elements from H to Au can be performed. Dr. Ralchenko also showed an example of access to spectral line databases using IVOA standards: SLAP (Simple Line Access Protocol) and the XML Spectral Line Data Model.

6 Conclusions and Recommendations

6.1 Status of Data Generation and Priorities in Data Compilation and Evaluation

- Some of the data needs and priorities from the request list of the 18th meeting are still valid. A number of the data needs have now been satisfied, and some new data priorities have been identified. Active and proposed CRPs are well positioned to address a wide range of these data needs. The current list of data priorities is summarized in Annex 3 and is available on the A+M Data Unit webserver: http://www-amdis.iaea.org/DCN/fusion_data.php.

- IAEA technical meetings, consultants' meetings, coordinated research programmes and individual consultancies make a significant contribution to both the data evaluation and quality control effort. All resulting A+M data are assembled and introduced into the ALADDIN database of the A+M Data Unit as soon as they become available.

- Over the past two years, use of short-term consultancies (several from within the Data Centre Network) in collaboration with staff efforts within the Data Unit have proven effective in addressing systems and software (ALADDIN, AMBDAS) problems.

6.2 Data Processing and Exchange

- All A+M Data Centres that maintain web sites have been very effective in delivering their data. Many of the data centres are ready to use the new exchange format in XML (AMDML) as presented by Yuri Ralchenko, when available. The first version of the XML format for AM/PSI data will be released in June 2008; results will be presented at the next ICAMDATA in China, October 2008.

- Requests on GENIE have been continuously increasing, as shown in the monthly statistics sent to the DCN members and the databases managers. GENIE is evolving in order to search new databases on the web, based on collaboration and communication between the data centres and the A+M Data Unit. The scope of GENIE should be enlarged to encompass more processes and molecular data.

6.3 Membership Status

L. Machado could not attend this meeting to present the BRAMPDAC activities regarding A+M data for fusion. The membership of Brazil will be reviewed at the next meeting. ADAS has also been invited to make a proposal to join the DCN.

6.4 Consultancies and Next Meeting

The DCN agreed to keep the meeting length at three days, and strongly recommends that data centre presentations should focus only on new issues related to fusion. Forty-five minutes was judged to be too long to present the activities of the data centres; durations of thirty minutes each would be more appropriate.

The DCN will continue to recommend specialists to present topics of immediate interest to the fusion community. An ITER representative was invited to the present meeting, as well as one expert on XML. A recommendation was made to invite another representative of ITER to the next meeting. The DCN does not contain expertise in molecular data, and therefore such a specialist or a representative of a data centre dealing with molecular data should be invited to the next DCN.

Annex 1

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (19th Meeting of the A+M Data Centres and ALADDIN Network)

3–5 October 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

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Annex 2

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (19th Meeting of the A+M Data Centres and ALADDIN Network)

3–5 October 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

Meeting Agenda

Wednesday, 3 October **Meeting Room: A27-74**

09:30 – 09:45	Opening (R.E.H. Clark, Head, A+M Data Unit, A. Nichols, Section Head, Division of Physical and Chemical Sciences, NAPC) Adoption of Agenda
Session 1:	Current Activities of the A+M Data Centres
Chairman:	J. Yan
09:45 – 10:30	W. Eckstein (MPIP)
10:30 – 11:00	***Coffee break***
11:00 – 11:45	Yu.V. Martynenko (Kurchatov Institute)
11:45 – 12:30	G. Mazzitelli (ENEA)
12:30 – 14:00	***Lunch***
Session 2:	Current Activities of the A+M Data Centres (Continued)
Chairman:	Y. Rhee
14:00 – 14:45	D. Kato (NIFS)
14:45 – 15:30	D. Humbert (IAEA)
15:30 – 16:00	***Coffee break***
16:00 – 16:45	A. Whiteford (ADAS)

Thursday, 4 October

Session 3:	Current Activities of the A+M Data Centres (Continued)
Chairman:	W. Eckstein
9:00 – 9:45	D.R. Schultz (ORNL)
9:45 - 10:30	Y. Rhee (KAERI)
10:30 – 11:00	***Coffee break***
11:00 – 11:45	K. Katsonis (GAPHYOR)
11:45 – 12:30	W.L. Wiese (NIST)

12:30 – 14:00	***Lunch***	
Session 4:	Current Activities of the A+M Data Centres (Continued)	
Chairman:	K. Katsonis	
14:00 – 14:45	T. Nakano (JAEA)	
14:45 – 15:30	J. Yan (CRAAMD)	
15:30 - 16:00	***Coffee break***	
16:00 – 16:45	D. Kato	"ITER AM/PSI Data Needs"
16:45 – 17:15	Yu. Ralchenko (NIST)	"XML Format for A+M Data"

Friday, 5 October

Session 5:	Data Issues
Chairman:	W. Wiese
9:00 – 10:45	Priorities in A+M data compilation (all participants) Data evaluation (all participants) Data for the Int. Bulletin on Atomic and Molecular Data for Fusion
10:45 – 11:15	***Coffee break***
Session 6:	DCN Issues
Chairmen:	R.E.H. Clark and D. Humbert
11:15 – 12:45	Review of Data Center Network Membership criteria Membership of Brazil and ADAS Plan of DCN activities for the near future ICAMDATA
12:45 – 14:00	***Lunch***
Session 7:	Demonstrations
14:00 – 15:30	Data Centre WWW and software demonstrations
15:30 – 16:00	***Coffee break***
Session 8:	Meeting Conclusions and Recommendations
Chairman:	D. Humbert
16:00 – 17:00	Formulation of meeting conclusions and recommendations Date of next meeting
17:00 –	*Adjourn of the Meeting*

Annex 3

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (19th Meeting of the A+M Data Centres and ALADDIN Network)

3–5 October 2007, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

Summary of Priorities in Data Compilation, Evaluation, Generation and Exchange for Fusion Energy Research

The long-term priorities in A+M and PMI data needs for fusion energy research are regularly reviewed during the IAEA Data Centre Network (DCN) Meeting on "Technical Aspects of A+M Data Processing and Exchange". The DCN also supports the development of a new standard for AM/PMI data exchange based on XML, as reliable and convenient tools for data exchange are essential with the development of Internet Technologies. The last DCN meeting was held in October 3-5, 2007 in the IAEA Headquarters in Vienna.

Atomic and Molecular Data

Spectroscopic Data

- Transition probabilities for Be and its ions are needed, as well as data for heavy elements like Fe, Cl, Mo and Cu.
- Transition probabilities for Na, Mg, Al, and Si are done for all ionization stages at the NIST Data Center for Atomic Spectroscopy. Data compilations for H, D,T, He, Li, Be, B, Ne, S, and Cs have been initiated.
- Energy levels, wavelengths, transition probabilities for metallic ions and high-Z impurities are needed.
  - W: compilation of some structure data (ionization energies, low lying energy levels etc.) is complete for all ionization stages of W. More detailed data are needed for most ionization stages.
  - Xe, Kr and Ar: There are urgent needs of data production for high ionization stages. First compilations for Kr and Xe have been completed, but they are rather incomplete. Argon is of interest for further work.
  - Data for Hf and Ta are identified as of importance.
- Complete spectroscopic characterizations of heavy noble gas ions are needed. Only Ne is in good shape.
- The DCN will enhance its expertise to address spectroscopic molecular data priorities. Some of the following data, where needs are identified, may already be available in some molecular databases.
  - Spectroscopic characterization of H_2, H_2*, H_2^+, H_3^+ and isotopic variants.
  - Impurity plasma edge molecules: CO, CO_2, CH_4, CH, C_2, BeH, BH, N_2, LiH, CsH and other hydrocarbons and radicals, including hydrogen isotopic variants.

Collisional Data for Plasma Edge Studies

This section includes neutral particle transport modeling and diagnostics, H-recycling and He-exhaust. All the molecular data are needed for different hydrogen isotopes, including mixed molecules like DT.

- Elastic collisions, charge transfer, inelastic collisions of H, H_2, H^+, H_2^+, H_3^+ with H_2 at low and intermediate energies (0 to 10 keV)
- H^- + H, H_2 (e.g. detachment, excitation, dissociation)

- Regarding interaction of the neutral beam with the plasma, collisions involving H* are of importance.
- Electronic excitation and ionization of vibrationally excited $H_2^*(v)$ and $H_2^+(v)$ in low-energy collisions with e (including dissociative processes and information on energy distribution of reaction products). The NIFS-DATA-73 and the APID vol. 13 (CRP on "Molecular Processes in Fusion Plasmas") are covering a significant part of these needs, as cross sections for H_2^+ and the rate coefficients for dissociation of $H_2^*(v)$. The CRP on "Atomic and Molecular Data for Plasma Modelling" also addresses this topic.

The two next items are largely addressed by CRPs (CRP on "Molecular Processes in Fusion Plasmas" and CRP on "Atomic and Molecular Data for Plasma Modelling") and other research efforts:

- Inelastic electronic collision processes of He, He^+, He^{2+} and excited states of H, He and H_2 at low energies.
- Inelastic collision processes of He, He^+ and He^{2+} with H, H^+, H_2, H_2^+ at low energies, including processes with excited H, He and H_2.

Despite considerable progress made in CRP work, there continues to be a need for data production and evaluation for collisional data for all hydrocarbons relevant to fusion devices:

- Further development of the databases for hydrocarbons, H_2O and CO, and Be-, B- oxides and hydrides (including their ions).
- For hydrocarbons, all processes with electrons and protons should be considered including vibrational excitation.
- Particle interchange reactions among primary species, C, O, metals and hydrocarbons. Some data are published in APID 13 on "Molecular Processes in Fusion Plasmas" and NIFS and FZ Julich Reports on hydrocarbons
- There is much interest in CH excitation and a need for state resolved data.

Collision processes of high-Z impurities. CRP on "Atomic Data for Heavy Element Impurities in Fusion Reactors" is addressing some of these issues, concentrating on W and the noble gases.
Data are needed in priority order for collisions of W, Mo, V, Ar, Kr, Xe with e, H^+, H, H_2.
Theoretical work on ionization per photon emission is needed to measure the neutral W influx.

From previous data priority lists, the following data needs have been addressed. Existing databases appear to be sufficient at this time and no new requests have been made recently:

- Elastic and momentum transfer ion-neutral and neutral-neutral collisions in the energy range 0.1 eV - 1 keV/amu, involving H, H^+, He, He^+, He^{2+}, H_2 and H_2^+.
- Ro-vibrational electronic excitation and attachment for D_2, T_2, DT.
- Completion of collisional databases for Be, B and their ions. It includes collision processes of Be^{q+}, B^{q+} with electrons, and quasi-resonant processes of Be^{q+}, B^{q+} with H, He and H_2.

Collisional Data for Neutral Particle Beam Heating

- Data for collision processes of the ions H_2^+, H_3^+ with e, H, H^+, H_2, H_2^+, He^{2+} from threshold to 1 keV.
- Data for collisional processes H^- on (H^-, e, H, H_2, H_2^+) in ion beam used (after neutralization) for plasma heating. (Pertinent energy range: from threshold to 150 keV). Data are needed for loss mechanisms in beams, including stripping.
- Charge loss for $H^- + H^-$ collisions at energies from 0 to 20 eV
- Data needed for elastic collisions between negative hydrogen and neutral molecule

Collisional Processes Related to Radiative Plasma

These data are important for determination of ionization balance and radiation losses. It would be very useful to formulate updated and new tables of cooling rates.

- **Plasma core region**

Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (Ti, V, Ni, Cr, Fe, Mo, W). Pertinent temperature range is from 100 eV to 30 keV. A large amount of data exists for Ti and Fe, but dielectronic recombination rate coefficients are not adequate for L-shell and M-shell ions even for Fe. The CRP on "Atomic Data for Heavy Element Impurities in Fusion Reactors" is addressing some of these issues. Current priorities are for W and noble gases.

- **Plasma edge region**

Data are needed for edge temperature (threshold to 500eV) charge exchange processes among intrinsic impurities and plasma components:

- collisions of X^{q+} (X = Cl, Ti, Ni, Cr, Fe, Mo, W, V) with H, H^+ and He^{2+}
- collisions of X^{q+} (q >= 5, X as above) with H, He, H_2, including state selective electron capture

Data are needed for all processes of N, N_2, Kr, Ne, Ar and Xe with e, H, H^+, H_2, H_2^+, He^+, He^{2+} and H^- (for the proposed radiative cooling scheme of divertors and radiative mantle).

Plasma-Material Interaction

Erosion

- Assessment of data needed for Be, carbon-based materials and medium- and high-Z materials (Ti, V, Mo, Nb, W, BeO). Data for physical sputtering yields are known. Energy dependence at normal incidence is satisfactory. Data for angle dependence is not as complete as for normal incidence. Data on sputtered energy (to allow the determination of the mean energy of sputtered atoms) also exist but have not been fitted, and not yet included in database. This can be done through consultancy.
- Data needed for mixed materials arising from Be, C and W.
- Need exists for chemical sputtering for carbon based materials. This can be addressed by the upcoming CRP on "Data for Surface Composition Dynamics Relevant to Erosion Processes".
- Investigation of erosion and target properties data for materials involved in ELMs and disruptions is important. Data will come more likely from plasma experiments, not from CRPs or DCN.

Hydrogen isotope and reflection, retention and release in fusion materials and codeposited layers

- H/D/T permeability, diffusivity, solubility, desorption rate and surface reactions. Materials of interest are W, Be, BeO, Mo, new CFC's, deposited and codeposited layers of these materials. Data on traps in materials. The CRP on "Tritium Inventory in Fusion Reactors" addressed much of this for Be, C and W.
- Angular and energy distribution of H, D, H^-, D^- scattering on surface (particularly on C) at glancing angles from 0 to 10^0 and energy from 50 keV to 1 MeV
- Charge state as well as electronic and ro-vibrational (molecular) states for reflected and sputtered particles may be important. Many data are now available for reflection of hydrogen isotopes as well as others such as noble gases, in the energy range of 10 eV – 100 keV.
- Mean range of impinging particles (and deposition profiles) are important to give information on the disturbed target region. Data can be made available for higher (>10eV) but data production is needed for kinetic processes for low energy (dependent on material temperature and properties).

Molecular Balance on Surfaces

There is a strong need of data in this area, emphasizing inclusion of molecular vibration in the initial state:

- Molecule and molecular ion formation and destruction with identification of product charge and quantum state.
- Data for hydrocarbons and H^- formation on surfaces, particle sticking, pumping, gettering, and recycling.

Material Properties

Data collection and generation are needed, but are difficult to address within CRPs and DCN:

- Data for dust formation from C, Be, W, Mo. A CRP will start in 2008 on dust formation and characterization.
- Mobilization of particles. Good diagnostics will be important.
- Gas bubble formation in wall material from protons and alpha particles formed by neutron reactions and directly from fusion plasma implantation.

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