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Summary Report of

IAEA Technical Meeting

Technical Aspects of Atomic and Molecular Data Processing and Exchange – 18th Meeting of the A+M Data Centres and ALADDIN Network

Prepared by

Denis Humbert

IAEA Headquarters, Vienna, Austria

10-11 October 2005

IAEA Nuclear Data Section, Wagramer Strasse 5, A-1400 Vienna, Austria

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Abstract

The IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange - 18th Meeting of A+M Data Centres and ALADDIN Network" was held on 10-11 October 2005, in Vienna, Austria. The discussions and presentations focused on the priorities in A+M data compilation and evaluation, and are summarized in this report. Conclusions and recommendations on the technical aspects of data processing, exchange and distribution are also presented.

January 2006

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1. Introduction

On 10-11 October, 2005, the biennial Technical Meeting was held to discuss "Technical Aspects of Atomic and Molecular Data Exchange and Processing - 18th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network". The objectives were to review the progress in A+M data related activities within the data centre network, the methods and procedures applied in the processing and exchange of data, and to coordinate the working plans for 2005-07.

Seventeen participants attended the meeting. All Data Centres were represented, except for KAERI. Representatives from each data centre presented a progress report on their current activities related to nuclear-controlled fusion. A report on KAERI activities had been prepared by Dr. Y. Rhee, and was distributed to the participants for information. The Network welcomed two new data center representatives: Dr. D. Kato representing NIFS (in place of Dr. T. Kato) and Dr. Jum Yan, the new representative of CRAAMD in Beijing, PRChina (replacing Dr. S. Yongsheng (retired)). Dr. L. Machado (Universidade Federal de Sao Carlos, Dpt de Fisica) also attended, and presented a proposal to establish a new data centre in Brazil to focus on atomic and molecular data for fusion (BRAMPDAC).

Dr. Yuri Ralchenko (NIST) and Dr. U. Fantz (Augsburg University), as specialist in data exchange and web databases tools and in molecular data needs for fusion, respectively, were invited to give presentations. Dr K. Katsonis (LPGP, University of Paris XI) attended the meeting as an observer, and presented his work on atomic data inside LPGP and the GAPHYOR data centre. The Agency was represented by Dr. A.L. Nichols, Dr. R.E.H. Clark, Dr. D. Humbert and Dr. A. Malaquias.

The full list of participants and data centres is available in Appendix 1.

2. Meeting Proceedings

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 AGM to the Data Centre Network. Knowledgeable consideration would be given to all new relevant developments that have occurred since the 17th AGM held in October 2003, and their advice would aid considerably in the network policies of the A+M Data Unit.

By adopting the proposed Agenda (Appendix 2), the meeting agreed to cover the following topics:

- current activities of the A+M data centres,
- data issues: molecular data needs, XML, priorities in data compilation for fusion,
- interfaces and web tools,
- membership status,
- conclusions and recommendations of the meeting.

2.1. Current activities of the A+M data centres

Progress reports were presented on the activities of individual data centres for the period October 2003 - September 2005. The main focus was atomic and molecular data of relevance

to fusion, including data compilation, evaluation and generation, WWW developments, data centre publications produced during the reporting period, and the status of on-going data centre programmes and plans for future work. These various presentations indicated that data centre activities followed the recommendations of the previous Advisory Group Meeting, both in terms of content and mutual cooperation. These reports are available on the A+M Data Unit web site: http://www-amdis.iaea.org/

Dr. Y. Rhee, KAERI:

Unfortunately, Dr. Rhee could not attend the meeting - his report on "Progresses of AMODS Databases in KAERI and Electron Impact Ionization Cross Sections" was distributed for information.

Dr. W. Wiese, NIST:

During the 2004 to 2005 period, the NIST Atomic Spectroscopy Data Center completed a number of critical data compilations and initiated several new ones. Tabulations of energy levels and wavelengths have been completed for Ar, Ga, Rb and Xe (always for all stages of ionization) and for Be II, Ne II and III, Ba I and II, and W I and II. Tabulations and critical assessments of transition probabilities were completed for all spectra of Na, Mg, Al and Si, and for Ne II to Ne IV and Fe I and II. Many of these compilations are much larger and of better quality than earlier NIST tables. They have been or soon will be incorporated into the principal Atomic Spectra Database (ASD) at NIST. Major projects are now in progress on other noble gas spectra, on the very light elements H to B, on S and Cl and on all of the 74 spectra of W. The NIST bibliographies are also constantly updated.

Dr. D. Kato, NIFS:

After presenting the new NIFS organization and the different bibliographical, numerical and graphics databases accessible through the NIFS web site (http://dbshino.nifs.ac.jp/), Dr. Kato reported on recent work at the A+M Data Research Center, consisting of data activities (compilation, evaluation and production), research and collaboration programmes, data publications (NIFS-DATA Series) and future plans.

Important work on data compilation has been published, and data incorporated into the NIFS databases (electron impact cross section, heavy-particle collisions and photon collisions, covering a wide range of atoms and molecules such as hydrocarbons, H_2O, H_2, D_2, O_2, N_2, CO, CO_2 and Ar). Cross sections have been evaluated for collisions of the hydrogen atom with ions: Li^{3+} (excitation, ionization and charge exchange) and carbon ions (charge exchange), as well for electron collisions with carbon atom and ions.

Many calculations and measurements have been performed, including:

- calculations of energy levels, radiative transition probabilities, and autoionization rates for boron- and carbon-like oxygen,
- measurements of absolute multi-electron transfer cross sections for I^{q+} (q = 10, 15, 20, 25) collision with Ne, Ar, Kr and Xe,
- numerical data on sputtering yield, reflection coefficients and mean range,
- theoretical and experimental determination of electron-capture cross sections of H^+ and O^+ collision with H_2, D_2 and hydrocarbons,

- calculations of cross sections for dissociative attachment, associative detachment and vibrational excitation of H(D)F, H(D)Cl, H(D)Br and H(D)I by electron impact.

NIFS also hosted the 4th ICAMDATA conference in 2004.

Dr. D. R. Shultz, CFADC, ORNL:

After providing an overview of the present organization of the Controlled Fusion Atomic Data Center (CFADC, http://www-cfadc.phy.ornl.gov/), Dr. Schultz described the natures of the important work done in data collection and production. Bibliographical data are regularly updated, and data related to fusion are sent to the A+M Data Unit. The CFADC answers direct requests from the fusion and plasma communities for data collection and production. A wide range of collected and evaluated data and collisional-radiative model software are made available through the CFADC web site (e.g., ADAS, MIRF data and Redbooks). Recently produced data include elastic scattering for transport modelling and diagnostics, a collisional database for molecular hydrogen, and data on chemical sputtering.

CFADC organized the workshop on "New Directions for Advanced Computer Simulations and Experiments in Fusion-Related Plasma-Surface Interactions" (PSIF), ORNL, Oak Ridge, Tennessee, March 2005. The center is also involved in projects such as the "Edge Coordinating Committee" (ECC) (www.mfescience.org/ecc) and the "US DOE Fusion Simulation Project". ECC co-ordinates advanced US fusion science through technical assessment, prioritization and coordination of edge plasma theory and modelling in close partnership with national experimental groups and international fusion programmes. The US DOE Fusion Simulation Project focuses on comprehensive edge plasma simulation ranging from the AM and PSI processes to particle transport and edge plasma phenomena simulation, including code integration, performance, validation and verification.

The upgrade of the ORNL Atomic Physics Facility (Multicharged Ion Research Facility (MIRF)) allows new particle-surface experiments, ion-atom and electron-ion collisions with higher and lower collision energies and improved fragment detection in order to study electron-molecular ion collisions.

Dr. Yum Yan, CRAMMD:

The activities of the China Research Association of Atomic and Molecular Data (CRAAMD) over the previous two years were presented, including data collection, calculation, measurement and assessment. Dr. Dong's group in Northwest Normal University have collected and calculated the energy levels and radiative transition properties for Ne- ($Z = 21 - 92$) and Ni-like ($Z = 31 - 92$) ions. These calculations were based on the MCDF method in which a large amount of basis states are included to take into account the electron correlation and relaxation effects. Dr. Chen's group (Fudan University) have calculated the electron impact ionization cross section and rate coefficients based on the relativistic distorted-wave Born approximation, with exchange within the framework of the configuration average. Dr. Qu's group (Graduate School of China Academy of Science) collected the charge transfer data for ion-molecules and ion-atom collision. Dr. Zhu's group (Science and Technology, University of China) collected and evaluated the elastic scattering data for electrons colliding with NF_3, SiH_4, C_2F_6, CF_3Br, C_2H_6, N_2, NO, H_2, O_2, Cl_2, HF and HCl molecules; inelastic excitation data of electron colliding with C_2H_6, N_2, NO, H_2, O_2, HCl and HF molecules, as well as the optical oscillator strength of N_2, NO, H_2, O_2, HCl and the generalized oscillator strength of N_2 and O_2. Dr. Mo's group (Tsinghua University) is collecting and evaluating

molecular ionization potential and vibrational energy level data of molecular ions that have been measured by the high resolution zero electron kinetic energy (ZEKE) photoelectron spectroscopy since 1984. Dr. Ding's group (Jilin University) is preparing a number of general Web pages to describe the molecular structure and processes with some typical data. Dr. Yuan's group (National University of Defense Technology) has calculated energy levels and radiative transition properties as well as the opacity of low-Z and several moderate- and high-Z (such as Br, Fe, Nb and Au) in local thermodynamic equilibrium (LTE) plasmas using the detailed term accounting (DTA) model. The related code developments for on-line calculation of the DTA opacity are also in progress. Besides integrating the data provided by the above mentioned groups and adding these data to the database (http://www.camdb.ac.cn/), a significant amount of data collection, calculation and assessment has been undertaken, for example:

electron impact ionization cross section of O-like ions;
systemic data (including energy levels, radiative transitions and electron collision processes) H-, He- and Li-like Argon ions; and
electron impact ionization and dissociation with H_2O, H_2, N_2 and O_2.

Data applications work was also carried out, such as identifying the lines of astrophysical transmission spectra, the diagnostic of emission spectra measured in inertial fusion energy experiments, and the calculation and comparison of the emission spectra of non-LTE plasmas. Last May, two of the databases were included in GENIE, the IAEA Web search engine for atomic data.

This work is supported by the CODATA Chinese Physical and Chemical Database Project, Chinese Research Association of Atomic and Molecular Data, National Science Foundation of China, National High-Tech ICF Committee of China, and Science and Technology Funds of CAEP.

Mr. D. Humbert, IAEA:

The 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 meeting, individual consultancies and staff efforts. Data are disseminated through the A+M Data Unit web site (http://www-amdis.iaea.org) using database interfaces, search engines (GENIE), and on-line numerical codes. All generated and evaluated data are published in issues of the APID series.

The policy is to maintain three active CRPs at any one time. Two CRPs are in their final phase of completion, with two APID volumes to be published: "Data for molecular processes in edge plasmas" and "Atomic and molecular data for fusion diagnostics"; while two further CRPs were initiated in 2005: "Atomic and molecular data for plasma modelling" and "Atomic data for high-Z element impurities in fusion reactors". A CRP on "Plasma surface interactions" will begin in 2006. The CRP on "Tritium inventory" will hold a final Research Coordination Meeting (RCM) in 2006.

A Technical Meeting on "Establishment of A+M computer code network (CCN)" was held during May 2005 in Vienna. The aim of assembling this network of institutes is to provide cost-free computational capabilities in the A+M areas relevant to fusion energy research.

During the course of September 2005, both the ADAS Steering Committee and the A+M Data Unit approved a joint-project for an "OPEN-ADAS" for atomic data.

The current version of GENIE includes searches of eight databases for atomic spectral properties and three databases for ionisation and excitation cross sections by electron impact. The scope of GENIE will be extended more towards processes and molecular data in 2006.

Two new numerical codes are available on-line (Section 2.2.3.).
New data are regularly added to the ALADDIN and AMBDAS databases, and their interface is updated. ALADDIN will have a major upgrade in 2006 (Section 2.2.3.). An XML schema for atomic and molecular data (AMDML) is also under development (Section 2.2.1.).

Dr. Yu. V. Martynenko, Kurchatov Institute:

Dr. Martynenko described different results for measured and calculated cross sections in ion-atom and ion-ion collisions (electron loss cross sections by negative hydrogen ions in their mutual collisions, and the interaction of highly-excited atoms with slow neutral atoms and ions), as well as particle-surface interaction data (tungsten sputtering at high temperature, hydrogen effect on metallic surface properties, and graphite submicron particle thermal radiation).

Two projects have been initiated to develop a computer code for Tokamak plasma processes. The Simplified Universal Numerical Code for atomic kinetics (SUNC) is a fast universal numerical code for the calculation of the radiative losses and the spectral line intensities over a wide range of plasma parameters and ion charges. A project entitled "Complex computer modeling of modern tokamak plasma processes" brings together the existing Russian codes for high temperature plasma in magnetic systems. This project will include new initiatives such as the "joint code for edge plasma" – a modelling code for the plasma edge region including convective transport across the magnetic field, atomic kinetic and radiation losses, and plasma surface interactions.

Dr. W. Eckstein, Max-Planck Institut fur Plasmaphysik, Garching:

Calculated atomic data were presented: energy levels of elements from Z = 1 to 82 of all charge states. Furthermore, new calculated values of sputtering yields, reflection coefficients, and penetration for many elements were discussed, including energy dependences and a few angular dependences. All data are available from the Max-Plank Institut fur Plasmaphysics using an anonymous secure ftp connection.

Dr L. Machado, Universidade Federal de Sao Paolo:

Dr. Machado presented details of the main objectives of the new Brazilian Atomic, Molecular and Plasma Physics Data Center (BRAMPDAC). BRAMPDAC will promote the Brazilian scientific and technological efforts related to the production of atomic, molecular and plasma physics data of interest to nuclear fusion research, provide easy access to the data via the WWW, and stimulate data exchange and collaboration between the Brazilian atomic, molecular and plasma physics communities.

Research efforts devoted to atomic and molecular physics of interest to fusion are important in Brazil, and Dr. Machado described some available data and on-going projects:

spectroscopic data for atoms (energy levels, transition rates) and molecules (energy levels, rotational, vibrational, ionization and dissociation parameters, transition rates);
electronic collisional with atoms, ions and molecules;
heavy-particle collisions (elastic, rotational, vibrational and electronic excitation, ionization and dissociation cross sections), and
plasma characterization (data on particle densities and local temperatures).

More than 1000 electronic data files have been catalogued and stored, and BRAMPDAC is now preparing the Web site. Databases and the Web interface to the data will be developped in collaboration with the A+M Data Unit of the IAEA.

Dr. E. Menapace, ENEA:

Dr. Menapace presented the contributions of the various Italian research institutes to the production of atomic and molecular data relevant to nuclear fusion research:

- data estimates and production involving electron-molecule, molecule-molecule, gas-surface interactions and transport cross sections in hydrogen plasmas, *M. Capitelli et al. (University of Bari)*;
- ionisation balance for optically-thin plasmas; rate coefficients for Cu, Zn, Ga and Ge ions, *G. Mazzitelli (ENEA), M. Mattioli (ENEA), P. Mazzotta (University of Roma)*;
- CHIANTI atomic database for spectroscopic diagnostics of astrophysical plasmas - new data are available for Fe, P, Cl, K, Ca, Co and Zn - freely available for research purposes.

Data requests from the Italian fusion community requests were briefly reviewed - mainly ENEA, CNR (National Council of Research) and Italian universities working on international fusion projects (ITER, Italian facilities and programmes, particularly FTU, IGNITOR and RFX).

Dr. H. Kubo, JAEA:

Both the Japan Atomic Energy Research Institute (JAERI) and the Japan Nuclear Cycle Development Institute (JNC) were merged on 1 October 2005 into a new independent agency called the Japan Atomic Energy Agency (JAEA). All atomic and molecular data activities for fusion research continue in JAEA. Significant recent activities have included the compilation, evaluation and production of cross sections for important collisions in cold divertor plasmas that are attractive for mitigating severe problems of concentrated power loading of divertor plates, and spectroscopic data for heavy atoms that can occur as impurities.

Cross sections for 74 processes in collisions of electrons with N_2 and N_2^+ have been compiled. The cross sections have been plotted as a function of the electron collision energy, and recommended cross sections were represented by analytic expressions to facilitate their practical use. These data will be included in the Japanese Evaluated Atomic and Molecular Data Library (JEAMDL) that is available through the Web at URL:

www-jt60.naka.jaea.go.jp/english/JEAMDL.

In addition to figures for approximately 900 collision processes, analytical functions written in FORTRAN programs are available on the Web for 284 processes. Cross sections for the production of various hydrocarbon molecules have also been measured, along with charge-

transfer cross sections of Be, B, C, Cr, Fe and Ni ions with gaseous atoms and molecules. Calculations of the cross sections of state-selective electron capture in collisions of C^{+4} ions with H* (n = 2) atoms have been made using a molecular close-coupling method. Band emission rates for CH/CD and C_2 produced from hydrocarbon molecules have been investigated in JT-60U divertor plasmas. Spectral wavelengths, energy levels, oscillator strengths, transition probabilities and ionization energies have been critically compiled for W I, II and Ga I-XXXI; compilations for W III-LXXIV and Ar I-XVIII are in progress. Measurements of the spectral lines from highly-ionized Xe and W are also in progress using the Tokyo-EBIT and JT-60U.

Atomic and molecular data activities in JAEA are being pursued in conjunction with many collaborators at NIST, Japanese universities, and other departments of JAEA.

Dr J. Bretagne and Dr. Katsonis, GAPHYOR and LPGP:

Recent GAPHYOR studies were presented by Dr. Bretagne, while Dr. Katsonis described the relevant activities of the LPGP research group dedicated to Atomic and Molecular Data for Modelling and Diagnostics.

GAPHYOR A+M data project includes: bibliographical data, numerical data and numerical codes for plasma modelling. Three French universities are involved in GAPHYOR: Université Paris XI Orsay, Université Paul Sabatier, Toulouse, and Université Paris XII, Villetaneuse. The bibliographical database is regularly updated, and the scope will be extended to bigger molecules. After a review of the data needs in nuclear fusion research, Dr. Bretagne defined the fields in which GAPHYOR is placing the effort to produce and collect numerical data. GAPHYOR is developing a series of standard numerical codes (e.g., typical case of Boltzmann equation solver), and rules will be defined to gain their access (source restricted, Web access).

Dr. Katsonis presented his recent work on atomic data related to fusion. Numerous data on argon and xenon have been produced, collected and evaluated (radiative transitions and cross sections). These data are used in a Collisional Radiative Model to study noble gas plasmas.

2.2. Additional topics

2.2.1. Yuri Ralchenko: XML and A+M 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 during the last DCN Meeting in October 2003, and is supported by the following institutions: IAEA, NIST, ORNL, JAEA and KAERI. Dr. Ralchenko presented the advantages of using XML as a new standard for exchanging atomic and molecular data. A first paper on AMDML was presented to the last ICAMDATA conference, October 2003, in Japan. AMDML now needs to be opened up to a larger audience. Contributions from the data centres would be very welcome (such as adding AMDML to the DCN databases). Collaboration was initiated with a member of IVOA who is developing a similar scheme in astrophysics. If efforts from both sides can be merged in 2006, a common publication will be proposed for ICAMDATA, October 2006, Paris.

2.2.2. Ursel Fantz: Discussion on molecular data for fusion edge plasmas and their data needs

On the basis of molecular processes in fusion edge plasmas, examples of available data were presented, and data needs discussed. Depending on the wall materials and the plasma recycling, hydrocarbons (or hydrides of boron, beryllium) and hydrogen molecules are of special importance in the understanding of chemical erosion and molecular assisted recombination. Emphasis was placed on the relevance of vibrational excitation, and thus on the requirements to have vibrationally-resolved data available. Needs for isotope relations were also addressed. Proposals are being made for the optimum arrangement of molecular data in the data centres.

2.2.3. Data centres WWW and software presentations

The opportunity was taken to demonstrate new tools, interfaces or databases available on the Web, as developed by the data centres.
(a) New ALADDIN, Denis Humbert

This new release of ALADDIN solves the hierarchical level problems for a request. All criteria are directly accessible on the same form. The user is informed after each selection on the number of data satisfying the request. This approach gives a better view of what is available in ALADDIN, and will be on-line by early 2006.

(b) Codes on the AMD Unit, Bob Clark

Two new web interfaces have been developed within the A+M Data Unit that use atomic physics codes. The first interface is accessible from the Web site of the A+M Data Unit (http://www-amdis.iaea.org/HEAVY/), and calculates cross sections for excitation and charge transfer in heavy-particle collisions (bare nuclei with hydrogenic ions) by means of the code developed by Dubois and Hansen. The second interface is linked to LANL Atomic Physics Codes (http://aphysics2.lanl.gov/tempweb/) and permits the calculation of atomic structure and electron impact excitation, and ionization cross sections.

(c) CRAAMD databases, Yum Yan

Numerical databases are available on the CRAAMD Web site (http://www.camdb.ac.cn/e/). The atomic database includes data that quantify atomic spectra, energy levels, autoionization and collisional processes (electron impact cross sections and heavy-particle collisions), while the molecular database includes ion-molecule collisions.

2.2.4. DCN membership

DCN members
Denis Humbert presented the updated list of DCN members (list is available on the A+M Data Unit Web site, and in Appendix 3). Following the previous meeting and actions undertaken by Ralchenko, Eckstein and Martynenko concerning the Weissmann Institute, Israel, Efremov Institute and TRINITII, Russia, respectively, there would appear to be no strong A+M data activities related to fusion being performed at these institutes. Furthermore, as no clear representative from these institutes could be found, the A+M Data Unit decided to remove them from the DCN membership.

Membership criteria
At the present time, no terms of reference exist regarding the role and activities that a data centre should be undertaking as a member of the DCN. This matter is important in deciding whether Brazil is qualified to join the DCN. "Terms of Reference" have been proposed to define the scientific scope and relevant activities of a data centre within the DCN:

AM/PSI DCN: Terms of Reference

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

Established programmes in the following:
- collection of data,
- dissemination of data,
- calculation and/or measurement of data,
- assessment/evaluation of data with the description of the adopted process.

After some discussions, no consensus has been reached to establish which programmes should be mandatory or only recommended as part of a data centre's activities. The A+M Data Unit will propose a "chart" based on the "Terms of reference" for discussion at the next DCN meeting.

Membership of Brazil
Brazil (represented by Dr M. Machado) attended the DCN meeting for the second time. One aim should be to welcome Brazil as a new member in the near future – their membership is of high interest and benefit to the DCN because of Brazil's strong research activities in atomic and molecular physics. Brazilian membership would also give the DCN a wider geographical representation. As no consensus has been reached regarding the role and activities of a data centre inside the DCN, a decision on the membership of Brazil had to be postponed.

2.3. Priorities in A+M data compilation and evaluation for fusion

A+M data compilations and evaluations for fusion were reviewed using priority lists from previous DCN meetings. Thus, a new list was generated by removing data needs that have now been fulfilled, keeping those that remain unfulfilled, and adding any new data requirements. There was also some agreed-upon merging and splitting of some collision categories, and the elimination of some previous needs that are now deemed to be redundant or irrelevant. The adjusted and updated data priorities that were identified and discussed are summarized in Appendix 4, and are available on the A+M Data Unit Web site:
http://www-amdis.iaea.org/DCN/fusion_data.php

3. Conclusions and Recommendations

3.1. Status of data generation and priorities in data compilation and evaluation

- Some of the data needs and priorities presented at the 18th AGM were concluded to be still valid. A number of the data needs have now been satisfied, and some new data priorities have been identified. The current list of data priorities is summarized in Appendix 4, 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 significant contributions to the data evaluation and quality control efforts. Data generated and collected are introduced into the ALADDIN numerical database as soon as they become available.

- Over the previous two years, use of short-term consultancies (several from within the Data Centre Network) working in conjunction with A+M Unit staff has been found to be very effective in tackling problems within system software (ALADDIN and AMBDAS).

3.2. Data processing and exchange

- All A+M data centres which maintain Web presentations have been very effective at delivering their own data. Once available, some data centres are ready to use the new exchange format in XML (AMDML), as presented by Ralchenko. An oral paper is scheduled for the next ICAMDATA, France, October 2006.

- GENIE has been on-line for 4 years, and user access increases regularly as shown in the monthly statistics sent to DCN members and databases managers. One aim is for GENIE to evolve continually in the search for new available databases on the Web, based on effective collaboration and communication between data centres and the A+M Data Unit. The scope of GENIE will be enlarged to more processes and molecular data.

3.3. Membership status

As no clear definition exists within the DCN regarding member status, no agreement has been reached concerning Brazilian membership. A charter will be prepared and presented at the 2007 DCN meeting, based on the agreed scheme (Section 2.2.3.) drafted by the A+M Data Unit in collaboration with the data centres.

L. Machado is invited to the next DCN meeting to present BRAMPDAC activities that involve A+M data for fusion. The membership of Brazil will also be properly reviewed at that time.

3.4. Next meeting and consultancies

DCN members recommended extending the meeting to 3 days. Data centre presentations should focus on new issues related to fusion. A talk on the working methods of a data centre may be of general interest, and a special issue on data evaluation will be discussed.

The DCN recommends inviting fusion specialists to present and discuss appropriate topics of interest. Two consultants were invited to the 2006 DCN meeting to give talks on XML and molecular data needs in fusion, and this arrangement had been extremely beneficial to all. DCN members recommended a similar procedure for the next meeting, and advised that a representative of ITER should be invited to attend.

Appendix 1

IAEA Technical Meeting on
Technical Aspects of Atomic and Molecular Data Processing and Exchange
18th Meeting of the A+M Data Centres and ALADDIN Network

10-11 October 2005, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Technical Meeting on
Technical Aspects of Atomic and Molecular Data Processing and Exchange
18th Meeting of the A+M Data Centres and ALADDIN Network

10-11 October 2005, IAEA Headquarters, Vienna, Austria

Agenda

Monday 10 October **Meeting Room: A-27-74**

09:15 – 09:30 Opening, Adoption of Agenda, A. Nichols, R.E.H. Clark, D. Humbert

Session 1: Current Activities of the A+M Data Centres

Chairman: Yu.V. Martynenko

09:30 – 09:45 D. Humbert, KAERI report from Y. Rhee
09:45 – 10:15 W.L. Wiese (NIST)
10:15 – 10:45 D. Kato (NIFS)
10:45 – 11:15 *Coffee Break*
11:15 – 11:45 D.R. Schultz (ORNL)
11:45 – 12:15 J. Yan (CRAAMD)
12:15 – 12:45 D. Humbert (IAEA)
12:45 – 14:00 *Lunch*

Session 2: Current Activities of the A+M Data Centres (Continued)

Chairman: Jun Yan

14:00 – 14:30 Yu.V. Martynenko (Kurchatov Institute)
14:30 – 15:00 W. Eckstein (MIP)
15:00 – 15:30 L. Machado (Univ. de Sao Carlos)
15:30 – 16:00 *Coffee Break*
16:00 – 16:30 E. Menapace (ENEA)
16:30 – 17:00 H. Kubo (JAEA)
17:00 – 17:30 J. Bretagne (GAPHYOR)

Tuesday 11 October

Session 3: Interfaces and Web Tools

Chairman: D.R. Schultz

09:00 – 09:30 Yu. Ralchenko (NIST)
"XML Format for A+M Data"

09:30 – 10:00 U. Fantz (Universität Augsburg)
"Discussion on Molecular Data for Fusion Edge Plasmas and Their Data Needs

10:00 – 11:00 Data Centre WWW and Software Demonstrations

11:00 – 11:30 *Coffee Break*

Coordination: R.E.H. Clark and D. Humbert

11:30 – 12:30 Review of Data Center Network Membership Criteria
Membership of Brazil
Plan of DCN Activities for the Near Future

12:30 – 14:00 *Lunch*

Session 4: Data Issues

Chairman: W. Wiese

14:00 – 15:30 Priorities in A+M Data Compilation and Evaluation (All Participants)

15:30 – 16:00 *Coffee Break*

Session 5: Meeting Conclusions and Recommendations

Chairman: D. Humbert

16:00 – 17:00 Formulation of Meeting Conclusions and Recommendations
Date and Duration of Next Meeting

17:00 – *Adjournment of Meeting*

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List of DCN Members

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Appendix 4

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

Atomic and Molecular Data

Spectroscopic Data

- Transition probabilities for the Be-, B-like isoelectronic ions and heavy elements like Fe are needed.
- Ne, Na, Mg, Al, and Si are done for all ionization stages at NIST ASDC. He, Li, Be, B, S, and Cs have been initiated, others are in the planning stage.
- Energy levels, wavelengths, transition probabilities for metallic ions, high-Z impurities
    - W: high ionization stages being initiated, low ionization stages are finished by NIST ASDC.
    - Needs for data production for W, Xe, Kr (in high ionization stages) in addition to needs for compilation/evaluation
    - W often has additives such as LaO, La_2O_5, and Re, so these should potentially be considered.
- Complete spectroscopic characterization of heavy noble gas ions. Ne almost done.
- 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, and hydrogen isotopic variants). The HITRAN database at Harvard CfA and other molecular databases may have some of this data.

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 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^+. Some combinations, e.g. $He^+ + He^{2+, +}$ on He, H_2 still not done. Excited states and higher energies still need to be done.
- Ro-vibrational electronic excitation and attachment for D_2, T_2, 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 CRP on "Molecular Processes in Fusion Plasmas" has produced initial work on cross sections for H_2^+. The rate coefficients for dissociation of H_2*(v) are calculated. The NIFS-DATA-73, APID issue in preparation is covering a significant part of these needs. The new 2005 CRP on "Atomic and Molecular Data for Plasma Modelling" initiated) also addresses this topic.
- Inelastic electronic collision processes of He, He^+, He^{2+} and excited states of H, He and H_2 at low energies. This is mostly addressed by the 2 CRPs:
    - CRP on "Molecular Processes in Fusion Plasmas"
    - CRP on "Atomic and Molecular Data for Plasma Modelling"
- 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:
    - CRP on "Molecular Processes in Fusion Plasmas"
    - CRP on "Atomic and Molecular Data for Plasma Modelling"
- Completion of collisional databases for Be, B and their ions. This will include collision processes of Be^{q+}, B^{q+} with electrons, and quasi-resonant processes of Be^{q+}, B^{q+} with H, He and H_2.
- 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 and the effect of this excitation on the dissociation processes, as vibrational excitation might affect dissociation. This is partly covered by concluded and active CRPs.
- Particle interchange reactions among primary species, C, O, metals and hydrocarbons. Data published for electronic collisions, CRP on "Molecular Processes" adding considerable data for hydrocarbons. NIFS and FZ Julich Reports on hydrocarbons.
- Collision processes of high-Z impurities in priority order (W, Mo, V, Ar, Kr, Xe) with e, H^+, H, H_2. CRP on heavy elements initiated in 2005.

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 needed for loss mechanisms in beams.
- Don't forget stripping.

Radiative Plasma Cooling

- **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 energy 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 new CRP on "Heavy elements" will address this topic.

- **Plasma edge region**

  - Charge exchange collisions of X^{q+} (X = Cl, Ti, Ni, Cr, Fe, Mo, W, V) with H, H^+ and He^{2+}. Pertinent energy range: is from 1 eV (or threshold) to 500 eV.
  - Collisions of X^{q+} (q >= 5, X as above) with H, He, H_2, including state selective electron capture.
  - All processes of N, N_2, Kr, Ne, Ar and Kr-ions with e, H, H^+, H_2, H_2^+, He^+, He^{2+} and H^- (for the proposed radiative cooling scheme of divertors).

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 on sputtering yields of these are partly available (i.e. for normal incidence).
- Sputtered energy (to allow the determination of the mean energy of sputtered atoms).

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

- H/D/T permeability, diffusivity, solubility, desorption rate and surface reactions. Materials: 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" addresses partly this topic.

Molecular balance on surfaces

- Molecule (molecular ion) formation and destruction with identification of product charge and quantum state. Data for H^- formation on surfaces, particle sticking, pumping, gettering, and recycling. (Emphasizing inclusion of molecular vibration in the initial state.)
- Mean range of impinging particles (and deposition profiles) would give information on the disturbed target region.
- Gas bubble formation in wall material from alpha particles formed by neutron reactions and protons from neutron reactions and implantation.

Material Properties

Data collection and generation needed

- Data for dust formation from C, Be, W, Mo.

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