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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 20th Meeting of the A+M Data Centres and ALADDIN Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

7–9 September 2009

Prepared by

Denis Humbert and Bas Braams

January 2010

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (20th Meeting of A+M Data Centres Network), 7-9 September 2009 at IAEA Headquarters in Vienna, are summarized. The meeting conclusions and recommendations on priorities in A+M data compilation and evaluation and on technical aspects of data processing and exchange are also presented.

January 2010

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1. Introduction

The IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing" (20th Meeting of the Atomic and Molecular Data Centres Network) took place 7-9 September 2009. The objectives were to review progress in A+M data related activities in the Data Centres, review methods and procedures for data processing, and review and coordinate the work plans for the next period.

Seventeen participants attended the meeting. All Data Centres were represented. The Network welcomed three new Data Centre representatives: Dr Izumi Murakami from NIFS in place of Dr Takako Kato (retired), Dr Chunglei Liu from CRAAMD in place of Dr Jun Yan, and Dr Konstantinos Katsonis from GAPHYOR in place of Dr Jean Bretagne (also retired).

Five observers attended the meeting. Dr Allan Whiteford from University of Strathclyde, UK, represented ADAS, candidate as new data centre in the Network. Dr Yuri Ralchenko from NIST, USA, was invited for his expertise on data exchange and database tools including XSAMS and XML. Dr Bob Clark, UT San Antonio, past Head of the IAEA A+M Data Unit, was invited for his expertise in web-based atomic physics calculation tools. ITER was represented by Dr Michiya Shimada. Dr Hyun-Kyung Chung of Korea attended the meeting as the future Scientific Secretary in replacement of Mr Denis Humbert who is leaving the IAEA at the end of September. The Agency was represented by Dr Robin Forrest, Dr Bas Braams and Mr Denis Humbert.

Dr Giovanni Mazzitelli of Frascati Laboratory, Italy, and Dr Bin Duan, 2nd representative of CRAAMD, could not attend the meeting. Dr Mazzitelli sent a report on the ENEA activities related to fusion for the past two years. Dr Bin Duan could not attend the meeting as the time between issuance of the invitation letter and the date of the meeting was too short to arrange a passport renewal and visa. The AMD Unit is aware of the complexity for consultants from some countries to obtain a visa to Europe and will take care in the future for the Russian Federation, China and at a lesser level the USA to start the invitation process sufficiently far in advance.

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

The meeting was opened by Dr Robin Forrest (Head, Nuclear Data Section, Division of Physical and Chemical Sciences, IAEA), Dr Bas Braams (Head, A+M Data Unit, Nuclear Data Section), and Scientific Secretary Mr Denis Humbert (Physicist, A+M Data Unit, Nuclear Data Section). They welcomed all participants and stressed the usefulness of this Technical Meeting to the Data Centre Network. They noted this meeting being the 20th of the network and noted the full turn-over of the A+M Data Unit with Dr Chung and Dr Braams replacing Mr Humbert and Dr Clark within a short period of time. 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 schema, priorities in data compilation and evaluation;
- Membership in the network;
- Interfaces and web tools;
- Meeting conclusions and recommendations.

2. Proceedings of the Meeting

The presentations at the meeting are available on the A+M Data Unit web site http://www-amdis.iaea.org/ via the links to the Data Centre Network and then to Meeting Reports and Presentations.

This being the 20th meeting, to mark the jubilee Dr Wolfgang Wiese of NIST, USA, who attended all 20 meetings, presented a brief history of the Data Centre Network. The Data Centre Network and the

activities of the IAEA in A+M data for fusion in general were initiated by Dr Alex Lorenz, then head of the Nuclear Data Section, at the request of the International Fusion Research Council (IFRC), with a meeting at Culham Laboratory, UK, 1-5 November 1976. (A message was received the morning of the present meeting that Dr Lorenz had passed away the previous Friday, 4 September.) This Culham meeting provided a recommendation to establish an A+M data centre network coordinated by the IAEA/NDS. The first meeting of the DCN took place in 1977, and subsequent meetings almost yearly since 1980. The priorities of the IAEA/NDS in atomic and molecular data recommended at the 1977 Culham meeting remain valid:

- To compile and publish international computerized indices to the literature on atomic and molecular 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; and
- To develop standardized computer input and output formats for the systematic compilation and the dissemination of bibliographic and numerical A+M data.

Highlights of the subsequent work of the network include the launch of the International Bulletin on A+M Data for Fusion and of the (CIAMDA) annotated bibliography of collision data, the adoption of ALADDIN ("A labelled atomic data interface") for data exchange, the development of the GENIE search engine, and most recently the adoption of XML as a standard for future A+M/PSI data exchange. Dr Wiese recalls that at the previous meeting of the network it had been agreed to drop "ALADDIN" from the title of the meeting, and the meeting took note of this for the future.

2.1 Current Activities of the A+M Data Centres

During the first meeting session all data centres presented progress reports on their activities in A+M data for fusion in the period October 2007-August 2009. This concerns the work done on data compilation, evaluation and generation, web developments, data centre publications produced during the reporting period, and the status of ongoing programmes and plans for future work. The presentations are summarized here. More information may be found at the Data Centre Network web pages under http://www-amdis.iaea.org/.

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

The energy and angular dependencies for the particle and energy reflection coefficients for a large number of ion-target combinations have been reported. Calculated values have been fitted by formulae with fewer fitting parameters than in previous investigations. The fitted curves are compared with available experimental data. The results are collected in an IPP report (Report 17/12, 2009) including tables with the fit parameters for the different cases. The calculated and experimental numerical values can be retrieved from public web pages of the IPP under the directory ftp.rzg.mpg.de/ftp/pub/ipp/eckstein/rep05/. For the report at IAEA special emphasis is given to fusion relevant examples.

Dr Eckstein is now retired from IPP Garching and the new code SDTrimSP is being maintained by Dr Andreas Mutzke at IPP Greifswald. This code replaces all earlier Trim.SP versions.

Yu.V. Martynenko, Kurchatov Institute, Moscow, Russian Federation

The main activities at Kurchatov on A+M Data are concerned with new data generation, computer code developments for tokamak plasma processes, and data acquisition systems. New data and studies over the past two years include:

1. Data related to neutral beam heating. Reactions involving D^- negative ions; D_2 molecules and D_2^- molecular ions have been experimentally observed.

2. Plasma radiation.
   - Ultra fast method of calculating the dynamic spectral line shapes, with application to radiation transport modeling;
   - Fast code nl-KINRYD for collisional-radiative kinetics of Rydberg atomic states;
   - Fast code ESMEABRR for bremsstrahlung and radiative recombination.

3. Data for tungsten and carbon surface change under high dose plasma exposure obtained in the LENTA linear plasma facility, in connection with the IAEA CRP on surface composition dynamics.

4. Experimental and theoretical studies of nanostructured deposited films in tokamaks.

5. Dust in tokamaks; dust charge and tritium retention issues; also study of discharge stabilization by dust injection into plasma.

There are new results in the data acquisition system; see http://cpunfi.fusion.ru/dassql/dasweb2.dll/showgl

G. Mazzitelli, ENEA, Italy

Dr Mazzitelli could not attend the meeting but sent a report on the activities of the ENEA, which have been focused on the production of atomic data relevant to impurity behavior in magnetic confinement fusion devices. Rates for ionization, radiative recombination and dielectronic recombination have been critically reviewed and missing data have been extrapolated from literature. This work has been done for all the elements up to germanium and also for krypton and molybdenum.

For the dielectronic recombination rates a simple formula with unique exponential factor is used for all the given elements. This allows impurity transport modellers to update the atomic package without modifying the underlying code by only changing the numerical coefficients used in the formulae.

At the moment, due to a lack of people and after the sudden absence of Mario Mattioli, it is only possible to maintain the web site.

A. Whiteford, ADAS, University of Strathclyde, UK

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS) over the web. Version 1.0 was released in July 2008. The primary objective of ADAS is support of the magnetic confinement fusion programme and the on-going development of ADAS is enabled by the ADAS Project and its membership. The OPEN-ADAS development has therefore a dual benefit, namely to enable non-members with an interest in fusion to download and use ADAS data, and also to provide ADAS Project members with a more intuitive searching mechanism for ADAS data.

ADAS and OPEN-ADAS are used extensively in transport modeling and in spectroscopic analysis, both in fusion and in astrophysical research. The project is managed at Strathclyde and is funded through memberships of universities and fusion laboratories. There are 28 members at present. OPEN-ADAS is a subset of ADAS focused on the needs of fusion diagnostics. Opacity data are already included. OPEN-ADAS does not include any of the ADAS analysis codes. Free registration is required to access OPEN-ADAS, and as of 1st August 2009 there are 124 registered users, 89 of them from non-ADAS sites.

I. Murakami, NIFS, Japan

At NIFS, theoretical and experimental work on atomic, molecular and plasma-wall interaction processes and related database work is carried out in the Atomic and Molecular and PWI Data Research Section in the Coordination Research Center. The Section maintains an A+M database that is regularly updated. In 2007-2009, the Section has been collecting collision data mainly for heavy

elements that are important for fusion research. The user interface of the A+M database was modified for the AMDIS excitation and recombination databases to treat large number of data sets. About 20-25% of the queries to the database now come through the GENIE interface. New web pages of evaluated photoabsorption cross sections and an online calculation of a collisional-radiative model for He-like ions are being prepared.

Excitation effective collision strengths for electron impact on Fe ions have been evaluated. This work is part of a collaboration on using Fe ion spectra to diagnose non-equilibrium plasma in fusion and in the sun. Extreme ultraviolet (EUV) spectra from plasmas in the Large Helical Device (LHD) at NIFS and in the sun have been analyzed. Line intensity ratios of Fe XIII, Fe XXI and Fe XXII lines and collisional radiative modelling were used for electron density diagnostics. Experiments using the Tokyo Electron Beam Ion Trap (EBIT) and a new compact EBIT measured EUV spectra of Fe ions. EUV spectra of W ions were also measured for LHD plasmas and the analysis is in progress. Ab initio calculations of dielectronic recombination processes were done for some Mg-like ions.

First-principles calculations for vacancy formation in bcc tungsten crystals and semi-classical calculations for excited neutral D reflected at Mo surfaces have been carried out.

D. Humbert, IAEA

The primary objectives of the IAEA 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 Coordinated Research Projects (CRP), technical meetings (TM), 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.

It is the goal of the Unit to maintain three active CRPs at any one time. Currently, three CRPs are in their final phase of completion, with two APID volumes in preparation (one for the CRPs on “Atomic and molecular data for plasma modelling” and “Atomic data for high-Z element impurities in fusion reactors” and one for the CRP on “Tritium inventory in fusion reactors”). The CRP on “Characterization of Size, Composition and Origins of Dust in Fusion Devices" held its first RCM in December 2008 and the one on “Data for surface composition dynamics relevant to erosion processes” held its second RCM in March 2009. The CRP on “Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions” will hold its first RCM in November 2009. It is planned to start a CRP on spectroscopic and collisional data for tungsten in plasma in 2010, and perhaps a CRP on characterization and control of H/He isotopic composition in 2010/2011.

Major improvements in the development of web tools and databases have taken place. The first version of OPEN-ADAS was released in June 2008. New data are regularly added to the ALADDIN and AMBDAS databases. After the major upgrade of the ALADDIN interface for collisional data, the interface for particle surface interactions was also upgraded. Both interfaces are now running the same version (2.3) of ALADDIN. A first version for the XML schema for atomic and molecular data (XSAMS) is ready for release. The development of web calculations tools is now coordinated by the IAEA Code Centre Network (CCN). Available capabilities provided by CCN members are summarized on the IAEA A+M Data Unit web site with links to their respective home pages (http://www-amdis.iaea.org/CCN).

The Unit organizes occasional workshops. A training workshop on A+M Data for Fusion Energy Research was held in Trieste, 20-30 April 2009, organized jointly with the International Centre for Theoretical Physics. A workshop on Challenges in Plasma Spectroscopy for Future Fusion Research Machines was held in Jaipur, India, 20-22 February 2008; it was organized jointly with the Birla Research Centre.

T. Nakano, JAEA, Japan

The Japan Atomic Energy Agency (JAEA) has been producing, collecting and compiling cross section data for atomic and molecular collisions and spectral data relevant to fusion research. The atomic and molecular data activities in JAEA are pursued by sponsored researches with Japanese universities and in collaboration with other department of JAEA

The electron capture cross sections of singly and doubly ionized tungsten ions by collision with H_2, CH_4, C_2H_6, He, Ne, Ar and Kr were measured at collision energies of 5, 10 and 15 keV. The state selective charge transfer cross sections of Be^{2+}, Be^{3+}, B^{5+} and C^{6+} by collision with H*(2s) and H*(2p) in the collision energy range between 62 eV/amu and 6.2 keV/amu were calculated with the improved molecular-bases close-coupling method. The state specific dissociative recombination cross sections for H_2^+ were calculated with the improved multi-channel quantum defect theory. The analytic expressions for the recommended cross section for the He collision systems (214 processes in these 4 years) were produced or revised in order to facilitate use of the data. The compiled data are being prepared for Web publication at the URL http://www-jt60.naka.jaea.go.jp/engish/JEAMDL/. The charge transfer data for 36 processes published in 2007 and 2008 have been compiled, and a database for the chemical sputtering yield data of impurity-doped graphite materials with hydrogen isotope collisions has been established. The 3s-3p and 3p-3d lines of $W^{\sim 60+}$ around 2 nm have been identified in 15-keV plasma in JT-60U.

C. Liu, CRAAMD, China

The China Research Association of Atomic and Molecular Data (CRAAMD) brings together scientists from 10 Chinese institutions. Activities of CRAAMD over the previous two years include data collection, calculations and measurements. The following are noted.

- Atomic energy levels and radiative transition rate of M-shell Au ions;
- Electron-ion collision excitation, ionization cross sections and rate coefficient (including inner-shell ionization);
- Dielectronic recombination rate coefficients;
- Cross sections of elastic and inelastic scattering of atom and molecule: Ar, Ba, SO_2, OCS, CF_2Cl_2;
- Molecular structure and spectra;
- Cross sections of heavy particle collisions;
- Ionization potential of molecular ions.

CRAAMD was a principal organizer of the ICAMDATA 2008 conference in Beijing.

The website for CRAAMD is http://www.camdb.ac.cn/. The database can also be accessed through the IAEA GENIE interface.

K. Katsonis, GAPHYOR, LPGP, France

The general objectives of the work of the past two years were the evaluation of pertinent atomic data based on experimental and theoretical studies, mainly of rare gas atoms and ions, and the use of those atomic data in plasma diagnostics and modeling applications. Plasma spectroscopy of Ne, Ar and Xe was carried out in various devices and conditions including a hollow cathode device available at the University of Ioannina, Greece, the DIVA reactor in LPGP, the WEGA stellarator of the IPPG of Greifswald, various plasma thrusters, and a beam-foil experiment specially conceived for the VUV region in IPNAS, Liège. The spectra were analyzed with line identification codes developed ‘ad hoc’ and compared with results from the GAPHYOR Collisional-Radiative (C-R) model. Systematic calculations and evaluations were carried out for atomic data pertaining to Ne, Ar and Xe atoms and their low ionization stages, which were used in the C-R models for diagnostics and modeling of plasmas of fusion interest.

Recent evaluations concerned the following:

(1) Structure and transition probabilities (A_{ij}), which are important in optical diagnostics of emission lines of plasmas. Generation of a huge number of A_{ij} is necessary for the complete C-R models. In evaluating these A_{ij} we compare results calculated using mainly the following theoretical methods:

I. Our Coulomb approximation code (CbA),
II. The Cowan Atomic Structure (CATS) code of LANL,
III. The Superstructure (SST) code, installed in Meudon observatory, and
IV. The MCDF GRASP code available in the IAPCM of Beijing.

Calculations II and III were carried out using different sets of configurations; we occasionally compared with results from IV, which describe the relativistic effects explicitly. Comparisons with the small number of available experimental data have also been made.

(2) Electron Collision Excitation Cross Sections (σEe) calculations and their corresponding Rate Coefficients (αEji) for various distribution functions. Special care was given to the αEji values because the theoretical spectra obtained by C-R models depend strongly on the accuracies of both transition probabilities and electron collision excitation data. We focused on the special case of electron impact excitation cross sections from the ground 2,3,5p and 3,4,6s transitory and metastable levels of the neutral Ne, Ar and Xe to the lowly excited levels of these three atoms. This work is now underway for argon and neon. In evaluating these σEe results calculations using the following theoretical methods were compared.

V. Distorted Wave (DW) approximation using the Los Alamos ACE codes.
VI. First Order Many Body Theory (FOMBT), also with the ACE code, especially near the threshold.
VII. Quasi-classical evaluations following numerical solutions of the few body problem.
VIII. The semi-empirical formula introduced by H.W. Drawin, as adapted by K. Katsonis for the rare gas atoms.

Calculations V and VI were carried out using different sets of configurations and the resulting cross sections compared. The comparisons of methods VII and VIII, which are based on experimental energies and on transition probabilities calculated with the Coulomb approximation, with NIST values, when available, are often satisfactory over the entire energy range and especially near threshold.

(3) Extension of the applicability of our 'zero-dimension' codes to treat the bulk of the plasma state and properties calls for their coupling with detailed kinetic codes such as EIRENE. Simplified C-R models of Ar and Ne, based on averaged structures of the atoms/ions, are under development.

W. Wiese, NIST, USA

The NIST Atomic Spectroscopy Data Center (http://physics.nist.gov/PhysRefData/) maintains annotated bibliographical databases and numerical databases, with special focus on spectroscopic data. The Transition Probabilities bibliographical database now covers literature from the years 1914-2009, the Line Widths and Shifts bibliographical database starts in 1992 and is up-to-date to 2007, and the Energy Levels and Wavelengths bibliographical database covers literature for the years 1908-2009.

Extensive work was done on the (numerical) Atomic Spectra Database (ASD), now at version 3.1.5. Critical evaluations of energy levels and wavelengths were performed for Na I through Na XI, K I through K XIX, Ga I through Ga XXXI; and Kr I through Kr XXXVI. Evaluations are in press or nearing completion for Ne IV, Cl V through XVI, Ar I through Ar XVIII, Cs I through Cs LV, and Ba III through Ba LVI. Compilations of transition probabilities were carried out for selected charge states of H, He, Li, C, N, Na, Mg, Al, Si, S, and K and further ones are in progress for Be, B, Cl, Ar, Cs, and Ba.

In ongoing work the bibliographic databases are being integrated with the Atomic Spectra Database, the principal numerical database of NIST. The Atomic Spectra Database is being updated with the recent numerical material from various NIST compilations. A completely new version of the Atomic Spectra Database is nearing completion (version 4).

NIST data tables are limited to reference data, i.e., data of certain minimum quality. Only one numerical value is presented for each quantity. This may be either from a single source, evaluated as being the most accurate one, or from an average of several sources of about equal reliability. For atomic transition probabilities (oscillator strengths), explicit accuracy ratings are given. For wavelengths and atomic energy levels the number of tabulated digits indicates the accuracy.

D. R. Shultz, CFADC, ORNL, USA

The Controlled Fusion Atomic Data Center (CFADC) of the Oak Ridge National Laboratory continued operation aimed at collecting, evaluating, and disseminating atomic, molecular, and particle-surface interaction (AM&PSI) data needed by both the U.S. and international plasma science communities. This work has been carried out within an overarching atomic physics research group which produces much of the required data through an active experimental and theoretical science program. The production of an annotated bibliography of AM&PSI literature relevant to plasma science continues to be among the most important activities of the data center, forming the basis for the CFADC on-line bibliographic search engine and a significant part of the IAEA A+M Data Unit's "International Bulletin on Atomic and Molecular Data for Fusion." Also chief among the data center's activities are responses to specific data requests from the plasma science community, leading to either rapid feedback using existing data resources or long term data production projects, as well as participation in IAEA Coordinated Research Programs including recently "Data for Surface Composition Dynamics Relevant to Erosion Processes" and "Atomic and Molecular Data for Plasma Modeling." Highlights of recent data production projects include the following: Experimental and theoretical data for inelastic electron-hydrocarbon reactions, large scale computational results for particle reflection from surfaces, measurements of chemical sputtering from carbon, inaugural experiments considering molecular ion collisions with neutral hydrogen, and expansion of the database of elastic and related transport cross sections calculated for intrinsic and extrinsic impurities in hydrogen plasmas.

Y. Rhee, KAERI, Korea

At the Laboratory for Quantum Optics at KAERI we extended our calculation of tungsten emission spectra up to W^{45+}. The MCDF computer code, which solves the relativistic Dirac-Fock equation, was used to calculate dipole transition probabilities for tungsten ions of charge states ranging from W^{33+} to W^{45+}, and to the calculation of electron impact ionization cross sections of W^{45+}. The results were compared with those of other groups to understand the validity of BEB model for a highly charged ion. Orbital parameters such as binding energies and occupation numbers, and transition probabilities between energy levels were calculated.

A brief introduction was given to the updated contents of AMODS database of KAERI as well as recent activities on the diagnostics and simulations of high density laser-produced plasma.

2.2 Other Presentations

During its meeting in October 2003 the DCN committee recommended the inclusion of presentations of general interest for controlled fusion energy research and to invite regularly an ITER representative. Dr Michiya Shimada represented the ITER project. Also Dr Yuri Ralchenko described the status of XSAMS and Dr Bob Clark described the work of the IAEA Code Centre Network.

M. Shimada: AM/PSI Data Needs for ITER

Requirements for modeling at ITER:

- Fitting formulae of evaluated data, Fortran codes;
- Estimated errors;
- A single web site as the gateway.

The plasma-facing materials foreseen at the start of ITER operation are W, C, Be; C in the form of carbon-fiber composites (CFC). However, when D and DT operation are started then only W and Be remain, and possibly W alone. The main atomic plasma species of interest are H, D, T, He, Be, C, W, O, N, Ne, Ar, Kr. Molecules of interest are H_2, H_2^*, H_2^+, H_3^+, H_2O, CO, CO_2, CH_4, CH_2, CH, C_2, N_2, Be hydrides, oxides and nitrites as well as other hydrocarbons and radicals. Less important for ITER: B, Li, and Cs and their hydrides and oxides. Be opacity is important and is not well addressed in the available data. Also photo-ionization is important in the divertor. For charge exchange accurate data up to 1 MeV are required.

With regards to plasma-surface interaction and erosion ITER is interested in Be, W, C and carbon-based materials, BeO, and mixed materials, including their dynamics. The CRP on dust formation is valuable. There are gaps in the available PSI data for reflection at low impact energy.

The main new data needs since 2007 are:

- More on tungsten, including data for bundled charge states for efficient modeling;
- Be opacity;
- Photo-ionization.

Yu. Ralchenko, NIST: XSAMS: XML Schema for AM/PSI Data Exchange

XSAMS stands for XML Schema for Atoms, Molecules, and Solids. It is intended to release XSAMS 0.1 within the next two weeks; an IAEA Consultants' Meeting on XSAMS immediately follows the present Data Centre Network meeting. The project has a strong partner in the Virtual Atomic and Molecular Data Laboratory, VAMDC, which is an EU project with funding for 3.5 years. Marie-Lise Dubernet is the lead person on VAMDC and XSAMS is their chosen method of data sharing. Yuri Ralchenko suggests that a CRP on XSAMS would be valuable.

R.E.H. Clark, UT San Antonio, The IAEA Code Centre Network

Computation is of increasing importance and new atomic data now come primarily from theory; this persuaded the IAEA A+M Data Unit to consider creation of a Code Centre Network, supplementing the long-standing Data Centre Network. A Technical Meeting was held at the IAEA in 2005 to bring together potential centres and inventorize methods and codes that can be made accessible through a web interface. Early examples include the Average Approximation codes of J. Peek for electron excitation of ions, the heavy particle collision codes of Dubois, Hansen, and Vainstein, and the Los Alamos codes of Cohen et al.; these three sets of codes can already be accessed through http://www-amdis.iaea.org/.

After a further exploratory meeting in 2008 the Code Centre Network (CCN) was formed. Information is available through http://www-amdis.iaea.org/CCN/. There are 12 participating centres. Each centre has summarized their expertise. Some centres have online calculations available now, others plan for future capability. Some centres offer to carry out large scale calculations upon request. The centres and their codes and contacts are listed on the CCN web page.

3. Data Issues

The priorities in A+M data compilation and evaluation for fusion were reviewed using the priority list from the previous DCN Meeting. The new list was generated by removing data needs that have been fulfilled, keeping those that require more work and adding new data requirements. The adjusted and updated data priorities are summarized in Appendix 3 below 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 experts in this field to future meetings.

The topic of data evaluation was briefly addressed. Evaluation is a difficult and time-consuming activity, and most of data centres lack resources for this effort. A recommendation is to provide

estimated accuracy (uncertainties, error bars) when possible. Traceability of the data should be mandatory. It was recognized that NIST has a strong activity in spectroscopic data evaluation.

4. DCN Membership

D. Humbert recalled the terms of reference for the AM/PSI Data Centre Network. The domain is atomic and molecular physics and particle surface interactions (AM/PSI). Data should be strongly relevant to fusion. A participating data centre should have established programs in one or more of the following:

- Collection of data
- Dissemination of data
- Calculation and/or measurement of data
- Assessment/evaluation of data

There was no contribution at the present meeting from the planned Brazilian data center, BRAMPDAC. It was decided not to pursue their membership in the DCN.

On behalf of the ADAS Steering Committee A. Whiteford requested that ADAS be admitted as a member in the Network. In the ensuing discussion an objection was raised connected with past financial support from the IAEA for OPEN-ADAS. On the other hand, the value of OPEN-ADAS for wide dissemination of atomic data was recognized, and it was decided to admit ADAS as a member of the DCN.

5. Data Centres Web Interface and Software Presentations

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

Dr Izumi Murakami showed the new NIFS database on recommended data for electron collisions and cross-sections for atom and molecule collisions.
List of available numerical databases:

- Excitation, upgrade of version
- Recombination
- Spectrum of Th-Ar hollow cathode lamps in the range 691 to 5804 nm.

Tool to fit data, for example AMDIS ionization.
The bibliographic database BIBLIO has regular updates.

Mr Denis Humbert, IAEA, showed the new ALADDIN interface for PSI data and the GENIE search engine.

Dr Yuri Ralchenko, NIST, presented the plasma kinetics databases SAHA (NLTE3) and NLTE4, which contain benchmark results for simulation of plasma population kinetics and emission spectra obtained from the contribution of the participants in the Non-LTE Code Comparison Workshops. FLYCHK, an online collisional radiative model where steady state and time dependant calculations for elements from H to Au can be performed, was demonstrated. Finally Dr Ralchenko showed an example of access to spectral line databases using IVOA standards: SLAP (Simple Line Access Protocol) and the XML Spectral Line Data Model. These databases are on the web at http://physics.nist.gov/PhysRefData/.

6. Meeting Conclusions and Recommendations

The list of data needs and priorities developed at the 19th meeting was reviewed. 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 provided in Appendix 3; it is maintained and updated on the A+M Data Unit web server at http://www-amdis.iaea.org/DCN/fusion_data.php.

All A+M Data Centers that maintain web sites have been very effective in delivering their data. Many of the data centers are ready to use the new XML Schema for Atoms, Molecules and Solids (XSAMS) exchange format. The first version of XSAMS should be released in September 2009.

Requests on GENIE increase regularly as shown in the monthly statistics sent to the DCN members and the databases managers. GENIE continually evolves to search new available databases on the web. In this matter, collaboration and communication between datacenters and the A+M Data Unit are very useful and efficient. The scope of GENIE should be enlarged to more processes and to molecular data.

Appendix 1

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (20th Meeting of the A+M Data Centres and ALADDIN Network)

7–9 September 2009, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

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Appendix 2

IAEA Technical Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange (20th Meeting of the A+M Data Centres and ALADDIN Network)

7–9 September 2009, IAEA Headquarters, Vienna, Austria

Scientific Secretary: Denis Humbert

AGENDA

Monday, 7 September **Meeting Room: F08-17**

09:30 – 09:45	Opening (Robin Forrest, NDS Section) Adoption of Agenda Presentation of the new IAEA A+M Data Unit Team
09:45 – 10:00	"A Brief History of the IAEA Data Centre Network", W. Wiese

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

Chairman: T. Nakano

10:00 – 10:30	W. Eckstein (MPIP)
10:30 – 11:00	Yu. Martynenko (Kurchatov Institute)
11:00 – 11:30	*Coffee break*
11:30 – 12:00	A. Whiteford (ADAS)
12:00 – 12:30	I. Murakami (NIFS)
12:30 – 14:00	*Lunch*

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

Chairman: I. Murakami

14:00 – 14:30	D. Humbert (IAEA)
14:30 – 15:00	T. Nakano (JAEA)
15:00 – 15:30	*Coffee break*
15:30 – 16:00	Chunglei Liu (CRAAMD)
16:30 – 17:00	K. Katsonis (GAPHYOR)
17:00 – 17:30	W.L. Wiese (NIST)

Tuesday, 8 September

Session 3. Current Activities of the A+M Data Centres (Continued.)

Chairman: W. Eckstein

9:00 – 9:30 D.R. Schultz (ORNL)
9:30 – 10:00 Y. Rhee (KAERI)

10:00 – 10:30 *Coffee break*

10:30 – 11:15 B. Clark (Univ. of S.A., TX) "Web Calculations Tools"
11:15 – 12:00 Yu. Ralchenko (NIST) "XSAMS: XML Format for A+M Data"

12:00 – 13:30 *Lunch*

Session 4. Data Issues

Chairman: D. Schultz

13:30 – 14:15 M. Shimada (ITER) "ITER AM/PSI Data Needs"
14:15 – 15:15 Priorities in A+M data compilation (all participants)

15:15 – 15:45 *Coffee break*

15:45 – 17:00 Data evaluation (all participants)
Web search engine: GENIE (D. Humbert)

Wednesday, 9 September

Session 5. Miscellaneous Topics

Coordination: D. Humbert

9:00 – 10:30 Review of Data Center Network Membership criteria
Memberships: ADAS and Brazil

10:30 – 11:00 *Coffee break*

11:00 – 12:30 Plan of DCN activities for the near future
ICAMDATA

12:30 – 13:30 *Lunch*

Session .7 Demonstrations

13:30 – 15:30 Data Centre WWW Database 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

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

A. Atomic and Molecular Data

Spectroscopic Data for Atoms

Transition probabilities for Be, C, N and O and their ions are needed, as well as data for heavy elements like Fe, Cl, Kr, Mo, Cu and W.

Transition probabilities for H, D,T, He, Li, Na, Mg, Al, Si and S are done for all ionization stages at the NIST Data Center for Atomic Spectroscopy. Data compilations for Be, B, Ne, Ar and Cs are in progress.

Energy levels and wavelengths 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 possible importance for erosion measurements and for spectral comparisons.

Complete spectroscopic characterizations of heavy noble gas ions are needed. Ne is in good shape and progress is being made on Ar.

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.

S*pectroscopic Data for Molecules*

Primary interest is in H_2, H_2^*, H_2^+, H_3^+ and isotopic variants.

Impurity plasma edge molecules: CO, CO_2, CH_4, CH, C_2, BeH_2, BH, N_2 and LiH 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). Much data have been produced, but much more are needed.

Data are needed for negative ion reactions H^-+H, H^-+H_2 (e.g. detachment, excitation, dissociation) and mutual neutralization H^-+H^+, H^-+H_2^+.

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).

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 hydrocarbons and other molecules relevant to fusion devices:
Further development of the databases for hydrocarbons, H_2O and CO, and beryllium and boron 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 Jülich Reports on hydrocarbons.
There is much interest in CH excitation and a need for state resolved data.
Regarding collision processes of high-Z impurities, the CRP on "Atomic Data for Heavy Element Impurities in Fusion Reactors" is addressing some of these issues, concentrating on W and the noble gases. A CRP on tungsten will be initiated in 2010.
Data are needed in priority order for collisions of abundant ions and neutrals of W, Ar, Kr, Xe, Mo and V with e^-, H^+, H, H_2. Amongst the W stages, the neutral and singly ionized are of especially high priority.
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.

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.
Regarding interaction of the neutral beam with the plasma, collisions involving H^* are of importance.
Data for collisional processes H^- on (H^-, e^-, H, H_2, H_2^+) in ion beam that is used (after neutralization) for plasma heating. (Pertinent energy range: from threshold to 1 MeV). 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 hydrogen molecule.

Radiative Plasma Cooling
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.

Core plasma collisional data
Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (W, Ar, Ne, Kr, Xe are highest priority, with V, Ti, Cr, Fe, Ni, Mo of lower priority). Pertinent temperature range is from ~1 keV 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" addressed some of these issues.

Edge plasma collisional data
Data are needed for edge temperature (threshold to ~500 eV) charge exchange processes among intrinsic impurities and plasma components:
Collisions of X^{q+} (X = W, Be, C, He, N, O, Li, B of highest priority, with Cl, V, Ti, Cr, Fe, Ni, Mo of lower priority) with H, H_2, He, H^+ and 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^+, and H^- (for the proposed radiative cooling scheme of divertors and radiative mantle).

B. Plasma-Material Interaction

Erosion

Assessment of data needed for Be, BeO, carbon-based materials and medium- and high-Z materials (W, Ti, V, Mo, Nb). 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.

Mixed materials will arise from Be, C and W. Without means of knowing the impurity flux, it is difficult to address this issue, see results from previous CRP on mixed materials. Characterization of the mixed materials is of interest.

Characterization of erosion products such as dust, films, flakes etc.

Need exists for chemical sputtering for carbon based materials. This is being addressed by the ongoing 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.

Hydrogen isotope 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, carbon based materials, 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 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.

Molecular balance on surfaces

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

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.

C. Material Properties

Data collection and generation are needed

Data on size distribution, composition, formation etc for erosion products (dust, flakes etc) containing C, Be, W. A CRP was initiated in 2008 on dust formation and characterization.

Tritium retention in erosion products.

Chemical properties of erosion products.

Mobilization of particles. Good diagnostics will be important.

Neutron induced damage, 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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