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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 22nd Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

4–6 September 2013

Prepared by

Hyun-Kyung Chung

December 2013

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

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Abstract

This report summarizes the proceedings of the IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (22nd Meeting of the A+M Data Centres Network) on 4-6 September 2013. Twelve participants from 8 data centres of 6 Member States attended the three-day meeting held at the IAEA Headquarters in Vienna. The report includes discussions on the data issues, meeting conclusions and recommendations and the abstracts of presentations presented in the meeting

December 2013

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1. Introduction

The 22nd IAEA Technical Meeting (TM) of the Atomic and Molecular Data Centres Network (DCN) on "Technical Aspects of Atomic and Molecular Data Exchange and Processing" was held at the IAEA headquarters, Vienna, Austria from 4th to 6th of September 2013. The objectives were to review progress in atomic, molecular and plasma-surface interaction (A+M/PSI) data related activities in the data centres and to formulate work plans related to data issues for the next period.

Nine participants attended the meeting from eight data centres and a representative from the Chinese Research Association on Atomic and Molecular Data at Institute (CRAAMD) of Applied Physics and Computation Mathematics (IAPCM, Beijing, China) could not attend the meeting. A member of DCN from the first days of IAEA Atomic and Molecular Data Unit, the Controlled Fusion Atomic Data Center (CFADC) at Oak Ridge National Laboratory (ORNL, Oak Ridge, USA) has closed down and its absence was strongly felt. Three new representatives replacing their retired predecessors were welcomed to the meeting: Dr Yu. Ralchenko for Dr W. Wiese at National Institute of Standards and Technology (NIST, Gaithersburg, USA), Dr A. Kukushkin for Dr Martynenko at Kurchatov Institute (Moscow, Russian Federation) and Dr D. Kwon for Dr Y. Lee at Korea Atomic Energy Research Institute (KAERI, Dae-jeon, Korea).

Two observers attended the meeting. Dr H. Sadeghpour of Institute of Theoretical Atomic and Molecular Physics (ITAMP, Cambridge, MA, USA) was invited to discuss collaboration opportunities with theoretical atomic and molecular physicists and Dr C. Hill of University of College London (UCL, London, UK) was invited for his expertise on data exchange and database tools. The Agency was represented by Dr R. Forrest (Section Head, Nuclear Data Section), Dr B. Braams (Unit Head, Atomic and Molecular Data Unit) and Dr H. Chung (Scientific Secretary). Staff members, Dr N. Otsuka and Dr R. Capote Noy of Nuclear Data Section (NDS) were guest speakers on the topic of nuclear data evaluation.

The full list of participants is available in Appendix 1 and the adopted agenda is listed in Appendix 2. Presentations are summarized in Section 2. Discussions of various issues on the following topics:

- Exchange information on current activities: data development and data exchange
- Activities on data evaluation: experiences, plans and encouragement
- Data exchange format: status of XSAMS development and implementation
- Bibliographical databases: changing environment, a review of role and effort
- Priorities for data development and evaluation, new meetings and information exchange

The summary of discussions and recommendations on future work plans are presented in Sections 3 and 4 in this report.

2. Proceedings of the Meeting

Welcoming participants, Dr R. Forrest (Section Head, Nuclear Data Section) acknowledged that the Data Centre Network (DCN) meeting of advisory nature is very valuable for the IAEA Atomic and Molecular Data Unit (the Unit) and the recent directional change in the DCN activities to enhance efforts in data evaluation is highly appreciated. Participants introduced themselves and the agenda in Appendix 2 was adopted without a change. Dr B. Braams reviewed meeting objectives.

Presentations were organized in three sessions: 1) Current Activities in the Atomic and Molecular Data Communities, 2) Current Activities in the Atomic and Molecular Data Centres and 3) Data Evaluation. Slides of presentations are available on the Unit web site http://www-amdis.iaea.org/DCN/ via the link to Meeting Reports and Presentations. Presentations are briefly summarized here, but much more detailed summaries are presented in Appendix 3.

2.1 Current Activities of Atomic and Molecular Physics Community

Atomic and molecular activities at ITAMP and beyond, H. Sadeghpour (ITAMP)

Dr H. Sadeghpour of the Institute of Theoretical Atomic and Molecular Physics at Harvard-Smithsonian Centre for Astrophysics (ITAMP-CfA, Cambridge, MA, USA) was invited to consult the Unit and DCN members on ways to enhance collaboration with atomic and molecular physics communities and data centres, particularly on the subject of critical assessment of theoretical atomic and molecular data. The ITAMP was established in 1989 with an objective to foster theoretical atomic, molecular and optical physics (AMO) in USA. It hosts concentrated workshops and topical group meetings, train postdoctoral fellows and receive visiting scientists and speakers. Research fields of current interest to AMO community such as charge exchange collisions, H^- photo detachment, collisions involving molecules and spin-flipping collisions were introduced.

The Virtual Atomic and Molecular Data Centre (VAMDC): Recent advances and future prospects, C. Hill (UCL)

Dr C. Hill of University of College, London was invited to give an advice on the implementation of XSAMS (XML Schema of Atoms, Molecules and Solids, http://www-amdis.iaea.org/xml/) to databases maintained by DCN members. He described the current status of the European project VAMDC consortium, which has established a standard query language and significantly developed the XSAMS data format for data exchange. The VAMDC project operates a portal website where 29 data base nodes may be queried through a unified interface at http://portal.vamdc.eu/. At the portal, XSAMS formatted atomic spectroscopic data are retrieved from databases. It is also possible to convert to a format compatible for a stellar atmosphere model if necessary. The follow-up project SUP@VAMDC consortium aims to incorporate databases from non-European projects and increase the user base.

2.2 Current Activities of Atomic and Molecular Data Centres

The session was dedicated to progress reports of data centres on data activities in the period of September 2011-August 2013. Representatives of data centres presented the work done on data compilation, evaluation and generation, web developments, data centre publications, and/or the status of ongoing programmes and future plans.

Update on the NIST atomic data program, Yu. Ralchenko (NIST)

Dr Yu. Ralchenko presented the summary of updates in the numerical and bibliographic databases, a new development in web interface for retrieval of ionization energies and total binding energies of ground states of all atomic spectra. Three new updates for the Atomic Spectra Database were released most recently in September 2013 and the latest version includes almost 215,000 spectral lines and 107,000 energy levels. Progresses are made on collisional-radiative calculations and high-precision atomic structure calculations. Data compilations (F V-VIII, Ne VIIX, Th I-III, Ag II, Mn II, In II, Cr

II, Th I and U I, Sr II-XXXVIII, Cr I-II, Ti I-II, Ne IV), newly evaluated data, an improvement of databases and production of high quality theoretical and experimental data were highlighted.

Atomic and molecular data activities at NIFS in 2011-2013, I. Murakami (NIFS)

Prof Murakami of National Institute for Fusion Science (NIFS, Toki, Japan) reported the development and maintenance of databases and research activities. NIFS collisional databases consisting of AMDIS, CHART, AMOL, CMOL, SPUTY, BACKS contain 684,589 collisional data in total (as of Aug. 26, 2013) and small databases are developed for specific processes of interest. A new database of bibliography compilation for 67 atoms and molecules by Prof M. Hayashi is now available. Research activities on atomic and molecular processes in plasmas of the Large Helical Device (LHD) and on tungsten atomic data are on the way.

Current activities of Data Center for Plasma Properties (DCPP), J. S. Yoon (NFRI)

Dr J. Yoon of National Fusion Research Institute (NFRI, Dae-Jeon, Korea) reported on the activities of Data Centre for Plasma Properties (DCPP). They have developed full-set data with simulation tools for low temperature plasmas, big data systems for fusion applications with emphasis on data evaluation. The center has been participating actively in the DCN coordinated activities by organizing group evaluation meetings and participating in the AMBDAS update activities.

Status of online database and analysis tool HYDKIN for plasma edge transport, D. Reiter (FZJ)

Dr D. Reiter of Forschungszentrum Jülich (FZJ, Institut für Plasmaphysik, Germany) reported that the TEXTOR tokamak is shut down and dismantled after 30 years of operation and linear magnetized plasma devices are being built and operated for plasma-material interaction studies under the power plant relevant nuclear conditions. The database HYDKIN has been developed to provide atomic and molecular data for fusion transport simulations of boundary layer plasmas. It also provides a useful online tool based on an eigenvalue analysis of the reaction matrix, which provides a sensitivity analysis of plasma chemistry models. Recently the database was extended to include Be and N containing atoms, ions and molecules relevant to ITER operation.

Overview of A+M data applications and data needs in JT60U spectroscopic studies, T. Nakano (JAEA)

Dr Nakano of Japan Atomic Energy Agency (JAEA, Naka, Japan) reviewed the recent spectroscopic results from JT-60U and provided the atomic data needs for these studies, particularly on carbon, neon and tungsten. Measured neon and tungsten spectral lines are significantly blended and theoretical calculations are often used for line identification. Unfortunately, the uncertainty of calculated wavelengths is so large that there is a great demand for high-precision experimental line lists. For radiative power evaluation, the visible lines from carbon transitions such as C^{3+} (3s-3p: 580.1 nm) are used and evaluated collisional excitation rates are needed for spectroscopic analysis.

The updating of OPEN-ADAS approach and recent work on excitation data and population modeling, M. O'Mullane (ADAS)

Dr O'Mullane reported on the update of OPEN-ADAS website and recent work on excitation data and population modeling. A new server was installed and IT security measures were implemented. A significant quantity of new data has been uploaded including new classes of data (photo-excitation and photo-ionization). ADAS baseline excitation data are being improved and non-Maxwellian datasets are being developed.

Status and development of KAERI atomic database, D. Kwon (KAERI)

Dr Kwon described the current status and development of atomic databases at Korea Atomic Energy Research Institute (KAERI, Dae-jeon, Korea) and research activities in atomic data. Organizationally, the data centre moved to join the nuclear data centre in 2012 from the quantum optics division where it began in early 1990s. Recent research has been focused on theoretical electron impact ionization and recombination cross-sections of Fe and W ions as well as photoionization cross-sections for Be-like and Mg-like ions. Calculated data are uploaded to a newly designed database PEARL (Photonic Electronic Atomic Reaction Laboratory, http://pearl.kaeri.re.kr).

Current activity in Kurchatov Institute and Russian Federation, A. Kukushkin (Kurchatov Institute)

Dr A. Kukushkin of NRC "Kurchatov Institute" (Moscow, Russia) has presented a survey of needed and available atomic, molecular and plasma material interaction (A+M/PMI) data for fusion applications as shown in Appendix 4. Applications include H-α diagnostics in ITER, D-α high-resolution spectral analysis in JET, and data analysis of film deposition in tokamak and adatoms formation and surface sputtering. PMI data needs have been extensively identified for hot spot studies: ion sputtering of metals with simultaneous electron irradiation, tungsten recrystalization and cracking under ITER-relevant heat loads, production of damaged materials and exposure in plasma, the studies of tungsten tiles under high-flux and high-fluence irradiation and the studies of a uniform layer of B_4C boron carbide safety.

Current activities of IAEA Atomic and Molecular Unit activities, H. Chung (IAEA)

Dr H. Chung presented an overview of the activities in the IAEA Atomic and Molecular Data Unit (the Unit) in the data production, exchange and evaluation. The server of http://www-amdis.iaea.org has moved to a cloud server for better IT security and web services. There have been 3 interruptions including the last of 6 months downtime and finally the site is back to normal in September 2013. Two coordinated research projects (CRP) are concluded, two CRPs are on the way, and two CRPs are newly organized in 2012 and 2013. A project to make ALADDIN numerical database available through VAMDC portal has begun and a new way of updating collisional data to the AMBDAS bibliographical databases is investigated. The Unit has organized a series of meetings on the topic of data evaluation and recommendations and the details of meeting outcomes were presented in the session on the data evaluation.

2.3 Data Evaluation

Experimental nuclear reaction data uncertainties – needs, concepts and documentation, N. Otsuka (IAEA)

Dr N. Otsuka reviewed concepts of uncertainties and covariances of experimental cross sections as well as the propagation of uncertainties to evaluated data uncertainties. Correlations in uncertainty components were discussed and the impact of correlated uncertainties in the final uncertainty evaluation was demonstrated. Needs of rigorous uncertainty evaluation and documentations were explained. An important task of the International Network of Nuclear Reaction Data Centres (NRDC) is to receive detailed information of experimental uncertainties from experimentalists, and compile it in the experimental nuclear reaction data library (EXFOR).

Unified Monte Carlo: An evaluation method combining experimental and modeling, uncertainties, R. Capote Noy (IAEA)

Dr R. Capote Noy described data evaluation methodology employed by the nuclear data community and the impact of covariances in evaluating a neutron reaction cross section. Based on Bayes theorem (1763) where the posterior is proportional to prior times likelihood, neutron reaction cross-sections (posterior) are evaluated by combining a properly weighted combination of experimental data (likelihood) with a well-defined theoretical model (prior) which has unknown parameters to which some prior probability density is assigned.

IAEA evaluation activities, H. Chung (IAEA)

Participants in the last DCN meeting agreed that data evaluation activities should be organized in the community and recommended IAEA to organize the community efforts on the data evaluation. In the last two years, IAEA has organized two consultants meetings and two technical meetings on data evaluation and established a roadmap towards a standard library of internationally agreed A+M/PMI data. Topics of presentations and discussions include: 1) current evaluated databases, 2) evaluation methods and experiences, 3) error propagation and sensitivity analysis, 4) theoretical data evaluation, 5) experimental data evaluation, 6) data centres evaluation activities and 7) uncertainty estimates of theoretical atomic and molecular data. Presentations and reports containing discussions and recommendations from the meetings are available in the http://amdis.iaea.org/DCN/Evaluation/.

EMOL group evaluation activities, B. Braams (IAEA)

Dr Braams described the EMOL, an EU-funded project for 3 years to develop methodology for analyzing, validating and recommending electron molecule collision data sets. The goal is to recommend self-consistent and complete data sets covering the entire energy range and all processes for about 12-15 data sets. For each evaluation performed by a group of 4-7 experts, relevant papers are assembled, classified by process and distributed to participants for reviews. Participants who reviewed the papers meet for discussion to come up with recommended data sets. Consistency checks, scaling, corrections and uncertainty assignments for recommended data sets are considered in the final result. It has been agreed with the Board of European Journal of Physics D (EPJD) that the evaluations will be published as well as data available in online archives.

Group research for the evaluation of CH_4, M. Song (NFRI)

Dr M. Song of National Fusion Research Institute (NFRI, Dae-Jeon, Korea) reported on the group research meeting for data evaluation of methane collisional processes. The concept of group evaluation was recommended in the joint IAEA-NFRI technical meeting on data evaluation in 2012 and the group of 8 people with various expertize (experimentalist, theoreticians and evaluators) met three times in 2013 and worked on the evaluation of CH_4 collisional data. Results of evaluated cross-sections with uncertainties, descriptions of evaluation methods will be produced.

3. Technical Discussions

Participants discussed on various issues related to data research: data evaluation, bibliographical data compilation, data exchange formats, database development projects, and the priorities in atomic, molecular and plasma-surface interaction (A+M/PSI) data compilation and evaluation for fusion applications.

3.1 Activities on Data Evaluation

The critical need of reference data or recommended data for fusion research echoed again in this meeting. A use of reference data will benefit, for example, plasma transport modeling community regardless of the data quality. Any transport code contains a complicated chemistry model that uses extensive sets of A+M/PSI data. Even with the chemistry model fixed, however, codes will differ from one another due to the highly non-linear nature of governing equations to describe plasma transport. Therefore, a use of reference data in a chemistry model eliminates at least the uncertainty due to different data uses and makes comparisons among transport codes more straightforward and hence better understand underlying transport physics.

For diagnostics, high-precision atomic and molecular data are required and critical assessment of data and benchmarks of codes for diagnostics are desirable. The most recent workshops on spectral line shapes in plasmas organized in cooperation with IAEA provide a great opportunity to benchmark codes with various assumptions to produce line shapes relevant for H-α diagnostics. It was noted that benchmarks for practical tasks are generally more successful and effective than for purely academic purposes. With a strong motivation from practical tasks, code benchmark workshops provide an effective venue for evaluation of theoretical data.

Since the last DCN meeting, much has been accomplished in data evaluation by community. Since an evaluation procedure by a group of experts was suggested in the NFRI-IAEA TM in 2012, it has already been producing internationally agreed evaluated data sets. Currently, several group panels are conducting evaluations of electron-molecule scattering data. EMOL, an EU-funded project plans 12-15 evaluations over the period 2013-2015. NFRI organizes group meetings for methane evaluation in 2013 and plan a series of evaluation meetings on new elements. Both projects will publish final evaluated and recommended cross-sections for total and individual molecular processes.

As data evaluation was performed by a group of evaluators in the similar format of a journal review panel, the objectivity and credibility of results increase, however, it was not easy for all experts to agree on a single result. Evaluators with different views and experiences are likely to have different opinions and it required intense discussions to settle the differences. Often, the discussions lead to a new understanding of physics or a need of new data to resolve the discrepancies. All the considerations and suggestions will be documented.

As a topic for the next group evaluation, molecules relevant to fusion applications such as BeH and BeH^+, the break-down chains of CH_4 and C_2H_6 (C_xH_y and $C_xH_y^+$) and N_2^+ were suggested. A group evaluation for electron-atom processes is currently planned for e-Be and e-Ne where high-precision, best available data of R-matrix and convergent close-coupling (CCC) calculations as well as the distorted wave calculations will be evaluated. It aims to produce a guideline or a workflow for evaluation as well as internationally agreed recommended data sets.

The starting point of any evaluation is the selection of data sets and the selection criteria were discussed. If evaluated data already exist, they provide the initial set of data for evaluation already. If not, a large amount of data should be collected and the qualified ones should be selected. The first criterion is the existence of uncertainties in the case of experimental data. However, theoretical data are hardly presented with uncertainties and it makes evaluation using both experimental and theoretical data sets extremely difficult.

In order to address the issue of uncertainty estimates of theoretical data, the Unit organized a TM of International Code Centre Network on this subject and plans to organize a meeting jointly with ITAMP (Institute of Theoretical Atomic, Molecular and Optical Physics), a leading organization in

theoretical atomic and molecular physics with broader community. The dates are set to be July 7-9, 2014, at ITAMP located in Cambridge, MA, USA.

A completely new way of data evaluation was proposed in this meeting, data evaluation by a very large group of users. Recently crowdsourcing has emerged as an alternative way of peer reviews for scientific work, motivated by successes of social network services. Casual reviews by article readers will not replace current refereeing system for journal publishing yet, but the success of arXiv.org, open-access to e-prints in a number of physics communities indicates that this new way of peer reviews are shaping up as an alternative solution to expert reviews. The quality of a paper submitted to arXiv.org is judged by citations and statistics. In the similar way, data are submitted to an open-access place, and the quality of data may be judged by data users in a statistical sense.

As the number of experts is decreasing in the field of data evaluation, this idea seems to have a tremendous potential and make every user an evaluator. In addition, it will bring data users and producers together in a community and bridge the gap between the two communities. On the other hand, it seems yet premature to adopt this method when data producers are not even used to the idea of their data being evaluated by experts, let alone by a group of non-experts. In addition, there is a risk that non-expert users evaluate data based on insignificant criteria such as ease of uses, completeness over energy ranges or availabilities instead of quality itself. Nevertheless, it would be worthwhile considering an option open to adopt advantages of both expert panel evaluation and user evaluation systems for the future.

3.2 Bibliographic Data Compilation

There is no question about the great value of maintaining the bibliographic database such as AMDAS. Test searches on Google scholar, DiRef database diatomic spectroscopy database, Computational Chemistry Comparison and Benchmark database (NIST) demonstrated how easy and fast the AMBDAS database can provide bibliographic information of data sets for $e+N_2^+$ dissociation processes. The question is how and who will maintain the database.

Since the CFADC at ORNL stopped providing the data for collisional processes and plasma-surface interaction, data centres have been seeking a way to collaborate on the issue and finally reached an agreement to resume the collection of bibliographic data for collisions as a joint activity. Four data centres of NFRI, NIFS, KAERI and IAEA volunteered to collect bibliographic data for electron, photon and heavy particle collisions as well as plasma-surface interactions.

The procedure was formulated as follows. Initially, queries based on well-defined keywords will be performed on the web of science or the similar services to find journal articles. The list will be first reviewed by the Unit to filter out irrelevant articles. Then articles in the filtered list will be collected and reviewed by scientists of each data centre. If an article contains collisional data or plasma-surface interaction data in tables or figures then the article will be classified according to the IAEA classification system (http://www-amdis.iaea.org/DCN/ProcessClassification.pdf).

An idea of involving students was discussed in bibliographical data compilation. Though analysis should be done by scientists, technical help can come from students for tasks such as article collection, transfer of data to SQL format and database update.

A numerical database of data sets contained in the articles of AMBDAS databases was discussed. The EXFOR database maintained by nuclear data community contains all experimental nuclear reaction data published by researchers worldwide. Experimental nuclear data contained in published articles are digitized and compiled by a group of nuclear scientists in the International Network of Nuclear

Reaction Data Centres Network (NRDC) coordinated by the IAEA Nuclear Data Section. The idea is great but it will not be feasible with the current limited resources in the Unit.

3.3 Numerical Database Development

There is a serious interest in a numerical database of high accuracy diatomic potential energy curves (PEC), which provide fundamental input properties for molecular processes as well as atom-atom (ion) collisions. DCN is supportive of the project to develop a new database of potential energy curves, dipole coupling coefficients and possibly matrix elements. The scope of database will include elements mainly for fusion and other applications such as cold atom collisions or astrophysics. Highly accurate potential curves and long-range coefficients are required for cold atom studies, which may provide a test bed for potential curves. Uncertainty analysis of PEC will be feasible when compiled data sets of the new database are compared for evaluation.

The Unit is interested in hosting a PEC database. It was suggested to pick a target for a feasibility study. Relevant bibliographical data will be collected and classified before numerical data are extracted and available in a functional or tabulated form. The database will be useful for researchers to deposit PEC data as supplementary information for collisional calculations.

DCN also discussed the improvement of plasma-material interaction databases, especially the uncertainties associated with Binary Collision Approximation (TRIM family) codes and their sensitivities to surface binding energy parameters. The widely used TRIM results on sputtering yields and reflection coefficients have changed over a period of time and the change seems solely attributed to the changes in surface binding energy parameter. Collaboration with atomic physics community in the field of atom-surface interaction, dynamic polarizability or sticking coefficients was suggested to benchmark the parameters.

3.4 Data Exchange Format

The XSAMS (XML Schema for Atoms, Molecules and Solids) project was first proposed by DCN in 2003 and developed by the XSAMS steering committee with the support from the Unit. Since the first version was launched in 2009, it has been actively used for data exchange through VAMDC project. However, the development of XSAMS project is not yet complete. The schema for atoms and molecules is in a mature state, but the schema for plasma-surface interaction data or kinetics needs more work. Currently, there is no immediate plan for the Unit to support the further development until the implementation of XSAMS is carried out and it is actively and widely adopted as a data exchange format by user communities.

A few data centres are interested in implementing XSAMS as an output format of data search and eventually making their databases available through the VAMDC portal. ALADDIN database at IAEA was modified to provide XML formatted data to VAMDC query, which was demonstrated in the DCN meeting. Currently, IAEA, NIFS, NIST and KAERI have a partnership with SUP@VAMDC project, the second phase of the VAMDC project which ended in 2012.

There was a debate on how much DCN should be involved in SUP@VAMDC project. The primary objective of DCN activities is to support fusion applications while the VAMDC project is mainly focused on astrophysics communities. The SUP@VAMDC project aims to provide fundamental atomic and molecular data to any science community including fusion community, industry plasma community or even biomedical community. As many fusion scientists turn to ADAS for their data needs, it is debatable how much relevance the VAMDC portal will have for fusion applications. It is however clear that the VAMDC portal provides a framework not only for researchers to retrieve

fundamental data sets ever so easily from databases worldwide but also for the datacentres to exchange data sets among themselves. It serves greatly the main goal of DCN that data centres seek ways to exchange data for collaboration.

Other ways of data exchange were briefly discussed. NFRI is interested in their database to be accessible through GENIE, a search engine at IAEA, but their web server needs to be moved outside the firewall. Many fusion scientists have a module to read ADAS data file for fusion applications. A conversion tool from XSAMS outputs to ADAS files would be valuable for fusion community to have a ready access to non-ADAS data.

3.5 Priorities in Atomic and Molecular Data Compilation and Evaluation

The review of long-term priorities in A+M/PMI data compilation, evaluation and generation has been conducted since the beginning at the IAEA Technical Committee Meeting on "A+M Data for Fusion Reactor Technology" held in 1992 and the list served as a reference for the A+M/PSI data producers to understand data needs of direct importance to fusion research. However, the list as it stands is too general to give specific information on priorities in processes and elements for data evaluation and production. In 2011, the Unit proposed to compose a new list of data needs discussed in various technical meetings and research coordination meetings and to incorporate inputs from the user community. An online survey was developed to obtain information on both data needs and available data sources from users, but it could not be completed due to the problems with IT security policies at IAEA.

Excellent examples of a way to collect information on the applications and availabilities of A+M/PSI data were presented by Dr Kukushkin as shown in Appendix 4. Communicating with his colleagues in Russia, he formulated a list of data uses, which consists of descriptions of fusion application, task to be performed, relevant publication, fundamental processes for consideration, sources of current data used in the application and specific data needs for the task. The examples provide a clear description of how specific data sets of fundamental processes and particular elements are used in a particular fusion application and how accurately they should be known. The list prioritizes immediately data needs in the context of fusion research, and makes it easier for producers and users of required data to have direct communication by providing detailed information on both sides of A+M/PSI data and fusion applications.

Motivated by the examples presented by Dr Kukushkin, it was proposed that the 7 domestic agencies of ITER member states should be contacted for the survey on data needs and availabilities from fusion scientists in their countries. The EU agency is responsible for neutral beam diagnostics and the Russian agency for spectroscopic diagnostics. Therefore domestic agencies will be in a good position to conduct a survey and obtain information from their scientists in the relevant tasks. Topical physics groups in the International Tokamak Physics Activity (ITPA) operated under the auspices of ITER are also good candidates to collaborate on this issue. A survey of data needs, task descriptions as well as current data sources from fusion scientists will help identifying the most urgent needs and priorities for evaluation and compilation.

In order to directly support the ITER/DEMO design activities, quantification of required accuracies, or “target accuracy” of data sets was proposed. There exists a limit in any design of fusion devices that the total uncertainties from all uncertainties of sciences and technologies used for the design should not exceed. For instance, the ITER Measurement Requirements (MR) stipulates the H-α and Visible Spectroscopy Diagnostic to provide 20% accuracy for the fuel ratio in the edge and 30%, for neutral hydrogen influx in the main chamber. Once the design accuracy is known, one can define the accuracy limit of the related fundamental data, for example, the accuracy of the charge exchange rates to meet

the ITER MR for H-α diagnostic can be prioritized to reduce the uncertainties of most sensitive data sets. Generally a sensitivity analysis can determine the "target accuracy", that is, the required accuracy where the propagation of data uncertainty should not exceed the limit of design accuracy on specific applications. Based on this information, the efforts of evaluation and compilation can be prioritized to reduce the uncertainties of most sensitive data sets.

4. DCN Membership

The terms of reference for the AM/PSI Data Centre Network are as follows: 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

The data centres of NFRI and FZJ which participated in the last meeting for the first time were accepted to the DCN membership without any objection. As old data centres stop data activities and new data centres are established, the DCN membership of existing data centres will be reviewed regularly and new research organizations with data centre activities will be actively sought out.

5. Data Centres Web Interface and Software Presentations

Dr Ralchenko, NIST, presented the new version of NIST atomic spectra database (ASD). More than 7000 lines of neutral tungsten are easily accessible by a new diagram of lines and levels holdings. Currently W and Fe lines are most populated. A new database of ionization energies was shown and a spectrum calculation consisting of NIST ASD lines was demonstrated for a given temperature based on the Saha-LTE assumption. For non-LTE spectra, FLYCHK code at NIST website can be applied for simple analysis.

6. Meeting Conclusions and Recommendations

DCN members reviewed and advised activities of DCN and the IAEA A+M Data Unit to benefit both DCN and fusion community on the topics of data exchange format, bibliographical data compilation, data evaluation, database development and data needs. This meeting was highly productive and the collaboration and communication between data centres and the Unit were highly valuable Recommendations and work plans in the future are summarized in this section.

6.1 Meeting Proposals

The following meetings and workshops are recommended in support of IAEA A+M Data Unit activities with an emphasis on data evaluation:

- A Joint ITAMP-IAEA Technical Meeting on uncertainty assessments of theoretical scattering data will be held in Cambridge, MA, USA, on the dates July 7-9, 2014. We expect 20-30 scientists working on the computational physics of electron-atom, electron-molecule and heavy particle collisions. The meeting is expected to provide a convenient venue for many USA scientists who have done much work in this field.

- An IAEA Technical Meeting on atomic, molecular and plasma-surface interaction data for fusion will be held in Dae-jeon (or Gun-San) in Korea on the dates of November 25-28 (or 29), 2014, following the national plasma meeting in Japan in the previous week. This meeting is the 4th in the series organized by this Unit in every 10 years. Approximately 60 participants were exclusively nominated by their government and attended the last meeting in 2002. Since all the previous meetings were held in Europe, it is appropriate to hold the next meeting in Asia to attract fusion scientists in the region where China, Japan and Korea are the member states of ITER. A plasma conference organized by the Japanese Physical Society, Japanese Society of Plasma and Fusion Science, and Japanese Society of Applied Science is scheduled in November 17-21 and the back-to-back meetings in Japan and Korea will help researchers of Europe and USA attending both meetings.

- An ICTP-IAEA conference is scheduled to be held during the week of November 3-7, 2014, at Trieste, Italy. The topics will include models and data for plasma-wall interaction in fusion devices. Approximately 30 participants with advanced knowledge on the topics are expected.

- The 16th international workshop on Radiative Properties of Hot Dense Matter will be held in September 29 – October 3 of 2014 in cooperation with IAEA in Vienna. The 4th technical meeting of international Code Centres Network (CCN) is on the agenda of 2014-2015.

- IAEA should continue training schools such as the previous ICTP-IAEA workshops or IAEA schools in India. There is no organization or entity other than the IAEA that can organize such a school for next generation scientists to enlighten the importance of A+M/PSI data for fusion applications. DCN strongly recommends workshops or schools to educate and enlighten young fusion scientists,

6.2 Data Issues

Work plans are recommended on a number of data issues and several steps were identified to reformulate the priority list of data evaluation and compilation.

- Coordinate the compilation and classification of bibliographical information for collisional and plasma-surface interaction processes
    - IAEA, KAERI, NFRI and NIFS will participate in the coordination of bibliographical data compilation
- Develop the numerical database for di-atomic potential energy curves relevant to fusion and other applications
- Encourage the implementation of the XSAMS as data exchange format.
    - With the completion of VAMDC project, IAEA should continue to work with XSAMS steering committee on the future of XSAMS development.
- Contact 7 domestic agencies to obtain detailed information on applications of their interest.
    - Obtain clear descriptions of a specific application, data needed by the application, current data used by the application and required sensitivities or measurement accuracy limits required by ITER design

    - Use the example list in the Appendix 4 or develop more focused template
- Define "target accuracy" of A+M/PSI data used for specific applications by sensitive analysis
- Document and inform community of the specific information on the measurement accuracies of ITER applications and target accuracies of required data sets
- Redesign the IAEA wiki pages for better presentation of data priorities by including:
    - Description of specific applications
    - Description of specific data needed for the applications
    - Currently available and used data sets
    - Completeness in data availability and data needs
    - Assessment of data qualities
    - Application design accuracy and data target accuracy (Sensitivity)
    - Recommendation from experts
    - Recommendation to data producers

6.3 Outreach Programs

DCN identified the need to enhance communication with A+M/PSI community and fusion community. More efforts in this regard were recommended.

- IAEA should encourage A+M scientists to organize an invited session or panel discussion session at DAMOP, ICPEAC, APS-DPP or APIP meetings on the importance of data evaluation and uncertainty estimates of theoretical data
    - It will provide a great opportunity to reach out to the broader A+M data community.
- IAEA should engage in activities of enlightening A+M/PSI physicists about fusion applications and the role of fundamental data and fusion scientists about the values and applications of A+M/PSI data research.
- IAEA should assist A+M/PSI community to recognize research activities of shared interest with fusion community and the relevance of their work.
    - While the A+M community often pursues to obtain the highest possible precision data, a lesser-quality data may still be perfectly suitable for some fusion applications.
- IAEA should keep a close contact with ITPA topical groups by attending their meetings and engaging them in the IAEA meetings.
    - It is critical to make fusion community aware that much more data are needed yet, on the contrary to the convenient belief of user communities that much more data have been produced.
- Collaboration among data centres is extremely valuable and should be actively pursued.
    - J. Yan of CRAAMD visited NIST in 2013 for 6 months and had a fruitful collaboration on evaluation of atomic structure and transition probabilities
- IAEA should continue to support and collaborate with the VAMDC, SUP@VAMDC projects, EMOL projects and other projects to engage atomic and molecular data research.
- DCN should consider working with ITAMP for the proposal to the Smithsonian Institution for archiving old reports containing data existing in data centres.
    - The Smithsonian Institution of USA holds an annual competition for grants for its Archives. Many old reports containing data exist in data centres and various laboratories. Reports from the CFADC at ORNL of more than 50 years of history should be found and archived.

Appendix 1

List of Participants

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Appendix 2

Agenda

Wednesday, 4 September **Meeting Room: A0531**

09:30 – 10:15	Opening (Robin Forrest, Nuclear Data Section Head) Introduction of Participants Review Meeting Objectives (B. Braams) Adoption of Agenda (H. Chung)
Session 1:	Current Activities of the A+M Data Communities
Chairperson:	H. Chung
10:15 – 10:55	H. Sadeghpour (ITAMP) : Atomic and molecular activities at ITAMP and beyond
10:55 – 11:15	***Coffee break***
11:15 – 11:40	C. Hill (UCL): The Virtual Atomic and Molecular Data Centre: Recent Advances and Future Prospects
Session 2:	Current Activities of Data Centres
Chairperson:	D. Reiter
11:40 – 12:05	Y. Ralchenko (NIST): Update on the NIST Atomic Data Program
12:05 – 12:30	I. Murakami (NIFS): Atomic and Molecular Data Activities at NIFS in 2011-2013.
12:30 – 14:00	***Lunch***
Chairperson:	M. O'Mullane
14:00 – 14:25	J.S. Yoon (NFRI) : Current Activities of Data Center for Plasma Properties(DCPP)
14:25 – 14:50	D. Reiter (FZJ) : Status of online database and analysis tool HYDKIN for plasma edge transport
14:50 – 15:15	T. Nakano (JAEA) : Overview of A&M data applications and data needs in JT-60U spectroscopic studies
15:15 – 15:35	***Coffee break***
Chairperson:	T. Nakano
15:35 – 16:00	M. O'Mullane (ADAS) : The updating of OPEN-ADAS and recent work on excitation data and population modelling
16:00 – 16:25	D. Kwon (KAERI) : Status and Development of KAERI Atomic Database

16:25 – 16:50 A. Kukushkin (Kurchatov Institute) : Current activity in Kurchatov Institute and Russian Federation

16:50 – 17:15 H. Chung (IAEA) : Current activities of IAEA atomic and molecular data unit

19:30 ***Social Dinner***

Thursday, 5 September **Meeting Room: A0531**

Session 3: Data Evaluation

Chairperson: Y. Ralchenko

09:00 – 09:45 N. Otsuka (IAEA) – Experimental nuclear reaction data uncertainties - needs, concepts and documentation

09:45 – 10:30 R. Capote Noy (IAEA) -- Unified Monte Carlo: An evaluation method combining experimental and modelling uncertainties

10:30 – 10:50 ***Coffee break***

10:50 – 11.10 H. Chung (IAEA) – IAEA evaluation activities

11:10 – 11.30 B. Braams (IAEA) – EMOL group evaluation activities

11:30 – 11.50 M. Song (NFRI) – Group research for the evaluation of CH_4

11:50 – 13:30 ***Lunch***

Session 3: Data Evaluation (continued)

Chairperson: J. Yoon

13:30 – 14:30 Coordinated activities on data evaluation (all participants)

Session 4: Bibliographical Data Compilation

Chairperson: I. Murakami

14:30 – 15:30 Coordinated activities on bibliographical data compilation (all participants)

15:30 – 16:00 ***Coffee break***

Session 5: Numerical Database Development

Chairperson: B. Braams

16:00 – 17:00 Coordinated activities on recommended numerical databases (all participants)

- A database of di-atomic potential energy curves
- A database of recommended electron-atom collisional data
- A database of plasma-material interaction data

Friday, 6 September **Meeting Room: A0531**

Session 6: Data Needs for Fusion Research

Chairperson: D. Reiter

09:00 – 10:20 Priorities in A+M/PMI data compilation and evaluation (all participants)

10:20 – 10:40 ***Coffee break***

Session 7: Data Exchange

Chairperson: Y. Ralchenko

10:40 –12:00 Data exchange format: xsams, adas, genie, (all participants)

12:00 – 13:30 ***Lunch***

Session 8: Review on Data Centres Network Activities

Chairperson: B. Braams

13:30 – 15:00 Plan of DCN activities for the future

- Coordinated activities on data evaluation
- Coordinated data collection for bibliographical database AMBDAS
- XSAMS implementation of DCN members
- Coordinated activities to establish a list of critical data needs for fusion
- Proposed meetings and workshops on AM/PSI
- Outreach to A+M/PMI scientists outside our community

15:00 – 15:20 ***Coffee break***

Session 9: Meeting Conclusions and Recommendations

Chairperson: H. Chung

15:20 – 16:00 Data centre WWW database and software demonstrations
16:00 – 17:00 Formulation of meeting conclusions and recommendations
Date of next meeting

17:00 – ***Adjourn of the Meeting***

Appendix 3

SUMMARY OF PRESENTATIONS

VAMDC: The Virtual Atomic and Molecular Data Centre: Recent Advances and Future Prospects

C. Hill and J. Tennyson
Department of Physics and Astronomy, University of College - London, UK

This presentation gave a summary of the current status of the VAMDC project: its achievements, standards and infrastructure. Since 2010, the VAMDC have established a standard query language, significantly developed the XSAMS data format for interoperable exchange of atomic and molecular data, and begun to operate a "portal" website at which 29 database nodes may be queried through an online interface (http://portal.vamdc.eu/).

To date, the VAMDC project has largely been focused on European databases (with the notable exception of the HITRAN database, which is managed by the Harvard- Smithsonian Center for Astrophysics), and a major goal of its follow-up, SUP@VAMDC, is to incorporate databases from non-European sources.

To this end, the members of the SUP@VAMDC consortium have been disseminating information about the project, running tutorials and workshops, and providing expertise to individual data providers who wish to set up a database "node", compatible with the VAMDC standards; this typically requires some customizing of the VAMDC node software and it is necessary for the database to be stored using some kind of relational database management system (e.g. MySQL).

In addition to a demonstration of the VAMDC portal itself, a case-study of the implementation of the VAMDC standards in an active research project was given: using the Spectroscopy Made Easy suite of spectral-fitting software, it is possible to query a VAMDC database node for (atomic) spectroscopic data, transform the resulting XSAMS document into a format suitable for input to a stellar atmosphere model, and then fit a stellar spectrum using the retrieved atomic line list to retrieve stellar parameters and atom abundances.

Future progress within the VAMDC project is geared towards increasing the user base, adding more database nodes, and writing more tools to convert XSAMS to various commonly-used data formats. In the longer term, it is envisaged that XSAMS and the VAMDC will cater for particle-surface interactions and solid-state properties.

Update on the NIST Atomic Data Program

Yu. Ralchenko, A. Kramida, J. Reader, C. Sansonetti, R. Ibacache, J.D. Gillaspy
National Institute of Standards and Technology

Over the last two years the Atomic Data Program has been actively advanced with addition of new evaluated data, improvement of databases, and production of high-quality theoretical and experimental data. In particular, three new updates for the Atomic Spectra Database were released, i.e., v. 4.1.1 in November 2011, major update 5.0.0 in July 2012, and the most recent v.5.1 in September 2013. The latest of these includes almost 215,000 spectral lines and 107,000 energy levels.

A new web interface is developed for retrieval of ionization energies and total binding energies of ground states of all atomic spectra. Ionization energies and ground states added or revised for all spectra of all elements up to Ds (Z=110). About 4900 of those ionization energies (5844 in total) are new, and about 400 have been updated. Uncertainties have been added or revised for all ionization energies.

The bibliographic databases has also been expanded and improved. Currently, the Atomic Energy Levels and Spectra database contains about 18,500 references, Atomic Transition Probabilities database contains about 8,800 references, and the Atomic Line Broadening and Shifts database contains about 6,800 references. The new bibliographic collections are annually submitted to IAEA.

A number of data compilations were published since Sep 2011, for instance, data on F V-VIII, Ne VIIX, Th I-III, Ag II, Mn II, In II, Cr II, Th I and U I, Sr II-XXXVIII, Cr I-II, Ti I-II, Ne IV.

We continue maintenance of the online collisional-radiative code FLYCHK (in collaboration with IAEA). Currently we have more than 600 users from various countries. Theoretical work concentrated on high-precision atomic structure calculations (C. Froese Fischer) and collisional-radiative modeling of EBIT and fusion plasmas (Yu. Ralchenko). We also maintain active collaborations with other members of DCN including IAEA, IAPCM, NIFS, and FZJ.

Atomic and Molecular Data Activities at NIFS in 2011-2013

I. Murakami
National Institute for Fusion Science (NIFS)

Dr Murakami of presented the current activities of the development and maintenance of databases, research activities related to atomic and molecular data and the publication of NIFS-DATA-reports during the last two years.

The NIFS databases of collision processes (http://dbshino.nifs.ac.jp) contain 684,589 in total (as of Aug. 26, 2013). The databases consist of AMDIS (electron impact ionization, excitation, and recombination cross sections and rate coefficients), CHART (charge transfer of atom – ion collisions cross sections), AMDIS MOL or AMOL (electron collision with molecules), CHART MOL or CMOL (heavy particle collision with molecules), SPUTY (sputtering yield of solid) and BACKS (reflection coefficient of solid surface). During the last two years, new data were added mainly for AMDIS, AMOL and CMOL. A list of bibliographies of which data are newly included in the databases is shown in the web page. The tables on species which data are stored in AMDIS EXC, ION, AMOL, and CMOL are updated. The AMDIS database is accessible through the GENIE search engine as the queries via the GENIE count as 20~27% of the total. Collaboration with the VAMDC project starts on implementing the e-infrastructure of the VAMDC to the NIFS databases.

In addition to the main collisional databases, there are small databases developed for specific processes. For example, databases of rate coefficients of electron dissociative attachment of molecular hydrogen, differential cross-sections of molecules by electron impact, differential ionization cross-sections of hydrogen by proton impact, sputtering yields, photo-absorption cross-sections are available. A new database of bibliography compilation for 67 atoms and molecules done by Prof M. Hayashi is now available. PDF files of the NIFS-DATA reports and IPPJ-AM reports are available.

There are two main research activities related to A+M data: 1) A collaboration group has worked for research on A+M processes in plasma using the Large Helical Device (LHD) and 2) a project on tungsten has progressed with atomic physicists and plasma physicists in Japan. Projects include EUV

and visible spectral measurement of W ions in Tokyo-EBIT, CoBIT and LHD, atomic structure calculations and collisional-radiative model of W ions and sputtering experiments of W target. EUV spectra of rare-earth elements and Bi are measured with LHD. A collaboration group organized with atomic physicists from Japanese universities have worked on atomic data, spectra and collisional-radiative models for W ions. Basic cross section measurements on charge exchange processes of W ions and H atom are to start.

Status of Online Database and Analysis Tool HYDKIN for Plasma Edge Transport

D. Reiter
Forschungszentrum Jülich GmbH, Institut für Plasmaphysik, Germany

A brief report was given on upcoming shut down and dismantling of the TEXTOR tokamak at FZ Juelich after this year, after 30 years operation, and also on the currently ongoing built-up and operation of linear magnetized plasma devices. One of them is located inside a hot cell laboratory to study plasma material interaction under the (fusion power plant relevant) nuclear conditions.

Atomic and molecular data are of relevance in fusion boundary layer plasmas, because reactive processes actively influence (and even control) the plasma flow and divertor dynamics in the near target surface domain in reactors.

These data are an important ingredient in fusion transport simulations of advective-diffusive-reaction type (codes such as B2-EIRENE (SOLPS) in EU or SONIC in Japan). Data at the most detailed level enter such transport simulations in kinetic (microscopic) model components, i.e. neutrals (atoms and molecules, molecular ions, and weakly ionized impurity ions such as e.g. W, N, C, Be, He), whereas the macroscopic (fluid) components use condensed, reduced information and atomic collision processes.

The database HYDKIN has been set up and is currently being developed to publicly expose the unprocessed raw A&M data used in B2-EIRENE. The underlying A&M dataset has either been compiled at FZJ in the past (e.g. the current hydrocarbon, and silane cross section databases), or data have been taken from publicly available other datasets (e.g. ADAS) or CR codes (H, H2, He) from NIFS.

The second purpose of the online tool HYDKIN is processing and analyzing data, prior to their activation in complex transport models. 1D (either time or, recently, also 1 spatial coordinate) test cases are solved, based upon an eigenvalue analysis of the underlying reaction master matrix. This enables a forward sensitivity analysis (evaluation of sensitivity coefficients defined as logarithmic derivative of a CR population density wrt. reaction rate coefficients).

The eigenvalue analysis carried out on plasma chemistry models in HYDKIN gives direct indications about the existence of underlying reduced chemistry models (e.g. by a separation of fast against slow modes). A targeted application here was a $H/H_2/H_2^+$ CR model, because presence of vibrational excitation at least of ground state H_2 (and isotopomeres) provides a rather continuous spectrum of time scales, strictly ruling out condensation of vibrational kinetics into bundled rates.

Recent extensions of HYDKIN datasets have started with respect to the Be, BeH, BeH+ system, and the N, N^+, N_2, N_2^+ N_2^- system, the former because of its relevance due to the choice of Be as ITER (and JET) main chamber material, the latter because of its possible important role as active edge plasma cooler in case of all metal divertors. Whereas the database wrt. the Be-family is rather sparse, the issue wrt. N, N_2,… is just opposite: the huge amount of data available (e.g. from atmospheric

research, space vehicle re-entrance issues, etc., requires primarily a critical evaluation and recommendation for the fusion community.

Another major data need as related to the ionization-recombination-radiation rates of tungsten from edge plasma (few eV) to core reactor temperatures (several 10 keV) . There are indications that significant progress has been achieved here in the last years, at least allowing to somewhat constrain the uncertainty in databases, which, however, due to lack of an overall critical evaluation and recommendation appears not to have been recognized and utilized in the fusion transport modeling community.

Overview of Atomic and Molecular data applications and data needs in JT-60U spectroscopic studies

T. Nakano
Japan Atomic Energy Agency, Naka, Japan

This presentation reviews recent important results in spectroscopic studies in JT-60U from low Z (C) to high Z (W) element and provides atomic data needs through the experience in these studies.

Carbon: in high-density and low-temperature divertor plasma with an X-point MARFE, it was found that C^{3+} and C^{2+} radiation contributed 60% and 30%, respectively, to the total radiative power. Volume recombination of C^{4+}, in addition to ionization of C^{2+}, was the source of C^{3+}, indicating that the volume recombination, which converted lowly radiative C^{4+} (He-like) to highly radiative C^{3+} (Li-like), was a key process to radiation enhancement in the low-temperature divertor plasma.

Neon: in Ne seeded divertor plasma, it was found that Ne radiation contributed up to 60% of the total radiative power. Similarly to C^{4+}, Ne^{8+} (He-like) volume recombination supplied Ne^{7+} (Li-like). This is one of the leading processes that enhanced the radiative power from highly charged Ne ions.

Tungsten: With increasing toroidal rotation velocity in the opposite direction to the plasma current, W accumulation in the core plasma was significant and the W density reached 0.1% of the electron density. The W density decreased with increasing toroidal rotation velocity in the same direction as the plasma current. The central heating by neutral beam or electron cyclotron wave was effective to reduce the W density.

Through the experience in these studies, atomic data needs are summarized as follows; carbon spectral lines were well isolated, and thus could be identified without help of theoretical calculation. In contrast, Neon and W spectral lines were difficult to be identified with only experimental line list database because of significant line blends. Thus, theoretically calculated spectrum was needed to identify the lines. However, because of inaccuracy of the calculated wavelength, for example 3% difference for Ne VIII 2s-2p spectral line from the measured wavelength, the experimental line list database is still needed in addition to the theoretically calculated spectrum. All excitation rate, used in collisional-radiative models, were taken from theoretically calculated data. Hence experimental data evaluation is important in particular for important transitions such as C^{3+} (3s-3p: 580.1 nm), which is a useful visible line for radiative power evaluation.

OPEN-ADAS developments since the last DCN

M. O'Mullane
ADAS, University of Strathclyde, Glasgow, UK

The first deployment of OPEN-ADAS was based on v3.0 of ADAS and made available a subset of the ADAS data in a number of ADAS classes. ADAS Data Format (adf) files for fusion relevant modelling and diagnostic interpretation in the following classes was provided:

- adf01 : Charge exchange cross sections
- adf04 : Resolved specific ion data collections
- adf07 : Electron impact ionisation rates
- adf08 : Radiative recombination rates
- adf09 : Dielectronic Recombination coefficients
- adf11 : Iso-nuclear source and power coefficients
- adf12 : Charge exchange effective emissivity coefficients
- adf13 : Ionisation per photon coefficients
- adf15 : Photon emissivity coefficients
- adf21 : Beam stopping coefficients
- adf22 : Beam emission coefficients.

The first 5 classes are fundamental atomic data and the remainder are effective coefficients, mediated via a population model to be used in data analysis of finite density, collisional plasmas. Approximately 4000 datasets, or 1.6Gb, made up the OPEN-ADAS database.

Technically OPEN-ADAS was a php presentation layer on top of an MySQL database. The ADAS datasets were queried to extract meta information and this was used for the searching. Free-form and data class specific search was provided. The final delivery was a complete dataset based on the philosophy of the ADAS system, where a complete set of data, useful for modelling is the starting point. This does demand that the user may need to undertake a post processing step in order to extract a particular piece of data, eg an ionisation rate or a transition probability, since these are delivered as an ensemble of data. It should be noted that computer code for reading each data class is also provided as a download. Given our resources, and practical experience in using atomic data for modelling, this is a reasonable balance of making data available and not diverting time into marginally useful work.

The original system had a registration requirement. Unfortunately the system was vulnerable to an SQL injection attack and was duly compromised. Although knowledge of the users profiles is useful, it is not strictly necessary since funding is not driven by the usual web metrics of unique users, volume of downloads etc. The cleanest solution was to remove any registration requirement and simply allow free download of the data. The restrictions prohibiting systematic data downloading, on re-hosting OPEN-ADAS sourced data and acknowledging the source of the data remain. Arrangements for institutions/modelling codes to use and distribute OPEN-ADAS data are welcomed.

OPEN-ADAS was taken down for a period of 6 weeks while the registration part was removed and the web code hardened against SQL injection attacks.

In the same timeframe between DCN meetings, the University of Strathclyde lead a support action under the EU Framework 7 programme on providing support for atomic data for fusion in Europe. The results of this work were planned to be disseminated as a set of documentation and as ADAS datasets. The wider distribution of these data is via OPEN-ADAS. As part of the activity the OPEN-ADAS

website was refreshed. The service of a professional web design company was used to re-design the user experience and to further harden the underlying web code. The new system was deployed in February 2013.

The distinction between fundamental and derived data was made clearer, the former being of more interest to the atomic data producers, the latter specifically designed for use by the plasma modelling and diagnostics community. New data classes were also added, specifically a more elaborated state resolved radiative recombination rate coefficients, photo-excitation and photo-ionisation rate date (adf48, adf38 and adf39). These are of particular interest to astrophysical models and ADAS has always reflected the substantial overlap of interests between the fusion and astrophysical data needs.

The data in the existing OPEN-ADAS data classes was brought up to date with v4.0 of ADAS. This included substantial new sets of calculations of excitation data in collision strength and effective collision strength forms. These are calculated in the same distorted wave model. The collision strengths will be used, within ADAS, to advance the population modelling of impurities in plasmas with non-Maxwell electron distributions. Derived coefficients with specified non-Maxwellian EEDFs may be added to OPEN-ADAS but the usability of such data must be studied before a release.

The current OPEN-ADS contains nearly 14000 files and is now 16.5Gb of data. Some highlights of the new data include:

- A generalized collisional-radiative set of data for silicon.
- A set of adf11 data for tungsten assembled for Asdex Upgrade.
- R-matrix collision data for He, Li, F, Na and Ne-like iso-electronic sequences for all elements up to zinc. Note that neutral and single ionised members are not included since these do not exhibit regular sequence-like behaviour.
- Distorted wave adf04 data for all elements up to zinc, with type 1 (collision strength/cross section) and type 3 (effective collision strength / rates) files.
- Iso-nuclear collections of R-matrix adf04 data for argon and neon.
- Revised beam emission coefficients for hydrogen. Note that there is a very modest change in the beam stopping data.
- The adf38, adf39 and adf48 data contains bare ion to Mg-like sequences for hydrogen to zinc and xenon.

Sources and references are in the datasets and a summary can be found in the ADAS release bulletin, available from the ADAS website, http://www.adas.ac.uk/bulletins.php.

Status and Development of KAERI atomic database

D.-H. Kwon
Korea Atomic Energy Research Institute, Dae-Jeon, Korea

Current status and development of KAERI (Korea Atomic Energy Research Institute) atomic database and recent activities of the atomic data research group were presented. Our atomic data group was begun in laboratory for quantum optics division, KAERI in the early 1990's but was moved to nuclear data center in KAERI from 2012.

Recent research works have focused on theoretical calculations for electron impact ionization (EII) and recombination cross sections of Fe and W ions which are essential in spectroscopic modeling for astrophysical and fusion plasma. The calculations have been carried out by FAC (flexible atomic

code) based on a DW (distorted wave) and IP-IR (Independent Process-Isolated Resonance) approximation, and compared with recent TSR (test storage ring) experiments. The resulting Maxwellian rate coefficients from our calculated EII cross section for ground state Fe^{11+} agrees with recent experiment as much as 15% better than the previously calculated one in CHIANTI database at the collisional ionization equilibrium (CIE) temperature regimes. Our method was extended to other P-like ions from P to Zn^{15+} and the EII rate coefficients show differences as much as 7-50% from those in CHIANTI database at the CIE temperature regimes. EII cross sections for W^{q+} (q=1-4, 17) were also calculated. Our calculated one for W^{17+} agrees with recent TSR experiment performed in 2011 but for W^{+}- W^{4+} show some discrepancies with TSR experiments done in 1990's. Photoionization cross sections for Be-like ions and Mg-like ions are also calculated by non-iterative eigen channel R-matrix method and compared with OP (opacity) results.

Our calculated data has been uploaded in newly constructed web database PEARL(Photonic Electronic Atomic Reaction Laboratory, http://pearl.kaeri.re.kr). We are going to add unitary correction of DW cross section to original FAC code and parallelize some routines of the original FAC related with R-matrix to improve accuracy and running time in the future.

Current Activity on Atomic, Molecular and Plasma-Material Interaction Data in Kurchatov Institute and Russian Federation

A.B. Kukushkin
NRC "Kurchatov Institute", Moscow, Russia

A brief survey of application of atomic and molecular (A+M) data and plasma-material interaction (PMI) data to fusion plasmas in the current and future experiments is given. The samples of survey on the generated, available and needed data are provided from various research groups in Kurchatov Institute and beyond (Russian Federation). Few examples of the tables for the survey of data generation and data use are attached to this summary.

For future fusion experiments the main accent is made on the use of the existing databases for the design of spectroscopic diagnostics for the tokamak ITER project. Among these examples are (i) the application of (A+M) data in the frame of the B2-EIRENE (SOLPS4.3) code simulations for the H-alpha (and Visible Light) Diagnostic in ITER [1] and (ii) the D-alpha high-resolution spectrometer data processing and interpretation in the currently running campaign at JET (JET ITER-like Wall experiments) [2].

The problem of PMI data needs for fusion research is discussed on the example of a quest for data accumulation for large molecules. This is illustrated with two examples: (i) the interpretation of data for the films deposited in tokamak T-10 [3], which demanded the quantum chemistry modeling of large molecules composed of a curved graphene [4], and (ii) a fuzz formation model [5] which demanded an analysis of adatoms formation and surface sputtering.

In the final part of report a special accent is made on the recent hot-spot evidences for the PMI data needs for fusion programme. These include (i) the ion sputtering of metals with simultaneous electron irradiation [6], (ii) tungsten recrystalization and cracking under ITER-relevant heat loads [7], (iii) complex experiment – production of damaged materials and exposure in plasma [8], (iv) the studies of tungsten tiles under high-flux and high-fluence irradiation [9], (v) the studies of a uniform layer of B_4C boron carbide safety covering on the MPG-8 graphite substrate under multi-pulse irradiation by the coaxial gun QSPU-T [10].

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Current Activities of IAEA Atomic and Molecular Unit Activities

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The main mechanism by which IAEA atomic and molecular data unit encourages new data production is a coordinated research project (CRP) of internationally renowned research groups on a focused topic. Two CRPs of "Characterization of Size, Composition and Origins of Dust in Fusion Devices" and "Light Element Atom, Molecule and Radical Behaviour in the Divertor and Edge Plasma Regions" are concluded and ready for final report and publication and the CRPs of "Spectroscopic and Collisional Data for W from 1 eV to 20 keV" and "Data for kinetic modeling of molecules of H and He and their isotopes in fusion plasma" are on the way. The CRPs on "Erosion and Tritium Retention for Beryllium Plasma-Facing Materials" and "Plasma-Wall Interactions with Irradiated Tungsten and Tungsten Alloys in Fusion Devices" are newly organized in 2012 and 2013.

In addition to CRP meetings, a series of technical and consultant meetings on data evaluation have organized to promote the critical assessment of atomic, molecular and plasma-material (A+M/PMI) data in the data producing communities and to collaborate internationally in order to produce internationally agreed data libraries of A+M/PMI data relevant to fusion applications. In cooperation with IAEA, three code comparison workshops have been organized in Vienna: the 7th Non-LTE Kinetics Code Comparison workshop, the 1st and 2nd Spectral Line Shapes in Plasmas Code Comparison workshops.

A project to implement XSAMS and make the ALADDIN numerical database available through VAMDC portal has begun. As the CFADC at ORNL closed down, a new way to collaborate with data centres to update collisional data in the AMBDAS bibliographical database was investigated. A comprehensive data set of atomic data using the flexible atomic code (FAC) has been generated for

atoms of Z=2 - 14. It includes collisional excitation and ionization, photoionization, radiative transition probabilities, autoionization as well as energy levels up to n=20.

Summary of EMOL Group Evaluation Activities

B. J. Braams with thanks to N. J. Mason (Open University)
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EMOL is an EU-funded project to develop methodology for analysing, validating and recommending electron molecule collision data sets. The project runs for 3 years (2013-2015) and about 12-15 data sets will be reviewed during that time. It is expected that each such review will result in a set of recommended data and a journal publication, and in addition the experience that is gained over the course of the project will result in guidelines for how evaluation may be carried out as a systematic group activity. The project is coordinated by Prof Nigel Mason of the Open University. The IAEA A+M Data Unit is not an official partner, but we cooperate in various ways.

EMOL is a part of a Roadmap for A+M data evaluation, recommendation and dissemination. In contrast to earlier evaluations of A+M data the project has been proposed and organized as a community activity. The community has somewhat the character of a journal board and initially there are 43 people on the "board". Each evaluation is a small group project carried out by 4-7 people who meet face-to-face once or twice in connection with the evaluation. (These meetings are usually attached to some other conference.) For each evaluation the aim is to provide recommended datasets that are self-consistent and complete, covering the entire energy range and all processes. It has been agreed with the Board of European Journal of Physics D (EPJD) that the evaluations may be submitted to that journal and it i expected that they will be published there and on the web. The evaluation approach follows Christoforou and Olthoff at NIST in the comprehensive nature (e.g. see their C3F8 evaluation published in J Phys Chem Ref Data, 1998).

Here is the present EMOL evaluations schedule, subject to change.

- H_2O: May 2013, Vienna.
- Biomolecules I, THF and nucleobases: May 2013, Gdansk.
- Fluorocarbons (*) I: July 2013, Japan.
- Fluorocarbons II: Sept 2013, Trieste.
- Fluorocarbons III: January 2014, Slovenia.
- N_2 (and N_2^+): December 2013, Vienna.
- SO_2 and Ozone: May 2014.
- N_2O: June 2014, Bratislava.
- NH_3: September 2014
- Biomolecules II Pyrimidine, THFA: December 2014
- Maybe still O_2, others.

(*) Fluorocarbons include CF_4, CHF_3, C_2F_4, C_2F_6, C_3F_8, C_4F_8 and SF_6

The first evaluation, of H_2O, was done in Vienna at the University on 8-10 May 2013, but the first day was jointly with our Code Centre Network meeting that took place 6-8 May at IAEA. (On Wednesday 8 May we met together at IAEA.) I (BJB) observed the process and found it very efficient. The review was based on an earlier one by Itikawa and Mason, 2005, and therefore only that review and more recent articles were considered. The various processes were assigned to the participants with 2 or 3 people for each process:

- Dissociation: S Matejcik, P Limao Vieira and B Marinkovic
- DEA: S Denifl, N J Mason and P Limao Vieira
- Elastic: B Marinkovic, G Karwasz and Y Itikawa
- Electronic excitation: G Karwasz, B Marinkovic and S Matejcik
- Emission: S Matejcik S Denifl and P Limao Vieira
- Inelastic: J Tennyson, G Karwasz and Y Itikawa
- Ionisation: S Denifl, S Matejcik and P Limao Vieira
- Momentum Transfer: G Karwasz, Y Itikawa and B Marinkovic
- Rotational excitation: Y Itikawa, J Tennyson and N J Mason
- Total: N J Mason, J Tennyson, G Karwasz
- Vibrational Excitation: J Tennyson, B Marinkovic and N J Mason

Following the meeting writing assignments were given and it was intended that the some of the participants would meet again at the Gaseous Electronics Conference in Princeton in October 2013 and then the review would quickly be finished.

Other reviews will follow the same pattern. The relevant papers are assembled and classified by process. The review team is assembled and divided into sub-teams. The participants study the papers at their home base and meet face-to-face for discussion and hopefully to agree on recommendations. After that meeting further consistency checks may be needed and scaling or other corrections may be considered. Then follows agreement on uncertainty assignments for the recommended data sets. A paper is produced for submission to EPJD and online archives and web pages are updated. (A website for the project is to appear in 2014.) Subsequent updates are expected about every 5 years.

At the A+M data Unit we attach much value to the EMOL project and following the overlap between our CCN and the water evaluation we will cooperate again on the nitrogen evaluation, for which participants will meet at IAEA in December 2013. (Nitrogen is an important gas for radiative cooling of fusion plasma.) We wish to work further with EMOL and with EMOL participants on the development of guidelines for valuation.

Group Research on Procedures for Evaluation of CH_4 Collision Processes

M.-Y. Song,
National Fusion Research Institute, Dae-Jeon, Korea

A demonstration of data evaluation by a number of people in a group was suggested at the Joint IAEA-NFRI Technical Meeting (TM) on Data Evaluation for Atomic, Molecular and Plasma Material Interaction Processes in Fusion in September 2012. Meeting participants recommended experts to take the task of evaluation and CH_4 collisional data as the evaluation topic. The purpose of the group evaluation activity is to establish the internationally agree standard reference data library for AM/PMI data.

Group Members are Itikawa (Japan), Grzegorz P. Karwasz (Nicolaus Copernicus University), J. Tennyson (University College London), Viatcheslav kokoouline(University of Central Florida), H. Cho(Chung-Nam National University),Y. Nakamura (Tokyo Denki University), J.-S. Yoon, and M.-Y. Song (National Fusion Research Institute).

The group met three times this year, on 23 - 25 January 2013, Gunsan, South Korea, 25 -27 June 2013, Deajeon, South Korea, 23-24 September 2013, Open University. UK. The group decided a working scope because not all data are available and the group divides the work.

The group plans to produce an evaluated data set of CH_4 collisional processes according to the analysis of previous evaluation papers presented by all participants. The results will be published with uncertainties and detailed descriptions of the data evaluation methods. Suggestions for future research topics will be made for data whose evaluation was impossible due to the lack of data.

Appendix 4

Application and Availabilities of Atomic, Molecular and Plasma-surface Interaction Data for Fusion

A+M Data Use (V.S. Lisitsa et al., NRC "Kurchatov Institute", Moscow, Russia

Problem	Task	Publication	Processes	Data Source	Data Needs
Integrated modeling of ITER scenarios H-alpha diagnostic in ITER	Simulator (fast routine) of hydrogen penetration from the wall in ITER, tested against B2-EIRENE	Proc. 39th EPS Conference, 2012, P4.093.	All processes with H_2 and H	Data file AMJUEL: Additional Atomic and Molecular Data for EIRENE	H_2 dissociation with H^* product, CX(n,l) Nl-cascade population
		Proc. 40th EPS Conference, 2013, P1.135.	Charge exchange of neutral H in excited states with protons		
Charge exchange recombination spectroscopy in ITER	Predictive modeling, Data interpretation		Selective populations of m sublevels in an atomic beam in a strong magnetic field		Cross sections in n,l,m
Thomson diagnostics in ITER divertor	Line and continuum spectral background on diagnostic chords	Plasma Physcis Reports, 2012, 38, 138-148	IR Hydrogen lines (P-7), Brems and photorec.	NIST	
	Impurity (nitrogen) line background	Submitted	IR line, Kinetics of 3d levels population	NIST, ADAS	

A+M Data Use (S.V. Polosatkin, Budker Institute of Nuclear Physics, Novosobrisk, Russia

Development of ion and neutral beam source for fusion

Task	Publication	Processes	Data Source	Data Need
Control of impurity Content in neutral beams	Instruments and Experimental Techniques **53** (2010) 253	Impurities ionization balance and atomic line emission	NIST ASD, ADAS	Impurities (C,O, Cu…) excitation in collisions with H_2 Isotopic effects in H-alpha excitation
Doppler-shift measurements of NB species content	JINST **8** P05007 (2013)	$H+H_2 \rightarrow H^*+H_2$ $H^++H_2 \rightarrow H^*+H^+_2$	ALADDIN ORNL-6086	Sublevel-resolved cross-sections of hydrogen excitation in collisions with H_2
Simulation of the beam generation and transport		$H_2+e \rightarrow H+H^++2e$ $H_2+H_2 \rightarrow H+H+H_2$		Distribution function of products of dissociation of H_2 (DH, D_2) in collisions with e and H_2

A+M Data Generation (Inga Yu. Tolstikhina *et.al.*, Lebedev Physics Institute RAS, Moscow, Russia)

Processes	**Method**	**Data Source / Code**	**Publication**	**Verification / Application**	**Problem**
Charge-changing collisions of tungsten and its ions with neutral atoms H, D, T, He, N, Ar and W	Adiabatic theory of transitions in slow collisions (hidden crossing method.), Born approximation and the classical energy-deposition model.	Codes: ARSENY, CAPTURE, DEPOSIT, RICODE	J. Phys. B: At. Mol. Opt. Phys. 45 (2012) 145201 Physics-Uspekhi, 56, 213 (2103)	Plasma modeling (near-wall, divertor), planning and interpretation of future experiments in fusion devices using tungsten as a material for the plasma-facing components	Influence of the isotope effect (mass dependence) on the charge exchange cross sections in slow collisions, ionization and charge exchange cross sections in a wide energy range, contribution of the multi electron ionization to the total cross sections
Influence of the isotope effect on the charge exchange in slow collisions of Li, Be, and C ions with H, D, and T			PHYSICAL REVIEW A 84, 012706 (2011)		
Collisions of Be, Fe, Mo and W atoms and ions with hydrogen isotopes: electron-capture and electron-loss cross sections			Submitted to JPB		

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