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Technical Aspects of Atomic and Molecular Data Processing and Exchange, 23rd Meeting of the A+M Data Centres

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

2-4 November 2015

Prepared by

Hyun-Kyung Chung

February 2016

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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" (23rd Meeting of the A+M Data Centres Network) on 2-4 November 2015. 10 participants from 9 data centres of 8 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.

February 2016

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1. Introduction

The 23rd 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 in Vienna, Austria, from 2 to 4 November 2015. 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.

Activities of eight data centres were presented: by Yu. Ralchenko of NIST (National Institute of Standards and Technology, USA), I. Murakami of NIFS (National Institute of Fusion Science, Japan), M. O'Mullane of ADAS (Atomic Data and Analysis Structure project, UK), P. Goncharov of SPBSTU (Peter the Great Polytechnic University, Russia) on behalf of A. B. Kukushkin (NRC Kurchatov Institute, Russia), D. Reiter of FZJ (Forschungszentrum Jülich GmbH, Institut für Plasmaphysik, Germany), J. S. Yoon of NFRI (National Fusion Research Institute, Korea), B. Braams of IAEA and D.-H. Kwon of KAERI (Korea Atomic Energy Research Institute, Korea). The presentation on KAERI was done by H. Chung as D. Kwon had to cancel the trip due to unexpected cause. The representative from the Chinese Research Association on Atomic and Molecular Data at Institute (CRAAMD) of the Institute of Applied Physics and Computation Mathematics (IAPCM, Beijing, China) could not attend the meeting due to difficulties with the nomination. T. Nakano of JAEA (Japan Atomic Energy Agency) did not participate due to lack of activity in data projects at JAEA after the Fukushima accident.

Four additional experts maintaining atomic and molecular databases for astrophysical and industrial plasma applications were invited to discuss their work in data evaluation and dissemination: R. Kisielius of ADAMANT database (Vilnius University, Lithuania), L. Pitchford of LXCat project (University of Toulouse, France), P. Young of CHIANTI database (George Mason University and NASA Goddard Space flight Center, USA) and M.-Y. Song on Methane evaluation project (NFRI, Korea). The Agency was represented by A. Koning (Section Head, Nuclear Data Section), B. Braams (Unit Head, Atomic and Molecular Data Unit) and H. Chung (Atomic Physicist and Scientific Secretary).

Discussions were held 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
- Cooperation on the maintenance of Bibliographical databases
- Priorities for data development and evaluation, new meetings and information exchange

The proceedings of the meeting are summarized in Section 2 and the summary of discussions and recommendations on future work plans are presented in Sections 3 and 4 in this report. The full list of participants is available in Appendix 1 and the adopted agenda is listed in Appendix 2. Presentations are summarized in Appendix 3. A Russian inventory of data needs is given in Appendix 4.

2. Proceedings of the Meeting

The new section head of the Nuclear Data Section, A. Koning welcomed participants and acknowledged the value of Data Centre Network (DCN) meeting. Participants introduced themselves and the agenda in Appendix 2 was adopted. Dr B. Braams reviewed meeting objectives.

The meeting proceeded with presentations by data centres on their current activities and by the additional experts on their databases and data evaluation activities. Slides of presentations are available on the Unit web site http://www-amdis.iaea.org/DCN/ via the link to Meeting Reports and Presentations. Detailed summaries of presentations are provided in Appendix 3.

2.1 Current Activities of Atomic and Molecular Data Centres

The session was dedicated to progress reports of the data centres on their activities in the period 2013-2015. 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.

Current status of the atomic data program at NIST

Yu. Ralchenko described the status of the atomic data program at NIST which hosts the Atomic Spectra Database (ASD) with 250,000 spectral lines and 109,000 energy levels, and three bibliographic databases of 19,220 references for energy levels and spectra lines, 9090 for transition probabilities and 6860 for line shapes and broadening. A new diagnostic module to produce density- or temperature-sensitive line ratios useful for plasma diagnostics was reported.

Atomic and Molecular Data Activities at NIFS in 2013-2015

I. Murakami reported the development and maintenance of NIFS databases containing 762,392 collisional data in total (as of Oct. 13, 2015). She also described research activities on light element atomic data, charge exchange cross-section measurements and spectroscopic measurement of highly charged ions using CoBIT and LHD devices. Spectroscopic study with development of collisional-radiative (CR) model is on the way.

Data and code updates in OPEN-ADAS and ADAS and ensuring traceability

M. O'Mullane reported on the new data sets, particularly radiated power calculations added to ADAS system as well as code updates with improvement in atomic structure activities and spectral fitting. Related to the Integrated Modelling and Analysis Suite (IMAS) for ITER, he described the current efforts on data traceability, provenance policy and data archives policy.

Current activity in Russia on atomic, molecular and PMI data

P. R. Goncharov provided an overview of atomic, molecular and plasma-material interaction (AM/PMI) data activity in Russia at 7 institutes. A summary of generation and use of AM/PMI data for fusion research was presented. Verification work on ITER relevant data issues was reviewed. Finally, data needs for specific applications are summarized in the table of Appendix 4.

Ongoing and pending data base activities at FZ Jülich

D. Reiter summarized current FZJ activities mostly focused on database maintenance and extensions of existing databases (molecular and surface reflection databases) used in fusion edge plasma modelling, particularly on raw data processing, condensation, their integration into transport codes and uncertainty propagation (sensitivity analysis). FZJ collaborates with IAEA AM Unit on evaluation activities.

Current Activities (2014~2015) of Atomic and Molecular Database at NFRI

J.-S. Yoon reported on the activities of Data Centre for Plasma Properties (DCPP) where their research focused on low temperature plasma full-set data generation with simulation tools, data evaluation and bibliographic data compilation with IAEA and big data systems for fusion applications. Experimental facilities for electron collisions with atoms and molecules and highly charged ion - matter interaction are under development.

Current Activities of IAEA Atomic and Molecular Unit Activities

B. Braams summarized the activities at IAEA A+M Data Unit: CRP (Coordinated Research Projects), meetings, publications, maintenance and development of databases and online codes. In 2014-2015, one CRP was concluded with a special volume published in Atoms journal and 4 CRPs are active. The Unit organized 17 meetings since last DCN meetings and produced 4 special volumes of publications. Data evaluation and uncertainty quantification have been top priority in unit's activities will remain so in the future.

Recent Progress of KAERI Atomic Database

Research activities on state-of-art calculations for electron ionization, recombination and photoionization data and spectroscopic measurement with collisional radiative (CR) modeling at KAERI atomic data center were summarized. Atomic database PEARL (Photonic Electronic Atomic Reaction laboratory, http://pearl.kaeri.re.kr) is updated with a better interface and also includes line ratios from CR modeling.

2.2 Databases and data evaluation

Experts shared their experiences with atomic and molecular databases used in astrophysical and low temperature processing plasmas and data evaluation activities.

ADAMANT: a platform for data users and producers

R. Kisielius described the database ADAMANT (Applicable DAta of Many-electron Atom eNergies and Transitions) that contains spectroscopic parameters and electron-ion interaction parameters for more than 1100 species (14 GB of data) mainly used for plasma spectral modeling. The data sets are calculated using the same computer code suites, same approximation for configuration interaction (CI) and relativistic effects, and identical multireference wavefunction.

LXCat: a web-based, community-wide project on data needed for modeling low temperature, non-LTE plasmas

L. C. Pitchford described the LXCat platform which provides an infrastructure for storing, accessing and manipulating electron and ion data for low temperature plasmas. There are 22 databases accessed on LXCat where the content is maintained by contributors. Available data sets include electron-neutral scattering cross sections, measured electron transport parameters as a function of E/N as well as ion transport and rate coefficients, ion-neutral interaction potentials and ion-neutral cross sections. The initial motivation, present objectives and the future strategy of LXCat were presented.

The CHIANTI atomic database

P. Young provided an overview of the CHIANTI atomic database and software package for spectroscopic diagnostics of astrophysical plasmas. Atomic data sets consisting of energy levels, radiative decay rates and electron effective collision strengths are selected from the published literature. Total ionization and recombination rates are also provided for calculating the ionization balance of astrophysical plasmas. Data evaluation is a critical component to CHIANTI and the best available atomic data set is provided for a single, coherent model for each ion. Data sources and evaluation procedures are published regularly.

Cross Sections For Electron Collisions With Methane

M.-Y. Song reported on the evaluation of electron collisions with Methane with a group of researchers Cross-sections of ionization, electron attachment, elastic, momentum transfer, vibrational and rotational excitation, electron excitation and dissociation as well as total cross-sections were compiled and evaluated and published in J. Phys. Chem. Ref. Data.

3. Technical Discussions

Issues related to data research and data centres were discussed: bibliographical data compilation, data evaluation, data exchange, database development, and priorities for data development and evaluation for fusion applications.

3.1 Bibliographic Data Compilation

The database AMBDAS of bibliographical information for atomic, molecular and plasma-surface interaction data has been maintained and distributed by the unit as a core activity of data centre network. Various data centres contributed to the compilation of bibliographical data since 1977 when the first volume of International Bulletin on Atomic and Molecular Data for Fusion was published. At present, NIST continues to provide bibliographic data for atomic levels and transitions; however there is no stable source of bibliographical data for fusion relevant electron, photon, heavy particle collision data as well as plasma-surface interaction (PSI) data.

In the last two years, the unit made an effort to compile bibliographical data of collision and PSI data in collaboration with members of data centres (M. Song of NFRI, I. Murakami of NIFS, D.-H. Kwon of KAERI) and consultants. As a result, electron collision and PSI data are compiled up to 2014 and 2013, respectively.

The procedure uses well-defined sets of keywords to find journal articles from web of science (http://apps.webofknowledge.com/) and relevant articles are selected based on abstracts. A list of selected articles is sent to NFRI, who retrieves articles and send them to IAEA. Articles are classified according to the classification system (http://www-amdis.iaea.org/DCN/ProcessClassification.pdf). Classified data are uploaded to the AMBDAS database.

Key words for atomic and molecular data were set up by H. Chung. U. von Toussaint (IPP-Garching, Germany) and A. Lasa (University of Helsinki, Finland) were invited to develop a set of keywords for PSI data, and 2 IAEA interns, H. Lee and K. Lim collected and classified journal articles using the keyword search. It was noted that an expert with at least a Ph.D is needed to classify articles in a consistent and rigorous way.

The unit invited M. Imai from Kyoto University to develop a set of keywords and explore other methods of collection and compilation of heavy particle collision data. He and NIFS will collaborate with the unit to compile the bibliographic data of heavy particle collisions. W.-W. Lee of KAERI was invited to classify electron collision data published in 2012-2014.

3.2 Activities on Data Evaluation

An overview of IAEA activities on the topics of data evaluation and uncertainty quantification was presented. Since 2012, the unit organized 10 meetings, including the joint IAEA-ITAMP (Institute of Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA) technical meeting on uncertainty assessment for theoretical atomic and molecular scattering data attended by more than 20 atomic and molecular physicists in 2014. After the

IAEA-ITAMP TM in Cambridge, MA in 2014, the unit is developing a guideline for uncertainty quantification of theoretical atomic and molecular data with experts in the field. The unit also organized meetings to produce evaluated data for electron-Be collision data and electron-W recombination rate coefficients data. In 2015, the 4th code centre network (CCN) meeting was held on the topic of uncertainty quantification for plasma-material interaction physics codes and models.

In addition to IAEA efforts for evaluation, there are several projects going on for data evaluation. One is eMOL project and the other is NFRI project. Both projects engage a group of experts with diverse background in theory and experiments. A group evaluation starts with a review of old review papers to find data needed for an update, proceeds with reading of recent publications and discussions at a meeting for recommendation of best data. They aim to produce a coherent, self-consistent ensemble of complete sets that can be readily used for modeling. It was noted that data sets such as swarm data or optical oscillator strengths are very useful to benchmark the complete set.

CHIANTI database developed for Solar spectra analysis has a unique position as a database to host one unique data set. The solar and astrophysical communities use the CHIANTI to identify lines and use them to determine plasma conditions. Occasionally, new observations will reveal unidentified lines or unexplained line intensities, then the CHIANTI team reviews the atomic model, improves data sets, and publish the new data set.

Uncertainty quantification (UQ) of theoretical data is not straightforward for most code developers. However, there is a change in attitude in the community to adopt UQ, particularly with a change of journal policy requiring UQ for theoretical papers claiming high accuracy or benchmarking high precision experiment data. Code developers of GRASP2K are planning to incorporate a module to assess uncertainty quantification and propagation of uncertainties as a routine output.

The results from top level collisional codes, CCC, RMPS and BSRM compared at the IAEA e-Be evaluation meeting showed remarkable agreement within 5-10% for most cases, which was taken as the uncertainties associated with the data sets. However, some resonance features in the results were deemed unphysical by authors while there was no obvious way of others to know that they were. It is necessary to address such hidden knowledge, numerical noises in a systematic fashion but there seems to be no obvious solution other than author’s own investigation.

The propagation of uncertainties of fundamental data to application result is of ultimate interest. There are examples to see the effects of uncertainties associated with atomic data on the line ratios used for plasma diagnostic and arbitrary uncertainty assignment is found not to change the final results dramatically. This implies that data users should have information on a few of critical data sets that influence the final results by a certain sensitivity analysis and the close communication between data users and data producers is clearly important in identifying and improving those data sets.

3.3 Data Exchange

The XSAMS (XML Schema for Atoms, Molecules and Solids) initially developed by the IAEA XSAMS steering committee has been actively used and further developed for data exchange through VAMDC (Virtual Atomic and Molecular Data Centre) project that developed a unified, secure, documented, flexible and interoperable e-science environment-based interface to 24 existing A+M databases. After VAMDC project ended in 2012, the work was carried by SUP@VAMDC project for two more years to coordinate collaborative studies and provide the supporting procedures that will develop a global e-infrastructure for the assembly, curation and access to A+M data.

Currently, IAEA, NIFS, NIST and KAERI have a partnership with SUP@VAMDC project. IAEA has been working with VAMDC to make ALADDIN database available as a VAMDC node. There is a minimum requirement to convert a database into a VAMDC node thanks to tools and protocols developed at VAMDC. SQL database is not mandatory for VAMDC node. Several data centres consider the option to make their databases available through VAMDC. Due to the XSAMS structure where the reference is a mandatory field, provision of data reference and citation are not an issue with VAMDC protocols.

The use of VAMDC interface is straightforward to retrieve a handful number of data. A retrieval of a complete data set often required by plasma modeling users is not ideal for VAMDC. Particularly, a self-consistent, comprehensive and possibly evaluated data set is preferred. ADAS or CHIANTI databases are better suited.

3.4 Priorities for data development and evaluation, new meetings and information exchange

In the last DCN meeting, a development of 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, was discussed. As a feasibility test, relevant bibliographical data are collected and classified and it was found that the classification is not trivial. The difficulty lies with assignment of molecular states, non-standard nomenclatures and vocabulary, and also hierarchy of top level classification (spectra, structure, photon, electron, heavy particle etc.) and the classification requires an educated judgement from the classifier. The conclusion is that the establishment of PEC database seems feasible; however, it will require a lot of enthusiasm and coordination of experts.

A need of major revision of hydrogen, helium, hydrocarbon databases used for CR (collisional-radiative) modeling for transport simulations developed by Janev and Reiter in 1990s was raised. Currently, a CRP on “Atomic and Molecular Data for State-Resolved Modelling of Hydrogen and Helium and Their Isotopes in Fusion Plasma” will address some issues with hydrogen and helium CR model. Nevertheless, there lack many data, particularly for electronically excited, vibrationally and rotationally resolved states, and hence scaling and educated guesses have been used to make up the missing data. Data sets consist of experiments, calculations, intuition and scaling laws and the assembled data is publicly exposed for validation. A few CR models exist and an evaluation is needed.

For tokamak plasmas, isotopes of H, D, T are major components and electron and heavy particle collision data involving H_2, D_2, T_2, HD, DT, HT of temperature ranges of 0.5 eV to 10-15 eV are of main interest. Depending on national programs, data involving Li is needed. There is a compilation of CCC electron-Li collision data compiled in 1999. Data of LiH and BeH are required mainly for diagnostics. Data of break-up chains and electronic transitions of molecules are needed. For ITER relevant research, data for Be molecules and break-up chains are needed. BeH molecules have been detected but BeH_2 have not been known spectroscopically.

Much of discussion was on the neutral beam related data. For stripping of fast neutral beams, there are two ready-to-use models, Janev model (1989) and Suzuki model (1997). However, none of the models are complete yet. Charge state dependent ADAS data sets are more flexible than both models where effective stopping coefficients as a function of electron density and beam energy are given and impurity effects are included. However, the ion impact excitation data and ionization from highly excited states need to be improved further. High quality data of proton impact data is also needed for fine-structure changing processes to allow an explicit mixing of fine-structure levels, for example, singlet and triplet states of He-like ions. Emission from higher-lying states is influenced by proton impact collisions. For neutral beam diagnostics, data of excitation between excited states, ionization from excited states, secondary processes from excited levels are largely missing or of poor quality.

IAEA is planning to organize a CRP on “Data for Charge Transfer Processes Related to Neutral Beams in Fusion Plasma” in 2016-2020. Data of neutral beam interaction with not fully stripped heavy particles, beam stopping power, data for charge exchange recombination spectroscopy (CXRS), beam emission spectroscopy (BES), beam stripping are of interest.

CXRS is used to measure impurity content in the fusion plasmas and the measurement accuracy should be in the order of 2 %. Therefore uncertainty propagation plays a critical role in neutral beam diagnostics and there are two aspects to be investigated: 1) the mechanism of uncertainty propagation to show a major effect in the results and 2) realistic assessment of atomic data input uncertainties.

BES diagnostics using motional Stark effect (MSE) measures local electric fields, though it relies on the line of sight and measurements of multiple optical components. Line splitting depends on the history of line of sight and hence validation is rather difficult for MSE measurement. Therefore data for line splitting and excited state population are generally important.

There was a discussion on the role metastable states, which is very difficult to validate in any diagnostics and hence frequently assumed, never measured. There are different views on the role of metastable states: it is critical to determine excited state population and it seems better with some amount of metastable population, on the other hand, as soon as ions enter into electromagnetic plasmas, the fields mix 2s and 2p states and hence metastable states will radiate within a fraction of seconds leaving no metastable states a few mm away from the boundary.

In a longer term, one should prepare for data needs not only for ITER but also for DEMO related problems. ITER is already being built and many diagnostics components are already assigned to member states for construction. Currently data related to material mix is of high priority and data compilation and prioritization is on the way as operation of diagnostics is still developing in various places. Apart from H, He, W and Be, data of Ne, Ar, N_2 are of interest. For DEMO, radiative power loss and spectroscopy of Ar and Xe are of interest, and data related to neutral beam stopping is of interest.

IAEA plans to organize a meeting on benchmarking and uncertainty quantification of atomic and molecular data, bringing experimentalists and theoreticians together on a well-defined problem. It is to strengthen the network of experimentalists working in the production of atomic and molecular data and promote interactions between experimentalists and theoreticians in defining the uncertainties of atomic and molecular data. Hopefully the network will provide a visibility for more funding opportunity for AM physicists in fusion applications and facilitate the transfer of knowledge of experimental programs that are fast vanishing due to retirements of experts.

4. Data Centres Web Interface and Software Presentations

Yu. Ralchenko, NIST, presented the new version 5.3 of NIST atomic spectra database (ASD). The version implemented a diagnostics tool for plasma conditions using line ratios. Currently, the line ratio is calculating using CHIANTI atomic data version 7.1. Saha-Bolzmann plot has been expanded to elements relevant to LIBS (Laser-induced breakdown spectroscopy). H. Chung demonstrated the electron collision data uploaded to AMBDAS database at IAEA.

5. Meeting Conclusions and Recommendations

The meeting was highly successful in reviewing the progress of data programs and working out the future plans of Data Centre Network (DCN) members. Participants reviewed and recommended future work plans for DCN members and IAEA. Reviews and recommendations are summarized in this section.

- Coordinate the compilation and classification of bibliographical information for collisional and plasma-surface interaction processes.

- IAEA, KAERI, NFRI and NIFS (with Kyoto University) will participate in the coordination of bibliographical data compilation.
    - NFRI needs more guidance in AMBDAS journal collections.
- Coordinate the activities of data evaluation
    - NFRI group evaluation and e-MOL group evaluation are on the way.
    - IAEA group evaluation of e-Be and e-W continues, and possibly starts a new activity on H and He data.
    - Evaluation for break-down chains is highly valuable for fusion research.
    - Experimental data of CH_x is available, however not curated properly for access.
- Develop a data library of evaluated and recommended data
    - IAEA should provide a depository of such data for public access.
    - IAEA compiled evaluated and recommended data published more than 20 years ago.
    - Core data should be updated.
    - A priority of evaluation and recommendation should be established.
- Promote a curation for data to meet the ITER demand
    - ITER prefers curated data; however, the data doesn't have to be fixed.
    - For example, ALADDIN is not a comprehensive source of any application domain and not easy for modeling uses. However, EIRENE is a practical source for a fusion modeling community to find a comprehensive data.
- Assemble data needs for fusion research
    - A list of data needs and used data sets provided by Russia data centres is highly useful.
    - The effort to provide such a list from other ITER member states is highly recommended.
- Provide a list of experimentalists worldwide to provide absolute cross-section measurements
    - A list of fundamental atomic and molecular cross-section measurement facilities is highly recommended.
    - A network of experimentalists in the fundamental atomic and molecular cross-section measurements will be valuable.
- Proposed meetings and workshops by DCN members
    - ICAMDATA, Gunsan, Korea, 25-29 September 2016
    - Fusion energy conference, Kyoto, Japan, 17-22 October 2016
    - Joint ICTP-CAS-IAEA School and Workshop on Plasma-Material Interaction in Fusion Devices, Hefei, China, 18-22 July 2016
- Encourage data projects of small funding opportunity
    - While national funding programs require a sizeable funding for a Ph.D, a postdoc or equipment and paperwork, a small funding of a size of 5000 € can establish a data project on a well-defined topic. The other merit is the reduced administrative work with the funding.
    - NIFS maintains university network for collaboration: 3 year project for data compilation and production. This year the topic is dissociation for H isotopes.
    - JAEA lost funding for collaboration projects after Fukushima accidents.
    - Russian network doesn't provide funding.
    - ADAS-EU has leverage of small funding for well-defined topics.
- Promote a data traceability issue
    - DOI mechanism for data is on its way.
    - Journals, editorial boards and referees should be encouraged to be vigilant about all data used in a paper to be reportable so that data producers can take a credit for their work.
    - Code developers should be encouraged to provide a code with reproducibility and version control.
- Enhance the IAEA web page with educational components
    - Educational materials for fundamental sciences related fusion industry are useful to attract young students and enlighten public.
    - IAEA Public relations and Physics section should be contacted to promote outreach programs for fusion research.

    - Connecting to Europe fusion programs (such as Eurofusion link) is valuable.
    - Educational materials to emphasize data issues and promote data and tools together will help experts in the new field interested in collaborations.
- Outreach to other communities
    - Astrophysics and solar physics community have much in common with fusion community in data needs.
    - Uncertainty quantification and evaluation is an important issue for all science and engineering fields. Cooperation with interested communities such as mathematics and computer science fields is desirable.

Appendix 1

List of Participants

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Appendix 2

Agenda

Monday, 2 November **Meeting Room: C0440**

09:30 – 10:10	Opening (Arjan Koning, Nuclear Data Section Head) Introduction of Participants Review Meeting Objectives (B. Braams) Adoption of Agenda (H. Chung)

Session 1: Current Activities of Data Centres

Chair: J. Yoon

10:10 - 10:40	Y. Ralchenko (NIST): Current status of the atomic data program at NIST
10:40 - 11:10	I. Murakami (NIFS): Atomic and molecular data activities at NIFS in 2013-2015
11:10 - 11:30	*Coffee break*
11:30 - 12:00	M. O'Mullane (ADAS): Data and code updates in OPEN-ADAS and ADAS and ensuring traceability when using ADAS data
12:00 - 12:30	P. Goncharov (SPBSTU): Current activity in Russia on atomic, molecular and PMI data
12:30 - 14:00	*Lunch*

Session 2: Current Activities of Data Centres (Continued)

Chair: I. Murakami

14:00 - 14:30	D. Reiter (FZJ): Ongoing and pending data base activities at FZ Jülich
14:30 - 15:00	J.S. Yoon (NFRI): Atomic and Molecular Data activities in NFRI
15:00 - 15:20	*Coffee break*
15:20 - 15:50	B. Braams (IAEA): Current activities of IAEA atomic and molecular data unit
15:50 - 16:10	D. Kwon (KAERI) by H. Chung: Recent Progress of KAERI Atomic Database

Session 3: Bibliographical Data Compilation

Chair: H. Chung

16:10 - 17:00	Coordinated activities on bibliographical data compilation (all participants)
19:00	*Social Dinner*

Tuesday, 3 November

Session 4: Data Compilation and Data Evaluation Activities in various applications

Chair: M. O'Mullane

09:00 - 09:40	R. Kisielius (Vilnius): ADAMANT: a platform for data users and producers
09:40 - 10:20	L. Pitchford (Toulouse): LXCat - an open-access platform for data needed for modeling low temperature plasmas
10:20 - 10:40	*Coffee break*
10:40 - 11:20	P. Young (GMU+NASA): The CHIANTI atomic database: an overview of data, software and applications
11:20 - 11:50	M. Song (NFRI): Evaluation of cross section for electron collisions with methane
11:50 - 13:20	*Lunch*

Session 5: Data Evaluation

Chair: H. Chung

13:20 - 13:40	H. Chung (IAEA): IAEA evaluation activities
13:40 - 14:40	Coordinated activities on data evaluation (all participants)

Session 6: Data Exchange

Chair: Y. Ralchenko

14:40 - 15:40	Data exchange format: xsams, adas, genie, (all participants)
15:40 - 16:00	*Coffee break*

Session 7: Numerical Database Development

Chair: 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

Wednesday, 4 November

Session 8: Data Needs for Fusion Research

Chair: D.Reiter

09:00 - 10:40 Priorities in A+M/PMI data compilation and evaluation (all participants)
10:40 - 11:00 *Coffee break*

Session 9: Review on Data Centres Network Activities

Chair: B. Braams

11:00 - 12:30 Plan of DCN activities for the future

- Network of AM/PSI Experimentalists
- 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

12:30 - 14:00 *Lunch*

Session 10: Meeting Conclusions and Recommendations

Chair: H. Chung

14:00 - 15:00 Data centre WWW database and software demonstrations
15:00 - 16:00 Formulation of meeting conclusions and recommendations
Date of next meeting

16:00 - ***Adjourn of the Meeting***

Appendix 3

SUMMARY OF PRESENTATIONS

Current status of the atomic data program at NIST

Yu. Ralchenko
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, two new updates for the Atomic Spectra Database were released, i.e., v.5.2 in September 2014 and v.5.3 in October 2015. The latest of these includes about 250,000 spectral lines and 109,000 energy levels.

The new compilations of spectroscopic data added to ASD include a very extensive Th I-III collection of levels and lines, new and/or updated data for W VIII, Sn II, Mo V, Cl II, Mg I, Cr I-II, Cu I, Fe V, Al I-VII. A large number of wavelengths and energies were corrected.

A new diagnostic module for a number of elements and their ions was added to ASD. This addition provides information on density- or temperature-sensitive line ratios that can be used for diagnostics of fusion and astrophysical plasmas. Another module extends the Saha/LTE interface to multi-component plasmas. A user can define an arbitrary composition of plasma to calculate spectra with the ASD data. This module would be especially useful for the laser-induced breakdown spectroscopy (LIBS) applications.

The three atomic bibliographic databases are updated regularly. Presently the total number of references is about 19,220 for energy levels and spectral lines, 9070 for transition probabilities, and 6860 for line shapes and broadening.

Theoretical calculations of atomic structure and collisional-radiative modeling of various plasmas contributed greatly to diagnostics of plasmas and identification of new spectral lines from various elements and ions. The number of users of the CR code FLYCHK approaches 800. Although calculation of charge-exchange interaction between highly-charged ions and neutral atoms and molecules was completed for a number of systems.

Atomic and Molecular Data Activities at NIFS in 2013-2015

I. Murakami
National Institute for Fusion Science (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, and BACKS contain 762,392 collisional data in total (as of Oct. 13, 2015) and small databases are developed for specific processes of interest.

Domestic working group with atomic and molecular physicists searched data mainly on light elements to update the databases (M. Kitajima et al.). Domestic collaboration programs are carried out on charge exchange cross section measurements for tungsten ions with helium (K. Soejima et al.), spectroscopic measurements of highly charged ions using compact electron beam ion trap (CoBIT) (N. Nakamura et al.), systematic study on EUV spectra of high Z elements with using the large helical device (LHD) and CoBIT at NIFS (F. Koike et al. and T. Higashiguchi et al.), and atomic data and model evaluation on Fe ions for Hinode / EIS using LHD (T. Watanabe et al.). EUV and visible lines of W XIII – W XV were measured with CoBIT in Univ. Electro-Communications (Kubota et al., Phys. Rev. A 92, 022510, 2015).

At NIFS spectroscopic study on tungsten ions has been carried out using LHD from EUV to visible wavelength range as well as developing the collisional-radiative (CR) model for tungsten ions. W IV – VII lines in VUV wavelength range were measured in LHD and time evolution of line intensities of W VI – XLVI were measured according to the change of the electron temperature of plasma (Oishi et al., submitted to Phys. Scr., 2015). EUV lines of W XXIV – XXII were used to determine tungsten ion abundances in LHD plasma and radiation power loss rates were estimated with the estimated abundance and the CR model calculations (Murakami et al., Nucl. Fusion 55, 093016, 2015). EUV spectra of lanthanides were measured in LHD plasmas and Yb XXXIX- XLI and Tm XXXVIII – XL lines were identified with CR model calculations.

Data and code updates in OPEN-ADAS and ADAS and ensuring traceability when using ADAS data

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

There is a new ADAS release each 9-12 months and OPEN-ADAS is updated shortly thereafter. The data archived in ADAS can be classified as either fundamental or derived: the former has a purely atomic nature while the derived data depends on macroscopic plasma parameters. ADAS population codes are developed to process relevant fundamental data into derived data suitable for plasma modelling and diagnostic interpretation.

The diversity of independent producers of fundamental atomic data is a concern since these data come from university groups and experimental facilities such as EBITs and storage rings, the number of which are diminishing. Fundamental data is calculated by ab initio computer codes and an increasing quantity of data archived in ADAS is the result of activity within our own university group, or close collaborators. Magnetic fusion may need to take on a funding role outside the usual national research bodies to maintain a supply of needed atomic data.

Since the last DCN meeting a significant quantity of electron impact excitation data has been added to OPEN-ADAS. In the R-matrix model, iso-electronic sequences for Be-like, B-like, Mg-like have been added to the existing (He-, Li-, Ne- and Na-like) adf04 archive. This is primarily the work of Luis Menchero and Nigel Badnell at the University of Strathclyde. In the less sophisticated distorted-wave (DW) model we have added all sequences from H-like to Ar-like for all elements up to krypton. The DW data is archived as Maxwell averaged effective collision strengths and as cross section data to model plasmas with non-Maxwellian electron energy distribution functions (EEDF).

R-matrix calculations for selected iron and tungsten ions have also been added.

Current development work includes the extension of the population models to deal with arbitrary EEDFs, an algorithmic approach to optimizing the calculation of total radiated power (cooling curves) and the inclusion of ion-impact collisions. As the atomic number increases, data in intermediate coupling picture is required and the effect of ion impact on the fine-structure populations must be explicitly added.

Traceability of data is an increasingly important topic. There are two domains of need: (1) guaranteeing the reproducibility of large scale plasma simulation codes which rely on atomic data (derived data

in ADAS characterization) as inputs, and (2) the provenance of database collections and the requirement of funding bodies for formal data management and lifetime planning for research outcomes.
ADAS is working with EUROfusion and ITER groups to address the first area. Data object referencing and longevity are concerns for all DCN members, and database/repository providers, which will become a much more prominent activity in the future.

Current activity in Russia on atomic, molecular and PMI data

P. R. Goncharov[1] and A. B. Kukushkin[2,3]
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An overview of the current activity in the Russian Federation on atomic, molecular and PMI data has been presented, including contributions from the NRC Kurchatov Institute, NRNU Moscow Engineering Physics Institute, A.F. Ioffe Physico-Technical Institute, Peter the Great Polytechnic University, Troitsk Institute for Innovation and Fusion Research, P.N. Lebedev Physical Institute, and G.I. Budker Institute of Nuclear Physics. The data are organized in the tables according to categories of “Data Generation”, with the accent on verification and application of the newly generated data, and “Data Use”, with the accent on the data needs for ongoing projects. Particular results were illustrated with detailed slides.

The data needs and data use for the spectroscopic diagnostics to be provided by the Russian Federation for ITER have been reviewed: (a) main chamber H-alpha (and visible light) spectroscopy and its verification on the JET-ILW tokamak; (b) edge charge-exchange recombination spectroscopy and its verification on the T-10 tokamak; (c) divertor Thomson scattering and the accompanying laser-induced fluorescence diagnostic, and their verification on the GLOBUS tokamak. The work in support to the ITER Core Thomson Scattering Diagnostics (EU) is also included.

The work on the verification of the issues of importance to other problems in ITER have been reviewed. This includes the tests of tungsten materials on the QSPA facility in TRINITI; the tests of plasma-facing-component materials and of hydrogen isotope retention at the cyclotron and the LENTA linear divertor simulator in Kurchatov Institute; the PMI data activity in NRNU MEPhI, including the stand for film deposition and material irradiation.
An overview of the use of atomic data in numerical modeling for ITER neutral particle diagnostics being developed in the Russian Federation, neutral particle diagnostics and other activities on the Globus-M spherical tokamak have been presented, as well as the extensive use of atomic data for pellet charge exchange (PCX) diagnostics on LHD in Japan, as a collaborative activity involving co-authors from NIFS, Japan, and Peter the Great Polytechnic University, Russia.
A brief review of the PMI data activity in the Russian Federation, as reported at the 18th Russian Conference on Plasma-Surface Interactions in Moscow, has been presented, including both the theory and experiments.

The survey enabled us to draw the following conclusions. First, the use of A-M data covers both the recognized databases (IAEA AMDU Databases, NIST, ADAS) and newly generated data. Next, the results of simulations by the suites of codes, e.g. B2-EIRENE (SOLPS-ITER), for reference scenarios of ITER operation have become a database widely used by ITER component designers. New A+M data may come from semi-analytic models for arising complicated problems (e.g. elementary process rates for many-electron, heavy-impurity atom and ions like, e.g., W in ITER) where the direct numerical modeling is either too cumbersome for providing the extensive databases or not very reliable for partially simplified simulation. The use of available PMI data, as a rule, assumes interpolation and/or extrapolation because of much less universality compared to A+M data. Generation of PMI data is rapidly growing along many lines. The benchmarking is more complicated compared to that for A+M data, however, is feasible for critical problems, e.g. melting of tungsten tiles. Experiments emulating ITER conditions (heat load, sputtering, etc.) seem to be the major line.

Ongoing and pending data base activities at FZ Jülich

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

Past activities at FZ Jülich on establishing own molecular databases (e.g. for collision processes between plasma electrons or protons and hydrocarbons up to C3H8 (and their ions) as well as of the Silane family SH4 and smaller, have ended, but the databases are maintained online under http://www.hydkin.de.

A similar attempt to build a database for breakup of BeH, BeH_2, and their ions in fusion plasma relevant conditions had been started some years ago. But despite the significant amount of material meanwhile being available in published literature, a comprehensive, internally consistent, complete chain of cross sections and rate coefficients for all competing fragmentation channels, to be used in modeling codes, could not yet be established, due to lack of resources.

The current FZJ activities on database maintenance and extensions of existing databases used in fusion edge plasma modeling (i.e. for those regions of the fusion plasma which are directly affected by the presence of molecules and wall recycled (or sputtered) atoms) are now mainly focused on raw data processing, condensation, their integration into transport codes and uncertainty propagation (sensitivity analysis).

The surface reflection database based on the BCA (binary collision approximation), i.e. various versions of TRIM-code results) is maintained under http://www.eirene.de/html/surface_data.html, and updated with further target projectile combinations upon request (latest new entry Oct. 2015: H,D,T on Al.)

This database differs from other surface reflection databases by the fully retained resolution wrt. reflected energy and angles, by storing these 3D velocity space distributions in a "conditional quantile format", (G. Bateman, PPPL report no. 1, 1980), which is particularly suitable for Monte Carlo transport code sampling of energy and angles of reflected (or sputtered) particles, for a given incident energy and angle.

Due to progress in computing speed and also transport code development the atomic/molecular data used in edge plasma modeling codes today can be far more detailed than before. This calls not necessarily for new raw data, but for reduced levels of condensation, more independent parameters in so called "effective rate coefficients", e.g. already 5 independent parameters ne, Te, ni, Ti, and E0 for an effective MAR (molecular activated recombination) rate coefficient. Major issues currently investigated are "physically correct" asymptotic behavior in all variables, proper behavior of the data when applied for the reverse processes (detailed balancing), either in case of fits or tables, and the possibility to directly integrate collisional radiative codes into transport modules without the intermediate step of multi-dimensional tabulation, or fitting (i.e. establishment of a CR model code library). This is established in the EIRENE Monte Carlo transport code so far only for the H,H+ system, and is currently being implemented for the H2 and He CR models. The ongoing data evaluation processes for electron collisions on Be, Be+ , by the AMS data unit of IAEA, if successful, will then also, hopefully, provide an evaluated underlying cross section database for such a collisional radiative code module for Be atoms, ions and ultimately their related molecules BeH, etc.…

Current Activities (2014~2015) of Atomic and Molecular Database at NFRI

J. S. Yoon
National Fusion Research Institute, Plasma Technology Research Center, Gunsan, Korea

J.-S. Yoon reported on the activities of Data Centre for Plasma Properties (DCPP) where their research focused on low temperature plasma full-set data generation with simulation tools. In general, 2~5 gas mixtures are used in low temperature plasma processing (ex. Semiconductor and display), however, complete and consistent datasets for electron scattering cross sections from most molecular species encountered in low temperature plasmas are limited to only few system. Thus, such a data needs from low temperature plasma industry in Korea, DCPP established electron impact total and dissociation cross section measurement system with Australian National University(ANU) and Sophia University in Japan. Also, they developed simulation tool for etching and deposition process in semiconductor including several mixture gas data module. It is now successfully adapted in several semiconductor industry. For fusion applications, they summarized their activities about data evaluation and bibliographic data compilation with IAEA. For data evaluation, NFRI operated small expert evaluation group and they evaluated cross section data for electron collision with methane. This result was summarized by M.-Y. Song in DCN meeting, and published in Journal of Physical and Chemical Reference Data, 44, 023101 (2015). Also, reported their ongoing research activities for Fusion and Plasma big data systems and experimental facilities for electron collisions with atoms and molecules and highly charged ion - matter interaction are under development.

Current Activities of IAEA Atomic and Molecular Unit Activities

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International Atomic Energy Agency, Vienna, Austria

The IAEA atomic and molecular data unit activities consist of data projects and data network activities. For data projects, the unit organizes Coordinated Research Projects (CRP), technical and consultants' meetings and publications for public access to data. Also the unit maintains data centre network of national data centres and code centre network of code developers. CRP is a main mechanism that the unit produces, compiles and evaluates data in collaboration with Member states. Researchers are brought together to work on a specific topic in a defined and coordinated fashion and the output of CRP is publications, meeting presentations, reports and books. In 2014-2015, a CRP on "Spectroscopic and Collisional Data for W from 1 eV to 20 keV " is concluded with a special volume in Atoms journal and 3 CRPs on "Data for kinetic modelling of molecules of H and He and their isotopes in fusion plasma", "Erosion and Tritium Retention for Beryllium Plasma-Facing Materials" and "Plasma-Wall Interactions with Irradiated Tungsten and Tungsten Alloys in Fusion Devices" remain active. A CRP on "Plasma Interaction with Reduced-Activation Steel Surfaces in Fusion Devices" started in 2015. The unit organized 9 meetings in 2015 and 8 meetings in 2014 and produced 4 special volumes on atomic, molecular and plasma-material data topics.

The unit maintains several databases such as ALADDIN numerical database and AMBDAS bibliographical database and as a code centre, the unit hosts online codes and code results. New additions to codes available through the unit's home page are FAC (Flexible Atomic Codes) and GRASP2K codes where documentations of FAC codes are updated and available. A new database on dust particles measured in fusion reactor is in development.

Since 2012, the unit has emphasized the importance of data evaluation and uncertainty quantification and organized a series of meetings on the matter. Initially meetings were focused on the strategy to promote data evaluation in the community and develop a methodology of evaluation. More recently, the unit is organizing meetings to produce evaluated data relevant to fusion research, for example, electron-Be collision data and electron-W recombination data.

Recent Progress of KAERI Atomic Database

D.-H. Kwon
Nuclear Data Center, Korea Atomic Energy Research Institute, Daejeon, Korea

We have carried out calculations for electron-impact ionization cross section of P-like isoelectronic sequences from P to Zn [1] and W^{17+} [2] and W^{+} [3] and dielectronic recombination of W^{45+} [4] using the flexible atomic code (FAC) based on a distorted wave approximation. Besides photoionization cross sections for Mg-like isoelectronic sequences from Mg to Ar except for P have been calculated by non-iterative eigenchannel R-Matrix method [5]. Our calculated atomic data have been uploaded on our Web DB (http://pearl.kaeri.re.kr) as graphical and numerical forms. The graphical plots are flexible in axis-range and scale variations on the Web and as well other available data can be plotted together with ours for comparison. We have also performed spectroscopic measurements in various plasma devices and the collisional-radiative (CR) modelling for the analysis. CR modelling for He I have been developed [8] and line ratio by the CR modelling as a function of plasma temperature and density can be obtained on our Web DB for selected transition lines at a given He gas pressure.
For ongoing works parallelization and a unitary correction of original FAC have been done, respectively, for large size DR calculations and for collisional excitation calculations of neutral atom.

[1] D.-H. Kwon and D. W. Savin, Astrophys. J 784, 13 (2014)
[2] D.-H. Zhang and D.-H. Kwon, J. Phys. B 47, 075202 (2014).
[3] D.-H. Kwon, Y.-S. Cho, and Y.-O. Lee, Int. J. Mass Spectrometry 356, 7 (2013).
[4] D.-H. Kwon and W. Lee, J. Quant. Spectrosc. Radiat. Transfer 170, 182 (2016).
[5] D.-S. Kim and D.-H. Kwon, J. Phys. B 48, 105004 (2015).

ADAMANT: a platform for data users and producers

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Over past three years (starting late 2012) a platform capable of producing large amounts of high-quality atomic spectroscopic data was assembled and a database ADAMANT (Applicable Data of Many-electron Atom eNergies and Transitions) was developed at Institute of Theoretical Physics and Astronomy of Vilnius University. The Institute has old traditions and huge experience in atomic theory, especially in investigation of multielectron ion spectroscopic properties. Hence it was decided to transfer created methods, algorithms and computer code suites into one platform capable of producing high-accuracy atomic data and preparing them for plasma modeling applications.

This task is realized by developing an open-access database (www.adamant.tfai.vu.lt) that contains theoretical spectroscopic parameters, obtained using our own original computer code suited or other well-established codes. The accuracy of determined atomic data is assessed and they are prepared for use in plasma spectra modeling. The database ADAMANT is arranged in such a way that it is easy to update and extend existing data sets in an automatic way. The User Guide gives basic information about the presented parameters, about the approximations and methods used to calculate atomic data. A possibility to add user comments or data requests is also foreseen.

The database contains spectroscopic parameters: level energies and level multireference wavefunction compositions; level lifetimes and Lande *g*-factors; radiative transition of various multipole order data: wavelengths, transition probabilities, oscillator strengths, transition line strengths. In addition to the discrete state data, we present electron-ion interaction parameters: autoionization probabilities, electron-impact excitation cross-sections, collision strengths, collision rates; electron-impact ionization cross-sections, strengths, rates; level-resolved dielectronic recombination rates. One of the most important features of our database is that the same computer code suites, same approximation for configuration interaction (CI) and relativistic effects, an identical multireference wavefunction basis is used in the calculated data set for a specific ion. This leads to a reduced workload for data application and simple data parsing for modeling codes. Today the database ADAMANT contains somewhat 14 GB of data for more than 1100 species. Those data are processed in a pipeline from the raw calculation data and can be served in several output formats (ASCII machine readable, HTML, ASCII ";" separated, HTML (formatted), XML VOtable standard).

Sizeable part of the data important in fusion plasma modeling (such as parameters for tungsten ions of various ionization degrees) are determined using quasirelativistic Hartree-Fock (QRHF) approach with transformed radial orbitals (TRO) describing virtually-excited electrons. For the lower-Z ions, a standard semirelativistic (Breit-Pauli) Hartree-Fock approximation can be adopted. For the ions important in the astrophysical plasma modeling ($Z \leq 30$), we employ the Flexible Atomic Code (FAC). The database contains radiative transitions and autoionization data for the ions with the vacancy in the inner 1s, 2s, 2p shells. These data are utilized in the spectral synthesis code Cloudy (www.nublado.org) and incorporated in its atomic and molecular database Stout. FAC is also deployed to calculate the autoionization parameters for the alkaline elements.

LXCat: a web-based, community-wide project on data needed for modeling low temperature, non-LTE plasmas

L. C. Pitchford, on behalf of the LXCat Team*
LAPLACE, CNRS and Univ. Toulouse, France

The LXCat platform is an open-access website (www.lxcat.net) which aims to provide a convenient infrastructure for storing, accessing and manipulating data for the electron and ion components of low-temperature (technological) plasmas. Anyone willing to contribute data can request an account and receive instructions for setting up a password-protected database on LXCat. The contents and maintenance of the individual databases are the responsibility of the contributors. The LXCat platform offers daily back-up and usage statistics. On-line tools are available for searching and manipulating data. An on-line Boltzmann solver allows users to calculate transport and rate coefficients in arbitrary gas mixtures is the cross sections for the individual components are available in one of the databases. At present, 22 databases contributed by groups around the world can be accessed on *LXCat*.

The available data types for electrons are electron-neutral scattering cross sections, both differential and angle integrated or "total" cross sections (mostly total cross sections) as well as measured electron transport parameters as a function of E/N, the reduced electric field strength, in a number of gases. Note that E/N is a good parameter in the limit of a cold gas, low degree of ionization, and homogeneous electric field. Some of the databases include "complete" sets of cross section data and thus can be used as input to a Boltzmann solver to obtain electron transport and rate coefficients as a function of electron temperature (for Maxwellian distributions) or as a function of E/N or average electron energy (for nonMaxwellian distributions). One such Boltzmann solver, BOLSIG+, can be run on-line. On-line comparisons using different databases are easily accomplished. The data types for the ions include transport and rate coefficients, ion-neutral interaction potentials and ion-neutral cross sections. Recently, a new database containing measured optical oscillator strengths for 75 species has been added to the site. From such data, and with a suitable model, electron-neutral cross sections for dipole transitions can be accurately estimated.

Usage statistics attest to a steady increase in the number of visitors and a glance at the titles of papers referring to LXCat show that researchers from many different scientific and technical areas make use of the data available on this site.

This presentation will include a brief discussion of the initial motivation, the present objectives and the future strategy of LXCat.

* The LXCat team members as of October 2015 are from Australia (I Bray, D Furst, L Campbell, M Brunger and S Buckman); Canada (A Stauffer, C Brion); France (MC Bordage, GJM Hagelaar, LC Pitchford, V Puech); India (B Chaudhury, S Chowdhury); Japan (Y Itikawa); Mexico (J de Urquijo); the Netherlands (J van Dijk); Portugal (LL Alves); Russia (I. Kochetov, A. Napartovich); Switzerland (S Pancheshnyi); UK (S Biagi, Quantemol team); and USA (K Bartschat, WL Morgan, L Viehland, O Zatsarinny).

The CHIANTI atomic database

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George Mason University, NASA Goddard Space Flight Center, USA

CHIANTI (http://chiantidatabase.org) is a freely-available atomic database and software package for spectroscopic diagnostics of astrophysical plasmas. Atomic data are selected from the published literature and evaluated to provide the best models for ions and neutrals. The principal data-sets are energy levels, radiative decay rates and electron effective collision strengths for modeling the level balance equations for electron densities in the low density regime (typically below 1013 cm-3). Additional data-sets include proton excitation rates, dielectronic capture rates, level-resolved ionization and recombination rates and two-photon decay rates. Total ionization and recombination rates are also provided for calculating the zero-density ionization balance in electron-ionized plasmas. Atomic data are also included for computing the free-free, free-bound and two-photon continua.
Data for 246 ions of elements up to and including zinc are contained in CHIANTI, and a particular focus is on the iron ions, many of which have atomic models containing several-hundred fine structure levels.

CHIANTI was first released in 1996 (Dere et al. 1997, A&AS, 125, 149) and version 8 was released in September 2015 (Del Zanna et al. 2015, A&A, 582, A56). The CHIANTI papers have received over 2000 citations, currently averaging 120-140 citations per year. CHIANTI is principally applied in solar physics, but there are many applications in astrophysics, including galaxy clusters, accretion disks, supernova remnants, stellar atmospheres and the Jupiter-Io plasma torus. In addition to spectral modeling, CHIANTI is also used by theoretical modelers for predicting radiative emissions from their codes, and it is also used by instrument teams for computing temperature response functions and performing calibration.

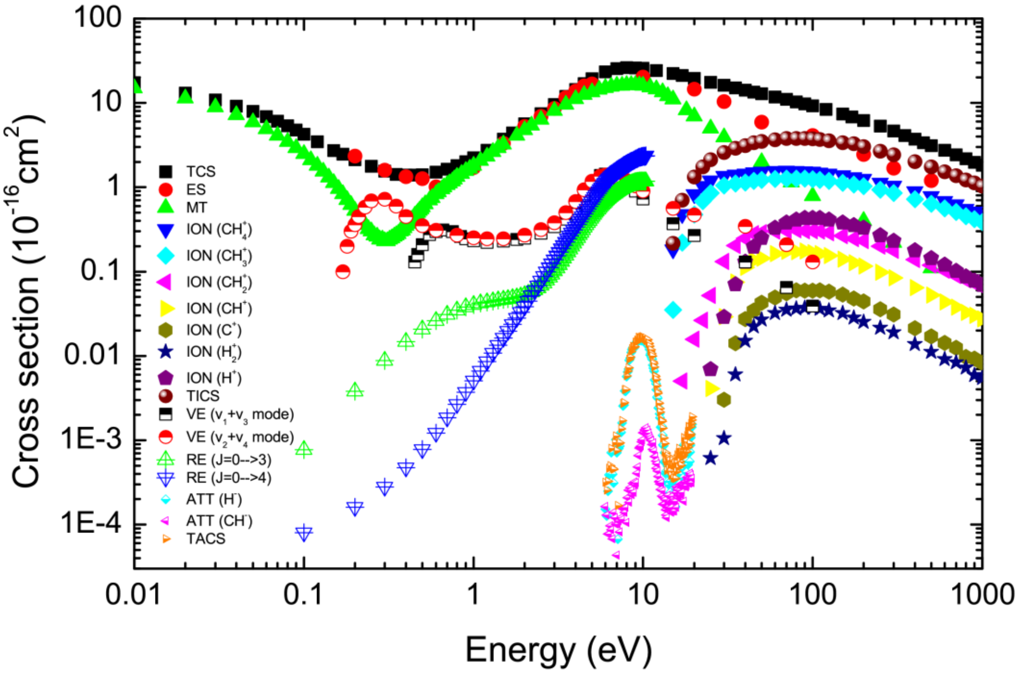
Data evaluation is a critical component to CHIANTI. The best available atomic data are selected, often from multiple sources, and combined to create a single, coherent model for each ion. A graphical assessment code is applied to each electron excitation transition to identify data irregularities. Benchmark studies are performed by the CHIANTI team members by comparing emission line emissivities with solar and stellar spectra to identify data anomalies and perform line identifications.
A CHIANTI Google Group is maintained as a forum for users to communicate with the CHIANTI team and for the team to send announcements.

Cross Sections For Electron Collisions With Methane

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

Methane (CH_4) is the simplest hydrocarbon molecule and has attracted significant interest as a target for low-energy electron collision studies. It has many technological and atmospheric applications as well as a fundamental importance as one of the testing grounds for the collision theories. Reflecting this importance, a number of compilation of cross section data have been published. Those publications, however, are rather old and a considerable number of new cross sections are available now.

In this report, cross section data have been compiled from the literature for electron collisions with methane molecules. Cross sections are collected and reviewed for total scattering, elastic scattering, and momentum transfer, excitations of rotational and vibrational states, dissociation, ionization, and dissociative attachment. The swarm method and data have also been included. For each of these processes, the recommended values of the cross sections are derived, and a part of them is presented in Fig.1 below. The literature has been surveyed through early 2014



Appendix 4

Data needs reflected in 2015 overview of A+M+PMI activity in Russia

Purpose	Needed Data
Hα diagnostics on ITER	Hydrogen isotope molecules dissociation with excited atoms as products Beryllium hydride molecules
ITER Thomson scattering diagnostics	Complex impurity molecules in divertor plasmas
ITER CXRS edge diagnostic	W lines intensity for all kinds of ionization stage in CXRS ranges: 468±8 nm 529±8 nm 656±10 nm
Theoretical studies of MARFE development for ITER-like impurity mixture (NRC Kurchatov Institute)	Elementary processes with high-Z impurities (W)
Diagnostics of edge plasma parameters on Globus-M/M2 spherical tokamak (Peter the Great Polytechnic University and A.F. Ioffe Physico-Technical Institute)	Improved data are needed for transition rates in the range of 2.0×10^{18} m^{-3} < n_e < 2.0×10^{19} m^{-3} and 10 eV < T_e < 250 eV
Measurements of the ion distribution function with an active PCX diagnostic (collaboration involving co-authors from NIFS, Japan, and Peter the Great Polytechnic University, Russia)	Calculation of the hydrogen Balmer-beta line shapes (in the vicinity of the line center 486.12 ±5 nm) in the multicomponent plasma such as 1/1 (for ablating polystyrene pellets) and 1/2 C and H (for ablating polypropylene or polyethylene pellets) mixture can improve results of the investigation. Required temperature range 0.5 – 15 eV Required electron density range 10^{16} - 10^{18} cm^{-3}
Doppler-shift measurements of NB species content (G.I. Budker Institute of Nuclear Physics)	Sublevel-resolved cross-sections of hydrogen excitation in collisions with H_2

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