https://doi.org/10.61092/iaea.rg9k-wjvd

INDC(NDS)-0801
Distr. LP,NE,SK

IAEA
International Atomic Energy Agency

INDC International Nuclear Data Committee

Technical Aspects of Atomic and Molecular Data Processing and Exchange
25th Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

30 September – 2 October 2019

Prepared by
K. Heinola
IAEA Nuclear Data Section

June 2021

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

Selected INDC documents may be downloaded in electronic form

from http://nds.iaea.org/publications

or sent as an e-mail attachment.

Requests for hardcopy or e-mail transmittal should be directed to

NDS.Contact-Point@iaea.org

or to:

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
PO Box 100
1400 Vienna
Austria

Printed by the IAEA in Austria

June 2021

INDC(NDS)-0801
Distr. LP,NE,SK

Technical Aspects of Atomic and Molecular Data Processing and Exchange, 25th Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

30 September – 2 October 2019

Prepared by

K. Heinola

IAEA Nuclear Data Section

Abstract

This report summarizes the proceedings of the IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (25th Meeting of the A+M Data Centres Network) on 30 September – 2 October 2019. 13 participants representing 12 national data centres in 9 Member States attended the three-day meeting at IAEA Headquarters in Vienna.

June 2021

Table of Contents

Abbreviations

A+M	atomic and molecular
AOCC	atomic orbital close-coupling calculation
CERN	European Organization for Nuclear Research
CR	collisional-radiative
CRP	coordinated research project
CX	charge-exchange neutral atom
DCN	Data Centres Network
DEMO	demonstration fusion reactor
DFT	electron density functional theory
DOI	digital object identifier
EBIT	electron ion beam trap
EUV	extreme ultraviolet
EX	excitation
FPP	fusion power plant
FW	first wall of a fusion device or reactor
ITER	international thermonuclear fusion device; next-step fusion device
JET	Joint European Torus
JET-ILW	JET's ITER-Like Wall project
LHD	Large Helical Device
MOCC	molecular orbital close-coupling calculation
OES	optical emission spectroscopy
PMI	plasma-material interaction
PSI	plasma-surface interaction
TDDFT	time-dependent DFT
TDS	thermal desorption spectrometry
TM	technical meeting
UQ	uncertainty quantification
VUV	vacuum ultraviolet

1. Introduction

The 25th 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 30 September to 2 October 2019. The objectives were to review progress in atomic, molecular and plasma-surface interaction (A+M/PSI) data related activities in the national data centres and to formulate work plans related to data issues for the next period.

Activities of ten data centres were presented: by Yu. Ralchenko of NIST (National Institute of Standards and Technology, USA), I. Murakami of NIFS (National Institute for Fusion Science, Japan), M.-Y. Song of NFRI (National Fusion Research Institute (presently KFE, Korea Institute of Fusion Energy), Korea), M. O’Mullane of ADAS (Atomic Data and Analysis Structure Project, UK), D.-H. Kwon of KAERI (Korea Atomic Energy Research Institute, Korea), P. R. Goncharov of SPbSTU (Peter the Great St. Petersburg Polytechnic University, Russia) on behalf of A. B. Kukushkin (NRC Kurchatov Institute, Russia), K. Heinola of IAEA, Y. Wu of CRAAMD (China Research Association of Atomic and Molecular Data, China), R. Barrachina of CAB (Centro Atómico Bariloche, Argentina) and C. Ballance of QUB (Queen’s University Belfast, UK). T. Nakano of QST (National Institutes for Quantum and Radiological Science and Technology, Japan) did not participate due to lack of activity in A+M data projects since the Fukushima incident.

An additional expert was invited to discuss their work on A+M data: V. Laporta of CNR Bari (Consiglio Nazionale delle Ricerche, Italy). His data centre is considered as a new member of the DCN and the membership status will be formally accepted in the next DCN meeting in 2021.

Two additional experts maintaining atomic and molecular databases for nuclear fusion and fission were invited to discuss their work in data evaluations and dissemination: D. Reiter of Heinrich Heine University Düsseldorf, Germany and who is currently an ITER Fellow, D. Brown of Brookhaven National Laboratory, USA.

A. Koning (Section Head, Nuclear Data Section), C. Hill (Unit Head, A+M Data Unit) and K. Heinola (Atomic Physicist, A+M Data Unit and Scientific Secretary) represented the IAEA. In addition, the first day of the TM had representatives from other Units of the Nuclear Data Section: J.-C. Sublet (Nuclear Data Services Unit) and R. Capote Noy (Nuclear Data Development Unit).

Discussions were held on the following topics:

- Exchange of information on data centre activities
- Data evaluation: experiences, plans and encouragement
- Cooperation of maintenance of bibliographical databases
- Priorities for A+M data for fusion applications
- Priorities for data development and evaluation, uncertainty quantification, new meetings and information exchange

2. Proceedings

The head of the Nuclear Data Section, A. Koning welcomed participants and emphasized increasing interest and need for atomic and molecular data. Participants introduced themselves and the agenda in Appendix 2 was adopted without change. K. Heinola 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.

Speaker summaries are provided in Appendix III and presentations are available on the A+M Data Unit web page at https://amdis.iaea.org/meetings/dcn-25/.

2.1 Current activities of Atomic and Molecular Data Centres

Yuri RALCHENKO (NIST, USA) described the atomic data research and database development at NIST. He reviewed the current NIST Atomic Spectra Database v5.6.1, which will be updated to v5.7 in October 2019. There are still gaps in the data for W, but which are hard to measure experimentally. The NIST LIBS Database (Laser-induced Breakdown Spectroscopy) was presented and its application to ITER was discussed. NIST maintains atomic bibliographic databases for i) atomic energy levels and spectra, ii) atomic transition probabilities and iii) atomic lines broadening and shifts, which updated regularly approx. in two weeks and which submitted to IAEA annually. NIST maintains the online computational tool for collisional-radiative modelling – FLYCHK, which has over 1100 users globally. Recently, NIST has published recommended cross-sections for electron-impact excitation and ionization for BeI, which comprise of analytical fits done with converged close coupling (CCC) and B-spline R-matrix (BSR) calculations. A new spectrometer with high energy resolution – a broad-band X-ray Microcalorimeter – has been installed on the NIST EBIT system in December 2018.

MURAKAMI Izumi (NIFS, Japan) reported the atomic and molecular data activities at NIFS in 2017 – 2019. The NIFS database on A+M and PWI was reviewed. There are no recent changes in the system, but new data has been added to databases AMDIS, CHART, AMDIS MOL (AMOL), CHART MOL (CMOL) and SPUTY. The A+M bibliographic database ORNL has not been updated since 2009. The AMDIS ION database is now integrated within VAMDC database and there are plans to implement AMDIS EXC to VAMDC next. A working group has been established with Japanese A+M physicists to update NIFS data e.g. for W and heavier elements as well as for light and heavy elements relevant for fusion reactor materials. Various smaller satellite databases are linked to NIFS, but there are no new entries during the last two years. NIFS carries out continuous experimental and theoretical studies on W ions, such as i) EUV, VUV and visible spectra measured with Tokyo-EBIT, CoBIT and LHD stellarator, ii) measurements at LHD using W pellets for unresolved transition array (UTA) of W^{24+}-W^{26+} emitted at EUV, which is very important for studying W in the edge plasma of ITER and iii) development of new hybrid CR model for W^{27+}-W^{34+} ions with recombination processes.

Mi-Young SONG (NFRI (presently KFE), Korea) reported on the A+M data center activities at the NFRI during period 2017 – 2019. Activities of the Fundamental Technology Research (FTR) Division were outlined. FTR Division comprises of Data Center for Plasma Physics (DCPP), which maintains a Web Database System for collision cross-sections, rate coefficients, electron collisions and heavy particle reactions as well as numerical and bibliographic data. Data relevant for fusion plasma-surface reactions, such as sputtering, sticking/adsorption/diffusion coefficients, are planned to be included by the end 2019. The AMBDAS database has been updated to include records up to 2018. NFRI's fundamental studies of A+M properties comprise of i) structures of molecules and their physical and chemical parameters, ii) electron collision processes with A+M (ionization, excitation, dissociation, etc with BEB method, R-matrix method and experiments (total cross-sections of electron scattering, dissociation cross-sections as well as plasma-material interactions) and iii) A+M properties of plasmas (plasma diagnostics with OES, CR modelling, analysis of OES data with Machine Learning to predict plasma state. Total electron scattering cross-sections for NO_2 has been obtained, next would be NH_3. Also, R-matrix method will be applied to calculations of elastic and excitation cross-sections of BeH_2, NH and C_4F_6 at low energies. NFRI carries out data evaluation activities through a working group of international A+M experts to establish an internationally agreed standard reference data library for A+M/PMI data. Completed evaluations of NF_3 and N_xO_y are followed by H_2O and N_2.

Martin O'MULLANE (ADAS, UK) reported on recent developments in ADAS and OPEN-ADAS. The project for calculations of W dielectronic recombination rate coefficients reported previously results for W^{56+}-W^{73+} and W^{38+}-W^{55+} and has been extended to cover W^{37+}-W^{28+} and W^{1+}-W^{13+}. Further, calculations for W^{14+}-W^{27+} were underway at the time of the DCN meeting. Calculations for thermal charge exchange (CX) with neutral plasma particles, H^0, at low interaction energies were reviewed and cross-sections for N^{q+}+H^0; q=1-7 were discussed. States of low-lying levels of W is problematic due to the significant number of metastable states and therefore computational methods need to be developed to handle these.

Duck-Hee KWON (KAERI, Korea) reported on the recent activities on plasma spectroscopy and atomic data in KAERI Atomic Data Center. Optical emission spectroscopy (OES) measurements were carried out at KAERI's capacitively-coupled plasma (CCP) device for low temperature and low density Ar plasmas and the results were combined with CR modelling. The obtained plasma T_e and temperatures were compared with the Langmuir probe measurements for ArI. In addition, OES and CR modelling was performed with KAERI Divertor Simulator, which allows high heat and high particle flux experiments. Emission of strong ArII lines was observed and simple CR modelling revealed large discrepancy with the OES results. More accurate CR modelling is needed and will be developed to include population kinetics such as recombination among ArI, ArII and ArIII

Pavel G. GONCHAROV (SPbSTU, Russia) on behalf of A. B. Kukushkin (Kurchatov Institute, Russia) reviewed recent works on atomic and PMI data for controlled fusion research in Russia. Activities of atomic data generation comprised of i) calculations with classical and quantum mechanical approaches of e^- capture and loss processes with heavy many-electron ions (e.g. Ar^{q+}… U^{q+}) with energies from 50 keV/u … 50 GeV/u, ii) one- and two-electron capture by He^{2+} from Ar atoms, iii) H and D scattering from amorphous Be, C and W targets, iv) radiative losses of α particles on W impurities as wells W migration in T-10 tokamak, v) spectral line shapes in fusion plasmas, vi) radiative transitions in atoms in hot dense plasmas under ultra-short electromagnetic pulses. Use of atomic data in fusion research comprised of i) CX collisions of H with C ions, ii) verification of interpretation methods of experimental Hα and visible spectroscopy data for ITER and JET-ILW, respectively, iii) cross-sections for CX reactions of H/D/T with Be and C for the ITER CXRS diagnostics of core and edge plasmas, iv) data for the operation of disruption mitigation/massive gas injection (MGI) diagnostics, v) CR models for HI and HeI, HeII in the framework of Laser-induced fluorescence and quenching diagnostics. Works on PMI data comprised of i) D retention studies in W under ITER-relevant transient conditions, ii) D co-deposition with metallic targets (W, Al, Mo), iii) analysis of Li content in co-deposits, iv) He retention in W at elevated target temperatures (up to 1200 K). The development of ITER diagnostics in Russia has revealed new A+M and PMI data needs.

Kalle HEINOLA (IAEA) summarized the activities at IAEA A+M Data Unit, which include CRP (Coordinated Research Projects), meeting organizations, book and report publications as well as the maintenance and development of databases and online codes. Much of the unit's activities has been focusing on remaking the A+M Unit's web pages in addition to launching new CRPs, workshops, databases and networks. Special mention is the crowdsourcing activity for visualizing and analyzing neutron-induced irradiation damage in fusion materials based on data hosted at the Unit's new database CascadesDB.

Yong WU (CRAAMD, China) presented the recent database activities at CRAAMD. The atomic spectra database comprises of ~20000 records with Al…Kr: C-like isoelectronic ions, Ne…Zn: Be-like isoelectronic ions, Ar…Zn: N-like isoelectronic ions and Cr…Kr: Ne-like isoelectronic ions. Cross-sections for heavy particle collisions involving CX and EX processes have been calculated for systems i) H^+, N^{q+}, O^{q+}, Ne^{q+}+H, ii) H^+, N^{q+}, O^{q+}, Ne^{q+}+He, iii) H^+, N^{q+}, O^{q+}, Ne^{q+}+H_2, iv) H^+, Li^{3+}+Li. Methodologies applied are atomic orbital close-coupling (AOCC), molecular orbital close-coupling (MOCC) and time-dependent DFT (TDDFT) and the results were benchmarked with experiments, where possible. TDDFT calculations provided cross-sections for He^{2+}+Ne and H^++H_2O processes. Data has been generated for atomic (e.g. Fe plasmas) and molecular (e.g. BeH^+, BH, H_2O) opacities as well as stopping powers for α particles in H_2 and Au plasmas.

Raúl BARRACHINA (CAB, Argentina) reviewed activities in many laboratories in Argentina working on Atomic, Molecular and Surface Physics in Argentina. They include the Bariloche Atomic Centre, a research facility of the National Atomic Energy Commission (CNEA), the Institute of Astronomy and Space Physics or IAFE, the Rosario Institute of Physics (IFIR) and the Southern Physics Institute (IFISUR) which cover a large range of processes, with different projectiles (ions, electrons, positrons, photons, etc.), targets (atoms, molecules, surfaces, etc.) and outgoing channels (elastic and inelastic collisions, charge exchange, ionization, transfer ionization, etc.). There is a plan to create a data centre DINAMO within the structure of CNEA and the objectives will be to provide fundamental data for nuclear and non-nuclear science (nuclear, atomic, molecular and optical (NAMO) research) and technological projects, and to coordinate the generation, collection and critical assessment of the required data by the different groups in Argentina.

Connor BALLANCE (QUB, UK) presented recent developments in the R-matrix calculations on the electron-impact excitation/ionization rates of W. Obtained results provide information for assessing the spectroscopic '*S/XB*' value, which is used for calculating the number of ionized particles per measured photon in the plasma. W is demanding for R-matrix codes: W requires a target description of several hundred of thousand levels due to its open *d* and shell system. This results to thousands of (coupled) channels for scattering (excitation/ionisation). Electron-impact excitation rates of WI calculated with R-matrix have been recently calculated and exist in the literature (and are implemented in ADAS) and results for WII will be made available by the end of 2019. However, electron-impact ionization (ground and metastable states) calculations of W are problematic due to the accuracy of the excited states. The ionization of highly-excited states of W influences the total effective ionization rate, which is seen in the CR calculations.

2.2 Proposed Data Centre Activities

One data centre, potentially joining the DCN, presented their data activities. Membership will be reviewed prior to the 2021 DCN meeting.

Vincenzo LAPORTA (CNR, Bari, Italy) presented *ab-initio* modelling research on electron-molecule scattering dynamics in non-equilibrium plasmas. The rotationally and vibrationally resolved processes included i) vibrational excitation, ii) dissociative attachment, iii) dissociative excitation and iv) dissociative recombination. Cross-section and rate coefficient results were presented for various systems e + N_2, $e + O_2$, $e + CO_2$, $e + BeH^+/BeD^+$, $e + H_2$, $e + ArH^+$, e + OH.

2.3 Data Needs for Fusion Research

Detlev REITER (Heinrich Heine University Düsseldorf, Germany, ITER Scientific Fellowship Network) summarized issues with CR and plasma chemistry modelling of fusion boundary plasmas. Current status of the elementary data matrix available for CR modelling of e/p + Be/BeH_y systems was reviewed and still unanswered or open questions were addressed. As an interim conclusion was presented that A+M and PMI data usage in fusion research is currently far behind the data availability. However, data applications in fusion require data sets, which are balanced, internally consistent, complete, conveniently available, etc. Existing and published reports/databases for plasma chemistry were reviewed: work done during Carbon era with C_xH_y molecules may pave the way for work with hydrides presently expected to be present in metal machines, such as Be_xH_y, N_xH_y, HeH^+, etc. The most important electron and proton collision processes e/p + $H/H_2/H_2^+$ required for fusion and CR modelling were reviewed. Importance of the isotope effect H/D/T for electron collision processes was highlighted, such as i) collapsing isotope effect in electron-impact excitation of H_2, D_2, T_2, HD, HT, DT and ii) dissociative attachment in H_2, D_2.

2.4 Atomic Data in the ENDF Library

David BROWN (Brookhaven National Library, USA) presented the current status of atomic data in the ENDF database. Various Monte Carlo -based particle and neutron transport codes (MCNP6, SCALE, GEANT4 etc) and nuclear isotope burn-up codes (ORIGEN, CINDER) have calculation modules, which use ENDF/ENSDF data. ENDF Library contains three sublibraries with an atomic focus: under domain Collisional Data are the photo-atomic and electro-atomic sublibraries, and under Spectroscopic Data is the atomic-relaxation sublibrary. Content and usage of ENDF atomic sublibraries were reviewed. Important report was given on the detected inconsistencies between the latest release version and the published version of ENDF/B-VIII.0. The latter contains erroneous binding energies, which are fixed in the latest release version, however, the latest release version is only available in EPICS2017 but not elsewhere, such as in NDS databases. Other version shortcomings were reviewed and gaps in data processing, reviewing, validation, etc activities as well as measures for future improvements were given.

3. Technical Discussions

Issues related to data research, data needs 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 following point were raised during the discussions about bibliographic information on A+M data:

- The A+M Unit's own bibliographic database AMBDAS has 50 000+ entries (https://www-amdis.iaea.org/AMBDAS/), but its interface is in need for an upgrade and that work is ongoing. AMBDAS contains approx. 10 000 duplicate entries and around 10 000 entries are without their Digital Object Identifiers (DOIs).
- Process classifications and notations used as search parameters in bibliographic databases were reviewed and revisited in a Technical Meeting in Nov 2019. The updated process classification list v2.1 is found at https://amdis.iaea.org/databases/processes
- The Harvard Astrophysics Data System (ADS) (https://ui.adsabs.harvard.edu/) is widely used in the astrophysics community
- NIST maintains atomic bibliographic databases, which are updated in regularly (in every ~2 weeks) and which data is annually submitted to IAEA
    - Atomic Energy Levels and Spectra Database (https://physics.nist.gov/cgi-bin/ASBib1/ELevBib.cgi)
    - Atomic Transition Probabilities Database (https://physics.nist.gov/cgi-bin/ASBib1/TransProbBib.cgi)
    - Atomic Lines Broadening and Shifts Database (https://physics.nist.gov/cgi-bin/ASBib1/LineBroadBib.cgi)
- NIFS has a bibliographic database, but that has not been updated since 2009
- NFRI has numerical data on collisional processes linked to bibliographical data and that data (up to year 2018) has been provided to AMBDAS for an update
- The SPECTR-W^3 database on spectroscopic properties of atoms and ions contains bibliographic database (http://spectr-w3.snz.ru/index.phtml), but its update frequency needs to be verified
- The previously available ORNL "Red Books" series on atomic data for fusion applications have in recent years become unavailable since closing down the corresponding web page. The AMD Unit has since then recovered the available "Red Books" found online and presently hosts Vols. 1, 3, 4, 5, 6-1, 6-2 and 6-3 at https://amdis.iaea.org/databases/.

- AMD Unit's new network for theorists and experimentalists Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP) is expected to result both data and bibliographic entries to the IAEA databases (https://amdis.iaea.org/GNAMPP/) in the future

3.2 Data Evaluation and Uncertainty Quantification Activity

There is a clear requirement for continuation of IAEA data evaluation activities. These have been co-ordinated by the DCN and a series of meetings that have been organized since 2012. These include consultancy meetings (CM) and technical meetings (TM) as well as collaboration workshops. The final report of the 24th DCN meeting reviewed the data evaluation activities since 2012. In 2012 the 1st TM on data evaluation identified issues such as lack of uncertainty quantification for theoretical data, lack of self-consistency checks in experimental data sets or lack of qualified data evaluators in the community. Since that meeting, IAEA promoted activities on uncertainty quantification (UQ) of theoretical data and data evaluation by editorial boards formed by group of A+M scientists. In 2016, a TM on "Uncertainty Assessment and Benchmark Experiments for Atomic and Molecular Data for Fusion Applications" was organized. However, since the TM for UQ and its final report publication[1], no major uncertainty estimate activities on atomic and molecular data have taken place by the A+M Unit. This is largely due to the unavoidable recruiting processes of the Unit's personnel. This issue was raised in the current DCN meeting and a potential new UQ activity was discussed.

The A+M Unit should continue promoting the philosophy for the importance of UQ quantification and transparently reporting the uncertainties within the provided data. The DCN discussed on the possibility of having a CRP on UQ issues but concluded it may not be required now. A code-comparison workshop is organized with the Neutral Beams CRP. Instead, promotional events could be organized in the form of ICTP workshop for young researchers, where participants would be introduced to the topics of UQ and error propagation with provided data and uncertainties. Also, intercomparison of computational methodologies may be included involving calculations with small-sized systems incorporating light atoms and molecules.

The DCN proposed more in detail an UQ activity, which would comprise of sensitivity analysis or uncertainty propagation of atomic structure and collision data on the final results. UQ in this area is complex due to the correlation between atomic structure and collisional cross-section data. A suggested possibility is a workshop or a TM on surrogate (simplified, not too challenging) model for UQ and error propagation (atomic structure to collision cross section: sensitivity analysis). The studied system was chosen to be Nitrogen and the activity would comprise of structural calculations (N, N_2, NH, …) and electron impact calculations (e + N, e + $NH_{1\text{-}3}$, …). NFRI expressed their willingness to contribute experimentally to the UQ of N activity. Uncertainties in the A+M data are crucial for modelling the divertor conditions of fusion reactor. In ITER it is expected that the plasma particle densities will be far greater than in any present tokamak fusion device. Ion collisionality is expected to increase up to two orders of magnitude. It has been assessed, that if the A+M data has even a small (~few percent) uncertainties, it may have a significant influence to the CR modelling and integrated modelling results of ITER divertor environment. The UQ of N will be discussed further at the next DCN meeting in 2021 and a potential supplementary meeting in connection of APiP conference in 2022 will be outlined.

As a subtask for CRP on Irradiated Tungsten, the A+M Unit organized a round-robin experiment for data validation of thermal desorption spectrometry (TDS) in collaboration with IPP-Garching and Osaka University. The TDS technique is critical to the measurement of hydrogen trapping and retention in fusion materials. However, the measured data have never been benchmarked. The TDS round-robin was organized to validate the TDS data and recommend the best practices of TDS measurements. However, results from this TDS round-robin experiment have not been published due to inconsistent and ambiguous results. The ultimate source for this outcome still needs to be scrutinized. A new TDS round robin has been planned in conjunction with a new CRP on Hydrogen Permeation. This time the round-

[1] J. Phys. D: Appl. Phys. **49**, 363002 (2016)

robin will be carried out with samples from 2 – 3 providers each representing a different method for sample preparation. Each provider prepares identical samples using their method and the samples will be distributed within the participants for TDS analyses.

There is a continuous concern on the financial support to the continuity of A+M activities on UQ and data evaluation and how to publicize them. It was recognized, that DCN members have been major supporting forces for the IAEA unit to pursue data evaluation activities. The IAEA DCN is expected to continue to play an important role in the quest of data evaluation and uncertainty quantification. It was considered that funding will eventually come if the community finds the activities important; visibility is crucial in this sense.

For data applications, it is important to ascertain what the target uncertainty is to be. Users should establish a list of important processes what is tolerated uncertainty etc. Integration of data user and data provider communities is very important. This question could be answered by the new GNAMPP network (https://amdis.iaea.org/GNAMPP/). Moreover, the data transferred from data providers to data users typically ends up as a black box within the codes used. There needs to be interaction between the providers and the end users, such as experimental spectroscopists and plasma modellers (transport, SOL, edge, etc). The data used needs to be commented, which is considered crucial and especially valuable for the recommended data.

Outreach issues:

- IAEA has no mechanism of bringing in new students etc. unless it involves developing countries. Financial support is limited.
- DCN could approve guest members, such as Universities working with fundamental A+M or PMI data
- A+M Unit continues encouraging users on the recognition of any A+M data used
- IAEA does not apply DOIs for their documents and hosted data. It is a widely expressed wish from the community that data used in research should be citable with a DOI. As an example, NIST provides DOIs for all the data at entry page. In addition, the data repositories at CERN are provided with a DOI. The topic with integrating DOI with data can be a topic for discussion at the next DCN meeting in 2021.
- The ICAMDATA conference is a good medium to bring the issues.

Appendix I: List of Participants

Connor BALLANCE, School of Mathematics and Physics, Queen's University Belfast, University Road, Belfast, BT7 1NN, UK

David BROWN, National Nuclear Data Center, Building 817, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

Raúl O. BARRACHINA, Centro Atómico Bariloche, Avda. Bustillo 9500, 8400 San Carlos de Bariloche, Rio Negro, Argentina

Pavel R. GONCHAROV, Research Laboratory for Controlled Nuclear Fusion, Peter the Great Polytechnic University, 29 Polytechnicheskaya st. 195251 Saint Petersburg, Russian Federation

Duck-Hee KWON, Nuclear Data Center, Korea Atomic Energy Research Institute, P.O. Box 105, 1045 Daedeok-daero, Yuseong-gu, Daejeon, Republic of Korea

Vincenzo LAPORTA, Instituto per la Scienza e Tecnologia dei Plasmi (ISTP), CNR, Bari, Italy

Izumi MURAKAMI, Data and Planning Center, National Institute for Fusion Science (NIFS), 322-6 Oroshi-cho Toki-shi, Gifu-ken 509-52, Japan

Martin O'MULLANE, Department of Physics and Applied Physics, University of Strathclyde, 107 Rottenrow, Glasgow, G4 0NG, UK

Yuri RALCHENKO, Atomic Spectroscopy Group, National Institute for Standards and Technology, 100 Bureau Dr., Stop 8422, Gaithersburg MD 20899, USA

Detlev REITER, Heinrich Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Mi-Young SONG, Korea Institute for Fusion Energy (KFE), 169-148 Gwahak-ro, Yuseong-gu, Daejeon 34133, Republic of Korea

Yong WU, Institute of Applied Physics and Computational Mathematics, Beijing, 100088, China

IAEA

Arjan KONING, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

Kalle HEINOLA, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

Christian HILL, IAEA Nuclear Data Section, Division of Physical and Chemical Sciences, P.O. Box 100, A-1400 Vienna, AUSTRIA.

Appendix II: Meeting Agenda

25th Meeting of the Data Centre Network

IAEA Headquarters, Vienna, Austria

30 September – 2 October 2019

Meeting room: M0E100

AGENDA

Monday, 30 September 2019

09:30 – 10:00	Arjan KONING, Christian HILL, Kalle HEINOLA: Welcome, introduction of the participants, adoption of the agenda

Session 1: Current Activities of the Data Centres I

10:00 – 10:30	**Yuri RALCHENKO**, *National Institute of Standards and Technology, United States of America* Atomic Data Research and Database Development at NIST
10:30 – 11:00	**MURAKAMI Izumi**, *National Institute for Fusion Science, Japan*
11:00 – 11:30	Coffee Break

Session 2: Invited Presentation

Chair: Arjan J. KONING

11:30 – 12:00	**David BROWN**, *Brookhaven National Laboratory, United States of America* Atomic data in the ENDF library

Session 3: Current Activities of the Data Centres II

12:00 – 12:30	**Mi-Young SONG**, *National Fusion Research Institute, South Korea,* A+M Data Center Activities in National Fusion Research Institute (2017~2019)
12:30 – 13:00	**Martin G. O'MULLANE**, *Department of Physics, University of Strathclyde, United Kingdom* Recent developments in ADAS and OPEN-ADAS: metals, influx and edge studies and web woes
13:00 – 14:30	Lunch

Session 4: Current Activities of the Data Centres III

14:30 – 15:00	**Duck-Hee KWON**, *Korea Atomic Energy Research Institute, South Korea* Recent Activities on Plasma Spectroscopy and Atomic Data in KAERI Atomic Data Center

15:00 – 15:30	**Pavel R. GONCHAROV**, *Peter the Great St. Petersburg Polytechnic University (SPbSTU), Russia* Recent Works on Atomic and PMI Data for Controlled Fusion Research in Russia
15:30 – 16:00	**Kalle HEINOLA**, *IAEA, Austria* Current activities of IAEA Atomic and Molecular Data Unit
16:00 – 16:30	Coffee Break
16:30 – 17:30	Coordinated activities on bibliographical data compilation (all participants)
19:30 – 21:30	Social Dinner: Gastwirthaus Pürstner, Riemergasse 10, 1010 Wien

Tuesday, 1 October 2019

Session 5: Current Activities of the Data Centres IV

09:00 – 09:30	**Yong WU**, *Institute of Applied Physics and Computational Mathematics (IAPCM), China,* Recent Database Activities of CRAAMD
09:30 – 10:00	**Raúl BARRACHINA**, *Centro Atómico Bariloche, Argentina* Roadmap on Atomic, Molecular and Optical Research at the Argentine Atomic Energy Commission
10:00 – 10:30	**Connor BALLANCE**, *Queen's University Belfast, United Kingdom* R-matrix excitation/ionization calculations for tungsten in support of magnetically-confined plasma diagnostics
10:30 – 11:00	Coffee Break

Session 6: Proposed Data Centre Activities

11:00 – 11:30	**Vincenzo LAPORTA**, *CNR Bari, Italy* Electron-molecule dynamics for non-equilibrium plasmas

Session 7: Databases and Data Exchange

Chair: Christian HILL

11:30 – 12:00	Data centre online databases and software demonstrations (all participants)
12:00 – 12:30	Data exchange format: XSAMS, ADAS, GENIE (all participants)
12:30 – 14:00	Lunch

Session 8: Data Needs for Fusion Research I

14:00 – 14:30	**Detlev REITER**, *Heinrich Heine University Düsseldorf, Germany*

	Issues with CR- and plasma chemistry modelling for fusion boundary plasmas
14:30 – 15:30	Discussion on A+M data needs for fusion applications (all participants)
15:30 – 16:00	Coffee Break

Session 9: Data Evaluation and Uncertainty Quantification

16:00 – 17:00	Discussion on coordinated activities on data evaluation (all participants)

Wednesday, 2 October 2019

Session 10: Data Needs for Fusion Research II

09:00 – 10:30	Discussion on priorities in A+M/PSI data compilation and evaluation (all participants)
10:30 – 11:00	Coffee Break

Session 11: Meeting Conclusions and Recommendations

Chair: Kalle HEINOLA

11:00 – 12:30	Plan of DCN activities for the future
12:30 – 14:00	Lunch

Session 12: Meeting Conclusions and Recommendations

14:00 – 15:00	Formulation of meeting conclusions and recommendations; Adjournment of the meeting

Appendix III: Summaries of Presentations

Atomic Data Research and Database Development at NIST

Yu. Ralchenko[1], A. Kramida[1], J.N. Tan[1], G. Nave[1], K. Olsen[1], J. Reader[1], Dipti[1], Hala[1], J. Ward[1], E. Takacs[2], R. Silwal[2], A. Gall[2], S. Saunders[2], Y. Yang[2]

[1]National Institute of Standards and Technology, Gaithersburg MD 20899
[2]Clemson University, Clemson SC

We present a detailed report on atomic data research and atomic database development at the National Institute of Standards and Technology (NIST) over the last two years (Oct 2017 – Sep 2019). Over this period, the most extensive database at NIST, the Atomic Spectra Database (ASD), had two major (5.5 and 5.6) and seven minor updates which brought the total number of critically evaluated energy levels and spectral lines in ASD to 111,865 and 276,555 respectively, with almost 118,000 transition probabilities. The Laser Induced Breakdown Spectroscopy (LIBS) database was improved, and a number of bugs were corrected as well. The bibliographic databases are updated regularly with the total number of classified references exceeding 20,000. All these databases are extensively use by the community and we will present the corresponding access statistics.

Our experimental program on measurement and analysis of atomic spectra has received a significant boost due to the installation of a state-of-the-art x-ray transition-array-sensor microcalorimeter on the NIST Electron Beam Ion Trap (EBIT). The very first measurements of spectra from highly-charged high-Z ions show excellent spectral resolution and sensitivity of the spectrometer. We will also present high precision spectroscopic measurements from neutral and low-charged ions. Finally, a detailed report will be given on our work on generation of recommended electron-impact excitation and ionization cross sections for neutral Be which is of high importance for the ITER spectroscopy.

Atomic and Molecular Data Activities at NIFS in 2017-2019

I. Murakami[1,2], D. Kato[1,3,] M. Kato[1], H. A. Sakaue[1], M. Emoto[1]

[1] *National Institute for Fusion Science, Toki, Gifu 509-5292, Japan*
[2] *Department of Fusion Science, The Graduate University for Advanced Studies, SOKENDAI, Toki, Gifu, 509-5292, Japan*
[3] *Department of Advanced Energy Engineering Science, Kyushu University, Fukuoka 816-858-, Japan*

NIFS has constructed and developed atomic and molecular numerical database for collision processes [1]. We report the current status of the atomic and molecular database and the development in 2017-2019. In total 822,378 data sets are stored in the databases (as of Sep. 5, 2019). AMDIS ION, one of our sub-database for electron-impact ionization cross sections, have been implemented to VAMDC [2]. Only element as a searching item works for query at the moment and further development is needed.

Various research activities related to the atomic and molecular data have been conducted. Tungsten spectra in wide wavelength region have been measured in plasmas of Large Helical Device with tungsten pellet injection. Visible M1 lines of tungsten ions were measured [3] and a collisional-radiative model with proton-impact excitation has developed for M1 transitions. Radial profile ofW24+ -W26+ ion densities were obtained using measurement by space-resolved EUV spectrometer [4]. Collisional-radiative model for tungsten ions have been developed with recombination processes [5]. Atomic structure of low charged lanthanide ions are examined for application to astrophysical plasma, “kilonova” [6-8]. The laboratory experiments by Laser Induced Break Down (LIBS) and charge exchange spectroscopy for low charged lanthanide ions have been tried to validate the theoretical calculations.

[1] NIFS atomic and molecular numerical database, URL=http://dbshino.nifs.ac.jp/
[2] M. L. Dubernet et al., *J. Phys, B: At. Mol. Opt. Phys.* **49**, 074003 (2016)
[3] K. Fujii et al., *J. Phys, B: At. Mol. Opt. Phys.* **50**, 055004 (2017)
[4] Y. Liu et al., *Japanese J. Appl. Phys*. **57**, 106101 (2018)
[5] I. Murakami, 11th ICAMDATA, invited talk (2018)
[6] G. Gaigalas et al., *Astrophys. J. Suppl.* **240**, 29 (2019)
[7] M. Tanaka et al., arXiv:1906.08914 (2019)
[8] D. Kato et al., *NIFS-PROC* **114**, 11 (2019)

A+M Data Center Activities in National Fusion Research Institute (2017~2019)

Mi-Young Song with FTR Division[1], H. Cho[2], G. P. Karwasz[3], V. Kokoouline[4], Y. Nakamura[5], J. Tennyson[6]

[1] Plasma Technology Research Center, National Fusion Research Institute, 37 Dongjangsan-ro Gunsan, Rep. of Korea
[2]Department of Physics, Chungnam National University, Daejeon 305-764, South Korea
[3]Institute of Physics, University Nicolaus Copernicus, 87100, Toruń, Poland
[4]Department of Physics, University of Central Florida, FL 32816 2385, USA
[5]6-1-5-201 Miyazaki, Miyamae, Kawasaki 216-0033, Japan
[6]Department of Physics and Astronomy, University College London, London WC1E6BT, UK

This presentation includes the research facilities of the NFRI Research Group of Korea and the data production techniques and data for plasma application. We investigated ways to produce collisional scattering cross sections of atoms and molecules by electron collision, and established a direct data production base through experimental measurements and developed a measuring device and measured total scattering cross section for e + Ar, N2O, CH_4 collisions at low electron energies. We obtained fundamental physical & chemical properties data of 193 basic physical property data for 21 kinds of C3Fy compounds and 89 basic data on the basic physical property data for 5 C4F8 isomers and 54 data for 3 kinds of L-PFC (X) compounds.

We have optimized the structure of molecules using the Density Functional Theory DFT (wB97X-D/aug-cc-pVTZ) using the Gaussian 09 program and the optimized geometry is used for the calculation and calculated various cross sections at low energies along with the detection of resonances using *ab initio* R-matrix method through Quantemol-N.

Our evaluation group strives to provide the data set as complete as possible. If there is no data, we are suggesting data studies to colleagues. We plan to make the Group data evaluation project for continuous activity.

DCPP web database system provides numerical and bibliographic data of atomic, molecular interaction. Also, the system provides functions for the efficient compilation, assessment, and grade evaluation process of atomic, molecular and plasma-material interaction data. We improved our system that focuses on user convenience. We plan to add plasma-surface reaction data in the near future.

We also collected approximate 1000 papers from journals a year to update AMBDAS. We need to change the data searching method to shorten the collection time, so we plan to find a way through the analysis of past search result

Recent developments in ADAS and OPEN-ADAS: metals, influx and edge studies and web woes

M. G. O'Mullane[1] and ADAS Contributors

[1] *Department of Physics, University of Strathclyde, Glasgow, G4 0NG, UK*

Since the last Data Centres Network meeting the focus for ADAS atomic data production has been on completing the dielectronic recombination (DR) calculations for tungsten and an increasing focus on data for other metals. Marker elements such as gold, innovative divertor concepts with liquid tin and quantifying the contribution of transition row elements to overall radiation motivate the upgrade of the existing baseline data.

The iso-nuclear set of tungsten DR data is not yet complete but the missing stages, W^{14+}-W^{29+}, are now bracketed with rates from a self-consistent calculation. Calculations are continuing but the open *4f* shell configurations are dense in levels. Code developments for tungsten DR and ionization have enabled a much improved baseline for other metals and this has been exploited to produce data for gold, tin, copper and nickel. Optimizing the atomic structure, following a metric of converging total power, has improved data for the radiation aspect of the cooling curve.

Influx studies on tokamaks rely on high quality atomic data, principally for excitation and ionization rates. Data has been added to ADAS for tungsten (W^0 - W^{4+}), Rhenium (Re^0, Re^+) and gold (Au^0, Au^+), based on the optimization of atomic structure based on the core polarization techniques of the ASPECT group of the University of Mons. Although we expect this to be superseded by superior collisional calculations having good baseline quality data enables plasma modelling to advance.

The edge, divertor and SOL of tokamak plasmas is an interesting environment for atomic processes. Intermediate coupling resolved collisional-radiative data for argon has been demonstrated with ADAS codes and data. A new set of ion-impact data, a new ADAS dataclass, and a code for generating such data are being finalized. Thermal charge exchange between neutral hydrogen (or deuterium) and lowly ionized charge stages can act as a recombination process. Data for nitrogen via this process has been added.

The public web face of ADAS is OPEN-ADAS which makes available fundamental atomic data and fusion relevant derived data. A recent penetration test, run by the University of Strathclyde which hosts the service, uncovered a number of vulnerabilities. The web code was overhauled and the service is now delivered over https. Keeping up with the quickly evolving nature of the web is a challenge and more stringent rules on data provenance will affect data providers.

Recent Activities on Plasma Spectroscopy and Atomic Data in KAERI Atomic Data Center

D.-H. Kwon and K.-B. Chai

[1] *Korea Atomic Energy Research Institute, Daejeon, 34057, Republic of Korea*

We have carried out optical emission spectroscopy (OES) in our own capacitively coupled plasma device which can be easily switched to an inductively coupled plasma device. The plasma temperature and density for Ar plasma in the device was been determined by a collisional radiative modelling (CRM) for the neutral Ar (690 – 830 nm) of the weakly ionized Ar plasma and compared with the Langmuir probe measurement (1.2 – 2.2 eV and 4.0×10^{9} – 8.0×10^{11} cm^{-3}) in order to test the reliability and uncertainty of the OES-CRM diagnostics [1]. In this density and temperature range electron impact de/excitation plays an important role in the population kinetics and the atomic data from the semi-relativistic Breit-Pauli B-spline R-matrix calculation [2] was used. We have also performed beam emission spectroscopy for more dense and hot Ar plasma in another divertor simulating plasma device which has been constructed for generation of high heat and particle flux similar to a tokamak divertor in KAERI. In our preliminary spectral measurement, lines at 400 – 500 nm are enhanced than those at 700 – 800 nm which indicates the dominance of Ar^{+} ion. We have calculated electron-impact excitation cross section and radiative transition rates for Ar^{+} ion and obtained a simply modeled spectra by the flexible atomic code. The detailed comparison of the atomic data with other available experimental [3] and theoretical data [4, 5] will be presented and discussed.

1. K.-B. Chai and D.-H. Kwon, *J. Quant. Spectrosc. Radiat. Transfer* **227**, 136 (2019)
2. LXcat plasma data exchange project database, *http://nl.lxcat.net*
3. A. Kramida, Yu Ralchenko, J. Reader and NIST ASD team (2018), *NIST Atomic Spectra Database (ver. 5.6.1)*, *http://physics.nist.gov/asd*
4. C. F. Fischer *et al., Atomic Data and Nuclear Data Tables* **92**, 607 (2006)
5. D. C. Griffin *et al., J. Phys. B: At. Mol. Opt. Phys.* **40**, 4537 (2007)

This work was supported by the National Research Foundation of Korea under Grant Nos. 2019R1A2C1009529 and 2017M1A7A1A03072768.

Recent Works on Atomic and PMI Data for Controlled Fusion Research in Russia

P.R. Goncharov[1,2], *A.B. Kukushkin*[3,4,5]

[1] *Peter the Great St. Petersburg Polytechnic University, 195251, Russia*
[2] *Ioffe Institute, 194021, Russia*
[3] *NRC Kurchatov Institute, 123182, Russia*
[4] *National Research Nuclear University MEPhI, 115409, Russia*
[5] *Moscow Institute of Physics and Technology, 141701, Russia*

An overview of the works carried out in Russia during the past two years on atomic and plasma-material interaction (PMI) data will be presented. Activities and newest results obtained at Ioffe Institute in St. Petersburg, P.N. Lebedev Physical Institute, NRC Kurchatov Institute, TRINITI, Moscow Institute of Physics and Technology, Moscow Engineering Physics Institute, Novosibirsk State University, and G.I. Budker Institute of Nuclear Physics, concerning the generation and the use of atomic and PMI data, will be described. A special emphasis will be made on the works in support of ITER diagnostics to be delivered by the Russian Federation, as well as domestic fusion projects. The subjects include:

- an overview of experimental data and theoretical methods for charge-changing processes of ion beams passing through gaseous, solid and plasma targets, including electron capture and electron loss processes with heavy many-electron ions, stopping power, isotopic effects;
- measurements of absolute total cross sections of one- and two- electron capture by He2+ ions from argon atoms and the studies of the applicability of various particle interaction potentials;
- calculations of interatomic potentials and reflection coefficients for scattering of particles at various surfaces (H, D – W, D–C, H, D – Be and others);
- simulations of heavy ions quasi-continuum (in the 4-8 nm spectral range), using the statistical model of atoms for elementary processes with many-electron atoms and ions in plasmas, including the new channels of radiative losses for heavy ions and the comparison with observations in magnetically confined fusion plasmas;
- development of a method for simulating the transition probabilities in ions for the problems of interaction of ultra-short electromagnetic pulses with hot dense plasmas and diagnostics of matter, including the inertially confined fusion plasmas, with free-electron lasers;
- development and verification of theoretical models of spectral line shapes (SLS) in plasmas, including the SLS models for high energy density plasmas of inertially confined fusion plasmas and the outline of the newest trends in the SLS community;
- progress in ITER Main Chamber H-alpha (and Visible) Spectroscopy, including the Zeeman spectroscopy of beryllium and the test of interpretation algorithms on JET;
- passive signal simulation for ITER charge-exchange recombination spectroscopy (CXRS) of the core and edge plasmas, including the CX data needs for Be at low collision energies in SOL;
- the use of data for fine structure of atomic levels in radiative-collisional kinetics and radiation losses simulation for edge plasmas in fusion facilities, including the radiation losses during massive gas injection for discharge quenching in ITER;
- progress on laser-induced fluorescence in ITER divertor, including the simulation of photon emission coefficients (PEC) under laser fluorescence;
- overview and highlights of the most recent Russian conferences on PMI;
- the work on Russian atomic spectroscopy information system in Novosibirsk and a number of other subjects.

Recent Database Activities of CRAAMD

Yong Wu,[1,2]
[1] *Institute of Applied Physics and Computational Mathematics, Beijing, 100088, P.R. China*
[2] *HEDPS, Center for Applied Physics and Technology, Peking University, Beijing 100084, China*

wu_yong@iapcm.ac.cn

China Research Association of Atomic and Molecular Data (CRAAMD) is constituted of about ten groups from universities and Institutes and works on collecting, producing and compiling Atomic and Molecular data (AMdata), which are needed from the related fields of astrophysics, Inertial Confinement Fusion (ICF) and X-ray Laser Research etc.

Recent progress of CRAAMD will be reviewed in the talk, in particular on the CRAAMD activities and the AM data production in the past two years. Extensive AMdata have been produced, compiled and assessed, including atomic and molecular spectroscopy, electron collisions with atoms and molecules, heavy particles collisions with atoms and molecules, atomic and molecular opacity, stopping power of plasma and so on.

I will also review the recent progresses of the AM group in Institute of Applied Physics and Computational Mathematics (IAPCM), mainly on the heavy particles collisions studies in collaboration with the group of Xinwen Ma from the Institute of modern physics, Chinese Academy of Sciences.

ROADMAP ON ATOMIC, MOLECULAR AND OPTICAL RESEARCH AT THE ARGENTINE ATOMIC ENERGY COMMISSION

*R. O. Barrachina**

Comisión Nacional de Energía Atómica, Argentina

The research in Atomic, Molecular and Optical (AMO) Physics at the National Atomic Energy Commission (CNEA) of Argentina has a long and continuous tradition, dating back to 1960, when the first laboratory in Argentina dedicated to AMO Physics was created in 1960 by Prof. Wolfgang Meckbach at the Bariloche Atomic Centre (CAB).

In a previous communication [1], the thematic scope and related experimental facilities, both in CNEA and in other laboratories in Argentina, have already been described. In this Roadmap, we will focus on how these activities are inserted within the framework of the various applications and technological challenges of CNEA. We will look back along the road, showing the evolution of AMO research in CNEA, overviewing the present status of the field, and addressing current and future challenges faced by those working in this broad and exciting area of research. The "Laboratory of Isotopic Separation" (LASIE), the "Centre for Proton Therapy" (CEARP) and the "Centre for Nuclear Medicine and Radiotherapy" (INTECNUS) are actual examples of CNEA projects that act as driving forces for AMO physics.

A myriad of stimulating research lines in Medical Physics, Heavy Ion Accelerators and Spectroscopy Techniques, to name just a few, add value and interest to the investigations carried out, for instance, in our 1.7 MeV tandem accelerator, with PIXE, RBS, ERDA and channelling capabilities, and a chamber for Cold Target Recoil Ion Momentum Spectroscopy (COLTRIMS), the Mass Spectroscopy facility (AMS), the two electrostatic accelerators of 100 and 300 keV, the time-of-flight system for ISS spectroscopy, the surface analysis equipment for XPS, UPS, AES and SIMS spectroscopy, and the STM and AFM microscopes.

Finally, we will also describe the advances in the creation of the "Argentinean Network for Nuclear, Atomic, Molecular and Optical Data and Codes", or DINAMO (for to its acronym in Spanish) and the participation of Argentina in the Data Bank of the Nuclear Energy Agency (NEA-OECD), and -in particular- in the Joint Evaluated Fission and Fusion (JEFF) collaboration, as well as in other international committees as BIMP and ICRM.

[1] R. O. Barrachina: "Atomic, Molecular and Optical Research in Argentina", 1st Meeting of the Experimentalists Network, IAEA Headquarters (Vienna, Austria, November 2018).

*

- Centro Atómico Bariloche and Instituto Balseiro, (8400) San Carlos de Bariloche, Río Negro, Argentina

- Comisión Nacional de Energía Atómica, Sede Central, Av. Del Libertador 8250, (1429) Buenos Aires, Argentina

- Phone: +54 294 4445100 int. 5408 (Bariloche), +54 11 4704 1479 (Buenos Aires); Email: barrachina@cnea.gov.ar

• Head of the Academic Area of the National Atomic Energy Commission, CNEA.

• Member of the Management Board for the Development, Application and Validation of Nuclear Data and Codes (MBDAV) of the Nuclear Energy Agency (NEA).

• Head of the Department of Interaction of Radiation with Matter, CNEA (2011 – 2015).

• Member of the National Director Committee for the Teaching of Radiological Protection, CoDiNEPRa.

• President of the Latin-American Network for Education in Nuclear Technology, LANENT (2011 – 2014)

R-matrix excitation/ionization calculations for Tungsten in support of magnetically-confined plasma diagnostics

C P Ballance[1], R Smyth[1], N Dunleavy[1], S D Loch[2], D Ennis[2] and C Johnson [2]

[1] CTAMOP, Queen's University of Belfast, UK, BT7 1NN
[2] Department of Physics, Auburn University, US, AL 36849

The collaboration between Queen's University and Auburn University has ensured that the relativistic atomic structure, electron-impact excitation/ionisation for neutral Tungsten and near-neutral ion stages may be validated against various collisional-radiative (CR) models and more importantly the observed spectra from the Compact-Torodial Hybrid (Auburn University) and the DIIID tokamak (General Atomics).

From the electron-impact excitation perpsective the Maxwellian averaged excitation rates for neutral tungsten [1] are available in the literature, and shall be presently available within the well-known adf04 file format utilised by the ADAS consortium. For singly ionised tungsten, an 800 level model is underway and should be available by the end of the year.

For electron-impact ground and metastable ionisation the path forward is less clear. There are various non-perturbative calculations including a groundstate ionisation configuration-averaged time-dependent close-coupling (TDCC) [2] calculation and a ground and metastable ionisation calculation employing the R-matrix with pseudostates method. Even though initial comparisons between methods is reasonable, preliminary collisional-radiative calculations reveal that the total effective ionisation rate is dominated by highly-excited state ionisation rather than the groundstate and first few metastables. Therefore SXB [3] ratios which are dependent on the effective ionisation rate will inevitably be a hybrid of explicitedly calculated groundstate and metastable ionisation and an imperical formula such as the ECIP (Exchange-Classical-Impact-Parameter) method.

[1] R Smyth et al, Phys. Rev. A 97, 052705 (2018)
[2] M S Pindzola et al, J. Phys. B, Vol 50 Nos. 9, 095201 (2017)
[3] Behringer, PPCF Vol 31 pp 2059 (1989)

This work in part was supported under the Queen's University consolidated grant awarded by the STFC.

Electron-molecule dynamics for non-equilibrium plasmas

Vincenzo Laporta

Istituto per la Scienza e Tecnologia dei Plasmi (ISTP), CNR, Bari, Italy

In my presentation, I will illustrate my research on electron-molecule dynamics at ISTP of CNR in Italy. I will focus in particular on vibrational-excitation, dissociative-attachment, dissociative-recombination and dissociative-excitation processes rotationally and vibrationally resolved. The electronic structures are obtained by using ab-initio quantum chemistry approaches implemented in computer codes like MOLPRO and UK–R-Matrix whereas the nuclear dynamics is studied within the theoretical models of Bardsley's local-complex-potential model, adiabatic-nuclei approximation and multichannel quantum defect theory. The latest results for cross sections and rate coefficients will be presented and discussed for ArH^+ [1], BeH^+ [2, 3], H_2, H_2^+, N_2 [4], O_2 [5], CO [6], CO^+, CO_2.

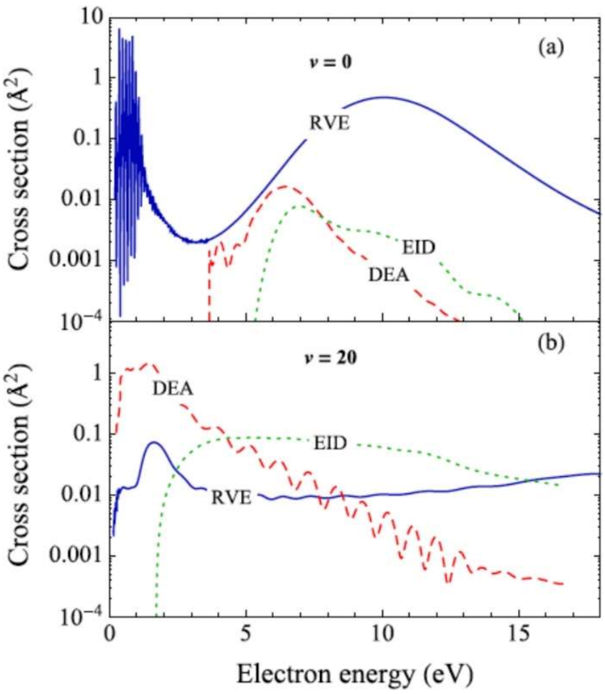

Fig. 1. Summary on electron-O_2 cross sections [5]: vibrational excitation (RVE), dissociative attachment (DEA), and dissociative excitation (EID) processes for the vibrational levels $v = 0$ (a) and $v = 20$ (b).

These researches are performed in view of many applications: in particular in aerospace (shuttle reentry in planetary atmospheres, electric propulsion); nonequilibrium plasma physics (combustion); controlled fusion reactors; astrochemistry (early Universe, interstellar medium) and chemical evolution of life just to name a few. Finally, some kinetics modelling will be also presented. Results are obtained in collaboration with the groups of I.F. Schneider (France), J. Tennyson (UK) and M. Panesi (US).

[1] A. Abdoulanziz, et al., MNRAS 479, 2415 (2018)
[2] V. Laporta, et al, Plasma Phys. Control. Fusion 59, 045008 (2017)
[3] S Niyonzima, et al., Plasma Sources Sci. Technol. 27, 025015 (2018)
[4] V. Laporta, et al. Plasma Sources Sci. Technol. 23, 065002 (2014)
[5] V. Laporta, R. Celiberto and J. Tennyson, Phys. Rev. A91, 012701(2015)
[6] V. Laporta, et al., Plasma Sources Sci. Technol. 25, 01LT04 (2016)

Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Tel.: (43-1) 2600 21725
Web: http://nds.iaea.org