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Technical Aspects of Atomic and Molecular Data Processing and Exchange

26th Meeting of the A+M Data Centres Network

Summary Report of an IAEA Technical Meeting

IAEA Headquarters, Vienna, Austria

1 – 3 September 2021

Prepared by

Dipti, K. Heinola, and C. Hill

IAEA Nuclear Data Section

October 2021

IAEA Nuclear Data Section

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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, 26th Meeting of the A+M Data Centres Network" held from 1 – 3 September 2021. 16 participants from 10 Member States (Argentina, China, Germany, Hungary, Italy, Japan, Republic of Korea, Russia, UK, and USA) and 5 representatives of the IAEA attended the meeting. The report includes discussions of the data issues, recommendations, and conclusions, as well as summaries of the presentations presented in the meeting.

October 2021

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1. Introduction

The Data Centres Network (DCN), coordinated by the Atomic Molecular Data (AMD) Unit, is a joint effort of national data centres for the collection, critical assessment, and generation of fundamental data for fusion applications. The heads of the data centres constitute a standing Advisory Group for advising the agency on the technical aspects of the atomic, molecular, and plasma-material interaction data, its processing and exchange.

The AMD unit holds a biennial meeting for analysis, coordination, and planning of all DCN activities at the IAEA Headquarters, Vienna. Due to the Covid-19 pandemic, the 26th biennial meeting of the A+ M Data Centres Network was held virtually from 1 - 3 September 2021. The Scientific Secretary is Kalle Heinola (Atomic Physicist, AMD Unit, IAEA) with the administrative support from Charisse Monfero. Invited meeting participants were members of the Advisory Group and guest experts.

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 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 (IAEA, Austria), R. Barrachina of CAB (Centro Atómico Bariloche, Argentina), C. Ballance of QUB (Queen's University Belfast, UK), and V. Laporta of CNR Bari (Consiglio Nazionale delle Ricerche, Italy). D. Reiter of HHU (Heinrich Heine University Düsseldorf, Germany) has retired from the DCN network and participated in the last meeting as a member. He will continue to contribute through other IAEA activities. Y. Wu of CRAAMD (China Research Association of Atomic and Molecular Data, China) was not attending the meeting this time.

Other experts were invited to discuss their work in the field of A+M data and its application in fusion science. B. Wei of Fudan University, China attended the meeting on behalf of Y. Zou and reported on his group's A+M data generation activities. Z. Mezei of ATOMKI Hungary discussed the topic of electron-driven molecule processes relevant to edge plasmas in fusion devices. J. Colgan and C. Fontes represented Los Alamos National Laboratory (LLNL), USA and J. Colgan reviewed his groups research's activities on plasma modelling relevant to fusion research as well as other fields of research.

A. Koning (Section Head, Nuclear Data Section), C. Hill (Unit Head, AMD Unit), K. Heinola (Atomic Physicist, AMD Unit), Charisse Monfero (Administrative assistant, Nuclear Data Section) and Dipti (Consultant, AMD Unit) represented the IAEA.

Discussions were held on the following topics:

- Status and recent developments of data centres in the last two years (Oct. 2019 – Sep. 2021)
- Future prospects of data centre activities
- Cooperation in the maintenance of bibliographical databases
- Requirements for the generation, validation, and compilation of A+M /PMI (Plasma material interaction) data for fusion applications
- Priorities for database development
- Uncertainty quantification of fundamental data for fusion plasmas and proposed new meetings

2. Proceedings

The head of the Nuclear Data Section, A. Koning welcomed the participants and emphasized the role of the IAEA Nuclear Data Section, AMD Unit and the DCN network in the field of fusion and data research. The participants introduced themselves and the agenda in Appendix II was adopted. K. Heinola reviewed the objectives of the meeting.

The meeting continued with presentations from data centres on their current activities and from the additional experts on their databases and data analysis activities. Presentation titles and summaries of presentations can be found in Appendix III. Presentation materials are available on the AMD Unit website under https://amdis.iaea.org/meetings/dcn-26.

2.1 Current activities of Atomic and Molecular Data Centres

Yuri RALCHENKO reported the recent progress in the database development and atomic data research at NIST over the last two years (Oct. 2019 – Sep. 2021). During this period, the Atomic Spectra Database (ASD), was updated twice (v5.7 and v5.8), bringing the total number of critically evaluated energy levels and spectral lines in ASD to 112,230 and 285,109 respectively, with 120,937 transition probabilities. Energy levels, spectral lines, and transition probabilities were added/updated for Fe III, Y VIII, Bi III, and Ac I-III ions. Energy levels and spectral lines were updated for neutral Be while wavelength uncertainties were added for singly charged Be ions. The energy conversion factors were updated to the 2018 CODATA Fundamental Constants. The Laser Induced Breakdown Spectroscopy (LIBS) database has been improved, and minor bugs have also been fixed. The major update to LIBS interface includes the ability to model the spectra of any ionization stage or combination thereof in ASD that was previously limited to the first three charge stages of an element. The online collisional-radiative modelling code FLYCHK is maintained by NIST which has about 1300 users from around the world. ASD's bibliographic databases are updated regularly (~ 2 weeks) with the total number of classified references 39,085, which are submitted annually to the IAEA. An overview of the development of NIST atomic databases, atomic data analysis, uncertainty assessment, and online tools was recently given in a publication in the journal Atoms. A new database of opacities, which is critically important for kilonova simulations, was presented. The database was developed in collaboration with the Los Alamos National Laboratory and made available online in 2021.

In addition to database work, NIST generated the experimental as well as theoretical atomic data and published papers directly related to fusion plasma. Recently, NIST reported on the first detailed theoretical analysis of charge exchange recombination spectroscopy based on interactions of the planned ITER neutral beams (diagnostic beam of 100 keV/u and heating beam of ~ 1 MeV/u) with highly charged ions of tungsten, which is one of the most important impurities in the plasma core. In addition, they provided atomic data required for calculating the intensities of the Stark components of excited hydrogen atoms in fusion plasmas. The electron beam ion trap (EBIT) facility at NIST has produced the spectroscopic data in the EUV to x-ray range for the precise wavelength measurements to probe the relativistic and quantum electrodynamics (QED) effects in high-Z elements, the polarization properties, and the isotope shift measurements in the highly charged ions to determine the nuclear properties of heavier elements, and so on. These benchmark data, generated under a well-controlled EBIT plasma, are crucial to test the advanced atomic theories as well as collisional-radiative (CR) models, as most of the data used for fusion plasma diagnostics is derived from theoretical methods.

MURAKAMI Izumi (NIFS, Japan) presented a detailed report on the AM + PMI databases and research activities related to atomic and molecular data at NIFS in 2019-2021. In the past two years, new data has been added to AMDIS, CHART, AMDIS MOL (AMOL) databases, increasing the number of records to 809,513; 7,707; and 5,943; respectively. In the databases CHART MOL (CMOL), SPUTY, and BACKS databases there have been no new entries in the last two years, while the A+M bibliographic database ORNL has not been updated since 2009. An overview on NIFS atomic and molecular numerical databases for collision processes has been provided in a recent publication in Atoms Journal.

In 2019, two new working groups were established with Japanese atomic and molecular physicists to compile and update the data on "Collisional data for light and heavy elements for fusion reactor materials" and "Construction of sputtering yield database for elucidation of tungsten damage process".

NIFS also reported on its measurements on tungsten ions as a contribution to the experimental database of line emissions as well as the study of W transport to improve the diagnostics in ITER's edge plasma. For instance, the forbidden visible M1 lines of W^{26+} and W^{27+} were identified in the measured spectra and used to investigate the spatial distributions in LHD plasma. Other work includes the measurements of spectra of different tungsten ions with LHD stellarator in a wide range of wavelengths, while the analysis is based upon the new hybrid CR model developed for W^{25+}-W^{39+} ions including recombination processes. Forbidden lines, e.g., E3 lines from W^{27+} and M1 lines of W^{8+} and W^{9+} as well as EUV and visible spectra from W^{6+} - W^{13+} were identified in the measurements performed at Compact electron beam ion trap (CoBIT) facilities. Spectral lines from other high Z elements, such as Pr and Nd were also measured in LHD.

Mi-Young SONG (KFE, Korea) reported on the A+M Data Center activities of the Korea Institute of Fusion Energy over the last two years (2019 - 2021). The activities of Fundamental Technology Division, which manages the Data Centre for Plasma Properties (DCPP) and develops plasma process analysis technology as well as virtual metrology and control technology, were described. The DCPP includes cross sections and rate coefficients for collisions with electrons, photons, and heavy particles. KFE supports the IAEA bibliographic database AMBDAS and updates of last two years will be provided to IAEA. New databases on plasma-surface reactions and thermodynamic properties are included in DCPP in the last two years. The total number of records in the DCPP have reached to 101,175.

Research on AM properties include experimental measurements of (i) total cross sections for electron scattering on atoms and molecules using magnetized electron beam (ii) elastic differential scattering cross sections (ii) dissociation cross sections (iv) biomolecule collisional data. On the theoretical side, (i) the structures of molecules and their physical and chemical parameters, (ii) electron collisional properties through the R-matrix and the BEB model. Total electron scattering cross sections for NO_2 and C_3F_6O were measured. Chemical and thermodynamic properties of NF_3O are being studied to replace SF_6 gas in circuit breakers which have a significant impact on global warming. KFE carries out data evaluation activities by a working group of international experts to establish an internationally recognized standard reference data library for A+M/PMI data. The recommended set of cross sections for electron collisions with molecules NO, N_2O, NO_2, and H_2O molecules is provided.

Martin O'MULLANE (ADAS, UK) presented recent developments in ADAS and OPEN-ADAS which include addition of new data in both databases, new models as well as extension of ADAS data formats. Baseline data based on empirical formulas are improved by replacing some data based on ab-initio calculations, for example, the ionization rates were obtained by configuration average distorted wave (CADW) instead of Lotz formula. The cooling factors were calculated for the elements from H to Bi using the ionisation, recombination coefficients in combination with the line power coefficients. Comparison of the radiated power from tungsten with different choices revealed convergence at high T_e while significant differences for temperature below 1 keV were attributed to emission from $4f^{(n-2)}$ complex ions W^{20+} - W^{27+}. Other work includes the R-matrix electron impact excitation data for C-like and N-like isoelectronic sequence for H to Kr elements. Calculations will be extended to H-like, He-like and O-like ions to complete the H-like to Mg-like isoelectronic sequence.

Duck-Hee KWON (KAERI, Korea) reported on the latest atomic data and CR modeling activities in KAERI Atomic Data Center. For the electron impact excitation process, the unitary correction for relativistic distorted wave (RDW) approximation was implemented in the flexible atomic code (FAC). Electron impact excitation cross sections for Ar and Ar^+ ions were calculated by solving the matrix elements in Born I (original FAC), II, and III approximations. Cross sections obtained with three approximations were compared with the experimental results available for neutral Ar as well as with various theoretical predictions such as BSR-500 (Ar), distorted wave (Ar), and multi-configuration-Dirac-Fock RDW (Ar, Ar^+). It was highlighted that benchmark data is needed to verify the theoretical results, particularly for Ar^+. In addition, they also performed optical emission spectroscopy (OES) and Langmuir probe measurements on an inductively coupled plasma (ICP) source for low-temperature and low-density He plasmas. The analysis is based on the CR simulations that solve the steady state balance equations, including non-linear effects such as radiation trapping, collisional ionization of heavy particles, and diffusion.

Recently KAERI also designed a divertor simulator to generate the ITER-level heat and particle fluxes to study fusion divertor technology. An applied-field-magnetoplasdynamic (AF-MPD) thruster concept is used to design a laboratory-scale divertor simulator and heat and particle fluxes were measured. Electron temperature and density were derived from the CR modeling combined with OES measurements. Results for EIE cross sections and CR modeling will be made available online at https://pearl.kaeri.re.kr.

Pavel R. GONCHAROV (SPbSTU, Russia, on behalf of A. B. Kukushkin (Kurchatov Institute, Russia)) reported on the recent activities of the last two years on the generation and use of atomic and PMI data for nuclear fusion research in Russia. Activities on the generation of atomic data for fundamental science and nuclear fusion includes (i) the measurement of total and partial cross sections for single electron capture by He^{2+} ions from H atoms using the method of collision spectroscopy based on the precision measurement of the kinetic energy of projectile ions after electron capture and (ii) calculations of sputtering yields and their angular dependencies for tungsten bombarded with Be and Ne ions using the molecular dynamics method. Activities on the online databases SPECTR-W^3 and Information System Electronic Structure of atoms (IS ESA) are ongoing, and the latest updates to the databases have been published in journal articles.

The need for atomic data for advanced diagnostics tools for fusion plasmas, such as the neutral particle analysis (NPA) method, has been described. They also published a review outlining the evolution of the NPA method over the past six decades. It is included as one of the primary ITER diagnostics and will provide information on deuterium-to-tritium isotope ratio and MeV ion distributions. The existing data requirements for the modeling of neutral fluxes from plasma include the cross sections for charge changing collision processes of H and He with impurity species such as Li, Be atoms. Further examples are the need for the orbital angular momentum-resolved cross sections for charge exchange (CX) between Be^{4+} and the neutral hydrogen for high-resolution spectroscopy in the visible range in ITER, the use of the sputtering coefficients of Be for hydrogen isotope irradiation on the first wall to determine the Be fluxes in the ITER tokamak. An overview of the recent activities on plasma surface interaction is also provided, which includes organization of conferences and studies on deuterium and helium retention in W and corresponding modifications of W-based materials.

Kalle HEINOLA (IAEA) provided an overview of the activities of the AMD Unit of the IAEA, which includes Coordinated Research Projects (CRPs), meeting/workshop organizations, report and scientific journal publications as well as the maintenance and further development of databases and online codes. Recent and ongoing CRPs include (i) hydrogen permeation in nuclear materials (2020-2025), (ii) atomic data for vapor shielding in fusion devices (2019-2023), (iii) data for atomic processes of neutral beams in fusion plasma (2016-2020) and (iv) plasma-wall interaction with reduced-activation steel surfaces in fusion devices (2015-2019). The unit recently set up new databases: CascadesDB (database of molecular dynamics simulations of collision cascades in materials relevant to fusion research), DefectDB (database for density functional theory calculations of radiation-induced defects in nuclear relevant materials), hcdb (hierarchical database for atomic, molecular and plasma-wall interaction processes for fusion energy research), Clerval (database of institutes, events relevant for nuclear fusion research), some of which are in the development phase. Details of the CRPs, databases, and the other activities are available on the unit's website https://amdis.iaea.org. The AMD Unit has a new group email *fusion-data@iaea.org*, which the Unit will be using extensively in publications, conferences and presentations with an aim to increase communication between the Unit and various fusion communities. Recipients of the new email address are the Unit Head and the Atomic Physicist.

Raúl BARRACHINA (CAB, Argentina) reviewed the activities of the Bariloche Atomic Centre, a research facility of the National Atomic Energy Commission which includes experimental facilities such as the 1.7 MeV tandem accelerator, 100 keV and 300 keV accelerators, and spectroscopic diagnostics tools, etc. as well as theoretical capabilities such as CDW (continuum distorted wave), C3 (Correlated three-body Quantum Distorted Wave) codes, Classical Trajectory Monte Carlo (CTMC), time dependent close coupling, to name a few. The Computer Program Services (CPS) and Nuclear Data Services (NPS) of the Nuclear Energy Agency data bank were described. Recent updates in the development of an open code C3 for calculation of cross sections for ionization of atoms and molecules by the impact of charged particles have been provided. The results obtained with the new ionization code were verified with the available experimental values, for example the differential scattering cross sections for ionization of Ar by the impact of 75 keV protons and of H_2 by the impact of 100 eV positrons were reproduced by the C3 code. The open code C3 is intended to complement the CDW-EIS (continuum distorted wave eikonal initial-state) code currently available in online format on the AMD unit's website.

Connor BALLANCE (QUB, UK) provided recent updates on electron impact excitation and ionization of the near-neutral stages of tungsten. The method uses detailed atomic structure calculations with GRASP0 code within multi-configuration Dirac-Fock approach for neutral and singly ionized tungsten, followed by electron-impact excitation cross section calculations using Dirac Atomic R-matrix code (DARC). Diagnostic lines from W^{0+} and W^{+} ions were predicted using the calculated atomic data in the CR codes and results for the neutral tungsten ions were compared with the measured spectra recorded at Compact Toroidal Hybrid (CTH) facility.

Electron impact ionization of near neutral stages is problematic because of the accurate representation of the highly excited states, which, in addition to the ionization from the ground state and first few metastable states, significantly contributes to the effective ionization rates. The correct description of effective ionization rates along with excitation data is crucial for the determination of SXB ratios or influx of tungsten impurities into the fusion plasma. The challenges of expanding the existing Method Dirac R-matrix with Pseudo States (DRMPS) code to calculate ionization cross sections for near neutral tungsten ions, which was previously applicable to hydrogen, were discussed.

Vincenzo LAPORTA (CNR, Bari, Italy) described the ab-initio calculations within the framework of the Local Complex Potential for the investigation of state-resolved electron-molecule dynamics. The rotationally and vibrationally resolved processes for electron-molecule scattering include i) vibrational excitation, ii) dissociative attachment, iii) dissociative excitation, and iv) dissociative recombination. Cross section and rate coefficient results for various systems relevant to fusion plasma applications were presented, namely $e^- + D_2$, $e^- + D_2^-$, $e^- + H_2^+$, $e^- + HD^+$, and $e^- + BeH^+/BeD^+/ BeT^+$. The vibrational relaxation time of D_2 is also calculated using the reaction rates, which is of key importance in understanding energy transfers in non-equilibrium plasmas.

Detlev REITER (Heinrich Heine University Düsseldorf, Germany, ITER Scientific Fellowship Network) provided an overview of the renewed interest in CX recombination data of H colliding with impurities injected into tokamaks. Impurities such as noble gases (Ne, Ar) or N_2 are introduced into the existing tokamaks in order to reduce the heat in the divertor region to a tolerable level. A recent study on the ASDEX upgrade provided strong evidence for the dominant role of CX recombination on radiative edge plasma cooling diagnostics. The status of the existing reports/databases for CX recombination was reviewed, and the main issues with accessing this atomic data for ITER are described. Reliable cross section datasets and a well-known scaling for highly charged ions such as H-like and He-like exist for high collision energies, but no trend or scale is available for weakly ionized atoms. There is lack of availability of data sources for collision energies in 5 - 200 eV, the most relevant energy range in the boundary region of fusion devices. The need of cross section data over rate coefficients is highlighted because the use of latter data in the modeling adds greater uncertainty independent of AM data which is due to non-LTE conditions in fusion edge plasmas generated by supersonic flow speeds and non-thermalized neutrals. The importance of studying the isotopic effect H/D/T for collision processes was emphasized.

2.2 Research activities of invited speakers' groups

Baoren WEI (FUDAN UNIVERSITY, China) on behalf of Y. Zou summarized the A+M data activities at Fudan University. The data generation activities include (i) absolute cross section measurements of single and double electron capture for O^{6+} ion colliding with CO_2, CH_4, H_2, N_2 at impact energies from 2.63 keV/u to 19.5 keV/u, (ii) measurement of state-selective capture cross section for collisions of O^{6+} ion with He, (iii) calculation of single and double charge transfer cross sections using time dependent density functional theory with molecular dynamics, (iv) Dielectronic and radiative recombination measurements for W^{q+} ions at the Shanghai EBIT facility which is important for tokamak plasmas, (v) measurement of the EUV and visible spectra of tungsten ions (W^{7+}-W^{15+}, W^{25+}-W^{28+}), and (vi) calculation of energy levels of multiply charged stages of tungsten and medium-Z elements with spectroscopic accuracy. The results were compared, where possible, with experiments to investigate the effects of electron correlations, relativistic, and quantum-electrodynamic (QED) corrections on atomic structure.

Zsolt MEZEI (ATOMKI, Hungary) presented his group's research activities on the electron-driven molecular processes that are relevant for the edge fusion plasmas. The Multichannel Quantum Defect Theory (MQDT) has been used to study the processes, namely dissociative recombination, elastic scattering, (ro-) vibrational excitation, vibrational de-excitation and dissociative excitation. For collisions of low-energy electrons with H_2^+, BeH^+, and their isotopologues, cross sections and rate coefficients of rotational and vibrational transitions were obtained. The results were compared with the available experimental and theoretical values and some important features such as isotopic and resonant effects were described. Cross sections for collisions of electrons with molecular cations such as LiX^+, BeX^+, WX^+ (X = H,…), BeH_2^+,… can be calculated based on the data requirements of fusion community.

James COLGAN (Los Alamos National Laboratory, USA) provided an overview of the Los Alamos Suite of atomic physics codes which is a set of atomic structure and plasma modeling codes. The plasma kinetics code ATOMIC has been used to calculate the opacity tables for the elements H through Zn in a wide range of conditions in the local thermal equilibrium (LTE) approach for astrophysical applications and the data is made available online. The LTE approach has also been used to model neutron star mergers and plasmas of interest to EUV lithography.

The plasma kinetics code has been extensively used for the spectroscopic diagnostics of various plasmas such as laser-produced and magnetically confined plasmas in non-LTE conditions. LANL regularly participates in the NLTE code comparison workshop and has performed atomic and plasma kinetic modelling for a variety of plasma conditions. An example of a test case in the NLTE workshop is the tungsten in the temperature range of 1200 -2400 eV and at magnetic fusion densities. Large-scale CR modelling calculations for W were submitted for different structure calculations using fully relativistic and semi-relativistic methods and its impact on the emission spectra and other properties such as radiative power losses were studied. LANL can provide the opacity data for other elements of interest to support the current CRP on vapour shielding.

3. Discussions

Issues related to data research, data needs and data centres were discussed: data generation, evaluation, and exchange, priorities for database development and maintenance, future activities of the data centres, bibliographical data compilation, and uncertainty quantification of fundamental data for fusion applications.

3.1 Data needs for fusion research and future activities of the data centres

NIST, USA

- The Atomic Data Center will continue to collect, evaluate, and disseminate accurate atomic spectroscopic data relevant to fusion and other research areas
- Evaluation of collisional data for Be II in cooperation with IAEA
- MCHF/MCHDF database will be revitalized.
- New data on Li-like satellites will be added

KFE, Korea

- Organize the dataset in DCPP by grouping the data in each molecule for user convenience

- Build a platform for the collection and sharing of research data to manage the data produced during plasma research
- Development of the reference standard for spectral properties of Ar, N_2, and O_2 plasma
- Establishment of research facility for plasma-surface reactions by 2023
- Evaluation of collisional data for N_2 and CO_2

SPbSTU, Russia

- Lithium is studied as the material of the first wall and divertor in the fusion reactors in recent publications. Data needs for the charge changing processes for collisions of H with Li ions include:

  Ion-impact ionization: $H + Li^{q+} \rightarrow H^{+} + Li^{q+} + e^{-}$ (q = 1,2)

  Three -body recombination: $H^{+} + Li^{q+} + e^{-} \rightarrow H + Li^{q+}$ (q = 1-3)

- Cross sections for electron capture by H^{+} ions for the modeling of hydrocarbon pellet clouds:

  $H^{+} + C^{q+} + e^{-} \rightarrow H + C^{q+}$ (q = 1-6)

  $H^{+} + e^{-} + e^{-} \rightarrow H + e^{-}$

  $H^{+} + H^{+} + e^{-} \rightarrow H + H^{+}$

- Orbital angular momentum (*nl*) resolved CX cross sections for collisions of Be^{4+} ions with neutral H:

  $Be^{4+} + H\,(n_{H}) \rightarrow Be^{3+}(nl) + H^{+}$

These requirements will be highlighted in the upcoming CRP on atomic data for injected impurities in fusion plasma.

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- Launch new CRP: “Atomic Data for Injected Impurities in Fusion Plasmas (2022-2027)”
  The objective of this CRP is to provide evaluated and recommended data for the principal atomic processes of injected impurities such as N, Ne, Ar, Kr and Xe in fusion plasma.
- Planned CRP on “Molecules in Edge Plasmas (2023-2028)”
- Development of the old ALADDIN database to improve search and data upload functionality, update of the process classification and an improved API
- The AMD unit will continue to develop the new databases: hcbd (https://db-amdis.org/hcdb), CascadesDB (https://cascadesdb.org), and DefectDB(https://db-amdis.org/defectdb).

Detlev REITER (Heinrich Heine University Düsseldorf, Germany, ITER Scientific Fellowship Network) pointed out

- unavailability of the CX recombination data for collision of H with impurities such as N, Ne, Ar, particularly for weakly ionized charge stages in the low-collision energy range (5 - 200 eV), that are most relevant in edge and divertor plasma regions.

The upcoming CRP of the AMD unit on atomic data for injected impurities in plasmas is expected to provide the required data.

3.2 Bibliographic Data Compilation

The following points were raised during the discussions about bibliographic information on A+M data:

- The AMBDAS bibliographic database (https://amdis.iaea.org/ambdas) of the AMD unit has entries for spectroscopic, atomic, and molecular and plasma surface interaction data. There are currently 51,106 references for materials relevant to fusion research. A new classification of plasma processes and search parameters were adopted which was reviewed at the IAEA technical meeting in 2019. The AMBDAS database is sustained through consultancies and collaboration with members of the DCN
    - spectroscopic data from NIST, USA
    - collisional data from KFE, Korea
- NIST maintains atomic bibliographic databases, which are updated regularly in about two weeks
    - 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 an atomic collision bibliographic database that was collected at ORNL (https://dbshino.nifs.ac.jp/nifsdb/ornl/top) since 1959 but that has not been updated since 2009. The database has a total of 78,097 entries.
- KFE has numerical data on collisional processes linked to bibliographical data which has been provided to AMBDAS for an update. KFE will develop a program to automate data collection and reduce sorting time.
- The Harvard Astrophysics Data System (ADS) (https://ui.adsabs.harvard.edu/) is widely used in the astrophysics community
- The SPECTR-W^3 database on spectroscopic properties of atoms and ions contains bibliographic database (http://spectr-w3.snz.ru/index.phtml).

3.3 Uncertainty Quantification of fundamental data for fusion plasma diagnostics

Experimental data for collisions of atoms, molecules, and heavy particles are very limited, and the cross-section data relate only to selected transitions at certain collision energies. For practical purposes such as plasma modeling, a large set of atomic and molecular data is required in a wide range of energies. Therefore, the theoretical methods have to meet such requirements, which has led to the development of advanced theoretical methods and sophisticated computational tools for the study of collision dynamics. The accuracy of the computed data can be determined from the benchmark data to some extent, but this is not always feasible. Therefore, one way is to quantify the uncertainty of the theoretical atomic data needed in fusion plasma diagnostics. The atomic and plasma physicists are now actively discussing the need to assess the uncertainty of A+M data and its impact on modeling results for fusion as well as other fields of research. However, finding an effective method to estimate the uncertainties of the computed A+M data is challenging for many reasons, such as accurate representation of atomic and molecular structures, various approximations in collisional calculations, validity of the different codes in different energy regimes, etc.

Due to the significance of accurate theoretical A+M data for the diagnostics of fusion plasma, the AMD unit has been promoting the uncertainty quantification activities through consultancy and technical meetings as well as through the organization of workshops since 2012. Although some progress has been made in the uncertainty quantification of A+M data, the field is still at an early stage for its application to fusion science, in particular to propagation of uncertainty in the theoretical A+M data to fusion models. In continuation of the unit's efforts, the last session of the DCN meeting was devoted to quantifying uncertainties in the atomic data for applications in fusion diagnostics and a proposed workshop on **"Algorithmic atomic uncertainties and their effect on plasma models"**. The detailed summary of this session is given below:

Martin G. O'MULLANE (Department of Physics, University of Strathclyde, United Kingdom) and **Connor BALANCE** (Queen's University Belfast, United Kingdom) presented details of the proposed workshop on Uncertainty Quantification which was previously discussed at the 24th DCN. Discussions have been ongoing between them and the IAEA to coordinate this activity since the last DCN meeting. The idea behind this activity is to add the uncertainties to atomic data and then propagate those uncertainties into plasma models. The primary objective of the activity is to develop robust and reliable methods/workflows to generate error bars for atomic quantities from the various codes and then to apply these uncertainties to the fusion models to determine the precision and any correlation between them that is necessary to affect the interpretation of the plasma model. The scope of the proposed activity would require the integration of atomic data producers and plasma(transport) modelers.

One of the possible ways is to understand the uncertainties by combining information from different theoretical methodologies and developing an algorithm to evaluate the uncertainties. Therefore, a test case relevant for magnetic fusion plasma research is decided in advance which requires ab-initio atomic physics calculations, CR population kinetics and then transport modeling. The studied system was chosen to be nitrogen, an important impurity for fusion plasma diagnostics and a simple atomic system compared to complex high-Z impurities. The activity would require structure calculations for Li-like, Be-like and B-like ions in the first step.

Participants from the DCN meeting provided important input for the proposed workshop. Some of the participants are also involved in the organization of the NLTE code comparison workshop and have shared their experiences. In NLTE workshop, test cases are defined a few months in advance and code results are submitted before the workshop. Submitted code results for defined cases are discussed in the workshop for the underlying atomic and plasma kinetics to understand differences and discrepancies when comparing code results. Over the past two decades, the NLTE workshop series has developed tools and techniques for verification and validation of advanced CR models which are difficult to validate and verify experimentally.

The key points to consider are listed below:

- Detailed workshop plan should be well-defined for networking of A+M physics experts and fusion plasma community, e.g., the parameters for the test case, plasma conditions, and the final quantities of interest should be clearly defined,
- To define the detailed formats of submissions in advance,
- Development of an intelligent method for comparing the various submissions which requires the establishment of well-defined database and interface.

Concluding remarks:

Uncertainties in the A+M data are critical for collisional radiative codes for fusion plasma transport applications, especially ITER, where plasma particle densities will be much higher than that of all current tokamak fusion devices and, therefore, the ion collisionality is expected to increase by two orders of magnitude. It has been estimated that even low uncertainties (~few percent) in the AM data can have a significant impact on the integrated modeling results of ITER divertor environment. Therefore, there is clear need for data evaluation and uncertainty assessment activities.

The IAEA can play an important role in bringing together the representatives from the atomic and molecular data producing and fusion data user communities that are essential for the success of the proposed activity. Thus, the uncertainty quantification activity will be announced at the upcoming 2nd meeting of the Global Network for the Atomic and Molecular Physics of Plasmas (GNAMPP2) to be held from 6 – 10 December 2021 (https://amdis.iaea.org/meetings/gnampp-2/), where the leading A+M physicists together with plasma physicists, representatives from ITER and other fusion devices using A+M data for fusion and other plasma applications will be invited. It was proposed to further discuss the test case and detailed plan of the workshop during the consultancy meeting of the CRP "Atomic properties of the injected impurities", which is tentatively scheduled for spring/summer 2022 and a potential workshop/consultancy meeting will be linked to the first RCM of the CRP to be held from 5 – 7 October 2022.

Appendix I: List of Participants

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Appendix II: Meeting Agenda

(Virtual) 26th Meeting of the Data Centre Network

IAEA Headquarters, Vienna, Austria

1 - 3 September 2021

Note: all times are given in Central European Summer Time (CEST, UTC+02:00).

AGENDA

Wednesday, 1 September 2021

14:00 – 14:15	**Arjan KONING, Christian HILL, Kalle HEINOLA** (IAEA, Austria) Welcome and Introduction
14:15 – 14:40	**Yuri RALCHENKO** (National Institute of Standards and Technology, United States of America) Report on the Recent Developments of the NIST Atomic Databases
14:40 – 15:05	**Izumi MURAKAMI** (National Institute for Fusion Science, Japan) Atomic and Molecular Data Activities at NIFS in 2019-2021
15:05 – 15:30	**Mi-Young SONG** (Institute of Plasma Technology, KFE, South Korea) A+M Data Center Activities in Korea Institute of Fusion Energy (2019 ~ 2021)
15:40 – 15:55	**Virtual Coffee Break**
15:15 – 16:20	**Martin G. O'MULLANE** (Department of Physics, University of Strathclyde, United Kingdom) Recent developments in ADAS and OPEN-ADAS
16:20 – 16:45	**Duck-Hee KWON** (Korea Atomic Energy Research Institute, South Korea) Progress of atomic data and collisional-radiative modeling in KAERI
16:45 – 17:10	**Pavel R. GONCHAROV** (Peter the Great St. Petersburg Polytechnic University (SPbSTU), Russia) Production, Uses and Needs of Atomic and PMI Data for Nuclear Fusion Research in Russia

Thursday, 2 September 2021

14:00 – 14:25	**Kalle HEINOLA** (IAEA, Austria) Overview of the activities of the A+ M Data unit
14:25 – 14:50	**Baoren WEI** (Fudan University, China) The A & M data measurement at Shanghai EBIT Lab

14:50 – 15:15	**Raúl BARRACHINA** (Centro Atómico Bariloche, Argentina) An Open Code Perturbative Model for Ionization Collisions
15:15 – 15:40	**Virtual Coffee break**
15:40 – 16:05	**Connor BALLANCE** (Queen's University Belfast, United Kingdom) Updates on the electron-impact excitation and ionization of the near-neutral stages of Tungsten
16:05 – 16:30	**Vincenzo LAPORTA** (CNR Bari, Italy) Electron-molecule collisions and vibrational relaxation times for fusion plasma applications
16:30 – 16:55	**Discussion**

Friday, 3 September 2021

14:00 – 14:25	**Detlev REITER** (Heinrich Heine University Düsseldorf, Germany) Renewed interest: charge exchange $H + A^{q+} \rightarrow H^{+} + A^{(q-1)+}$
14:25 – 14:50	**Zsolt MEZEI** (Institute for Nuclear Research, Hungarian Academy of Sciences (ATOMKI), Hungary) Electron-driven molecular processes in the edge plasmas of fusion devices: new state-to-state cross sections and rate coefficients
14:50 – 15:15	**James COLGAN** (Los Alamos National Laboratory, United states of America) Collisional-Radiative Modelling of Tungsten Plasma
15:15 – 15:40	**Virtual Coffee break**
15:40 – 16:30	**Martin G. O'MULLANE (**Department of Physics, University of Strathclyde, United Kingdom) **and Connor BALANCE** (Queen's University Belfast, United Kingdom) Algorithmic atomic uncertainties and their effect on plasma models

Appendix III: Titles and Summaries of Presentations

Presentation materials available at https://amdis.iaea.org/meetings/dcn-26/

Report on the Recent Developments of the NIST Atomic Databases

Yuri Ralchenko

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

In spite of the pandemic effects on research world-wide, the NIST atomic databases were consistently expanded and updated since the previous DCN meeting. We will report on the latest upgrades of the Atomic Spectra Database (ASD) and the LIBS database, development of the new database on opacities of lanthanides that are critically important for kilonova simulations, recent work on EBIT x-ray and EUV spectra analyses, and the current projects on atomic data compilations.

Atomic and Molecular Data Activities at NIFS in 2019-2021

Izumi Murakami[1], Daiji Kato[1], Masatoshi Kato[1], A. Hiroyuki Sakaue[1], Tomoko Kawate[1], Masahiko Emoto[1], Tetsutarou Oishi[1], Chihiro Suzuki[1], Priti[2], Nobuyuki Nakamura[2]

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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 2019-2021. In total 825,997 data sets are stored in the databases (as of Aug. 2, 2021). Number of the data sets for AMDIS EXC and AMOL are increased much during this period. A new working group for data compiling and producing on sputtering yields has started since 2019.

Various research activities related to the atomic and molecular data have been conducted and we mainly have work on tungsten spectra. Tungsten spectra in wide wavelength region have been measured in plasmas of Large Helical Device (LHD) with tungsten pellet injection. Spectral lines of W^0 – W^{46+} ions are measured [2-5]. Extreme ultraviolet spectra of other high Z elements, such as Pr and Nd were also measured in LHD [6,7]. Collisional-Radiative models have been developed to identify and examine properties of spectra for W ions in plasmas [4,5]. E3 lines of W^{27+} and M1 lines of W^{8+} and W^{9+} are measured and identified by using compact EBIT devices [8,9].

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[4] I. Murakami et al., Nucl. Mater. Energy 26, 100923 (2021)
[5] D. Kato et al., IAEA FEC28 (2021); submitted to Nucl. Fusion (2021)
[6] C. Suzuki et al., X-Ray Spectrom. 49, 78 (2020)
[7] C. Suzuki et al., Atoms 9, 46 (2021)
[8] H. A. Sakaue et al., Phys. Rev. A 100, 052515 (2019)

A+M Data Center Activities in Korea Institute of Fusion Energy (2019~2021)

Mi-Young Song

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

This presentation includes the research facilities of the KFE Research Group of Korea and the data production techniques and data for plasma application.

DCPP [1] 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. About 1000 papers are collected in the first collection, and through the filtering process, about 100 data are finally secured for AMBDAS updates.

We studied the chemical and physical properties of candidate gases for the development of new alternative gases by utilizing our research base for the past two years. We established a direct data production base through experimental measurements and developed a measuring device and measured total scattering cross section for e – N2O[2], C3F6O collisions at low electron energies. We have optimized the structure of NF3O 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.

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. So We evaluated the cross section for electron collisions with H2O [3] and generalized the definition of cross section in this year. In the future, N2 and CO2 molecular evaluation will be conducted through the operation of the evaluation group.

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[1] DCPP (Data center for Plasma Properties), https://dcpp.kfe.re.kr

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Recent developments in ADAS and OPEN-ADAS

Martin O'Mullane

Department of Physics and Applied Physics, University of Strathclyde, 107 Rottenrow, Glasgow, G4 0NG, UK

Progress of atomic data and collisional-radiative modeling in KAERI

Duck-Hee Kwon, Kil-Byoung Chai, Minkyu Lee and Sung-Ryul Huh

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We have implemented unitary correction [1] for relativistic distorted wave (RDW) approximation of electron-impact excitation (EIE) in the original flexible atomic code. The EIE cross sections for Ar and Ar^+ are calculated by the unitarized RDW code and compared with others by more sophisticated R-Matrix calculation and experiments (Ar), and other DW calculation (Ar^+).

A collisional-radiative (CR) modeling for low temperature He plasma was developed, which solves nonlinear steady-state balance equations including radiation trapping and heavy particle collisional ionization [2]. The electron temperature and density diagnostics by the CR modeling and optical emission spectroscopy was compared with Langmuir probe measurements.

A novel applied-field MagnetoPlasmaDynamc (AF-MPD) thruster device simulating particle and heat fluxes in divertor for plasma surface interaction (PSI) study has been constructed in KAERI and the performances have been measured [3,4]. A CR modeling for H plasma to determine the plasma parameters is under developing. Our results about the EIE and the CR modeling will be uploaded on our web site https://pearl.kaeri.re.kr in the near future.

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Production, Uses and Needs of Atomic and PMI Data for Nuclear Fusion Research in Russia

Pavel Goncharov[1, 2]

[1]Peter the Great St. Petersburg Polytechnic University, 195251, Russia

[2]Ioffe Institute, 194021, Russia

An update on the activities carried out in Russia during the past two years on atomic and plasma-material interaction (PMI) data will be presented. The overview covers the newest results obtained at Peter the Great St.Petersburg Polytechnic University, Ioffe Institute, P.N. Lebedev Physical Institute, NRC Kurchatov Institute, Moscow Engineering Physics Institute, Novosibirsk State University, and G.I. Budker Institute of Nuclear Physics. The main emphasis is on the works in support of ITER diagnostics to be delivered by the Russian Federation, as well as the activities in the framework of the Russian Federal project on fusion and plasma technologies. Online databases and Russian topical conferences will also be overviewed.

Overview of activities of the A+M Data Unit

Kalle Heinola

International Atomic Energy Agency (IAEA), PO Box 100, 1400 Vienna, Austria

This presentation summarizes activities of the IAEA A+M Data Unit during 2019-2021. This comprises of reviews of ongoing and planned Coordinated Research Projects (CRPs), meeting organizations (Technical Meetings, Consultancy Meetings and Workshops), publications as well as the maintenance and development of present and future databases. Unit's activities have been focusing on maintaining and launching new CRPs, databases, networks and workshops as well as remaking the A+M Unit's web pages.

The A&M data measurement at Shanghai EBIT Lab

Baoren Wei

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An Open Code Perturbative Model for Ionization Collisions

Raúl Barrachina

National Atomic Energy Commission (CNEA), Bariloche Atomic Center, Argentina

Due to the COVID 19 pandemic, the Bariloche Atomic Center, like the rest of the facilities of the National Atomic Energy Commission of Argentina, has remained closed, except for essential tasks as the production of radioisotopes, the irradiation plants, the nuclear medicine centers, etc. In this context, the three accelerators and the remaining experimental facilities of the Laboratory for Radiation Interaction with Matter have largely remained in a state of maintenance. For its part, theoretical studies have continued to be carried out remotely.

In this communication, one of these theoretical undertakings will be discussed, which proposes the development for its use in an open-code format, of a computer program for the calculation of the cross section for the ionization of atoms and molecules by the impact of charged particles. This proposal seeks to complement the CDW-EIS code currently available in online format at the website of the AMD unit of the IAEA.

During the presentation, we will review the basic principles of the open-code concept and will discuss the improvements that the new program implies with respect to the existing CDW-EIS.

Updates on the electron-impact excitation and ionization of the near-neutral stages of Tungsten

Connor Ballance

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A summary will be given as to the progress of electron-impact excitation and ionization work using the parallel DARC (Dirac Atomic R-matrix Codes) for neutral and singly-ionized Tungsten. The electron-impact excitation for neutral Tungsten [1] has been compared with observations taken at the CTH (Compact Toroidal Hybrid) experiment at Auburn University and reported in Johnston et al 2019 [2].

Collisional Radiative (CR) modeling or the generation of a synthetic spectrum requires a metastable approach to the analysis, yet simple line ratios have been ascertained that have predicted CTH temperatures. Combined with ground and excited state ionization cross sections it is hoped that these may be used to provide SXB ratios or a theoretical determination of the impurity influx from Tungsten from plasma-facing components, though there are outstanding issues.

The electron-impact excitation of WII (Dunleavy et al, in preparation) shall follow the same approach followed for neutral Tungsten. Ideally, from an experimental perspective it is beneficial to have spectral lines from different ion stages emitting within wavelength window.

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Electron-molecule collisions and vibrational relaxation times for fusion plasma applications

Vincenzo Laporta

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

In my presentation, I will illustrate my researches on non-equilibrium plasma physics and electron-molecule collisions 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. These researches are performed in view of many applications: in particular in aerospace (shuttle reentry in planetary atmospheres, electric propulsion), combustion, controlled fusion reactors, astrochemistry (early Universe, interstellar medium) and chemical evolution of life just to name a few.

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 H2 [1], D2 [2], H2+ [3], ArH+ [4] and BeH+ [5, 6]. Finally, vibrational relaxation times in state-to-state approach [7, 8], will be also presented.

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Renewed interest: charge exchange $H + A^{q+} \rightarrow H^+ + A^{(q-1)+}$

Detlev Reiter

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Active plasma edge cooling in current and future magnetic fusion reactor with deliberately injected impurity gases such as N_2, Ne, Ar, Kr, etc. provides a key mechanism to deal with otherwise excessive plasma (heat) loads on exposed parts of the reactor chamber, such as divertor targets. The role of charge exchange recombination collisions $H + A^{q+} \rightarrow p + A^{(q-1)+}$ has since long been studied, and its potentially significant influence on overall fusion edge plasma conditions has explicitly been demonstrated recently (again) in dedicated ASDEX-UPGRADE experiments (Dux et al., J. Nucl. Fus. 60 (2020) 126039). Current attempts to relate and quantify these results for ongoing ITER predictive and (future) interpretative studies have so far been hampered by gaps in both: the available basic cross section data bases and in processed data formats (with often missing key parameter dependencies in rate coefficients).

Analysing the NIST and IAEA cross section data bases for these processes shows: The NIST data base (report NIFS Data 102, 2008) appears to be the most complete publicly available cross-section data set, but it is missing the data for N, and O impurity plasma components, and, due to its particular fit format, does not allow easy extension to fusion edge plasma relevant energy ranges (from threshold to some 100 eV collision energy). Here extension to lower energies, and an asymptotically correct low energy limit in fits or tables, appears to be the most pressing data issue.

The IAEA cross section database for these reaction channels dates from the mid-nineties of the past century (APID Vol 4, 1993), and, apart from further completion (e.g.: towards N ions plasma component) the low energy limit of these datasets needs to be re-evaluated and validated against more recent theoretical and experimental data and also with respect to low energy consistency with experimental thermal rate coefficients, when the latter are available e.g. from thermochemical tables.

The suitable data format for processed data (rate coefficients) is highly case dependent, ranging from beam-Maxwellian, double Maxwellian formats and retaining dependencies allowing for isotopic scaling as well as T_e to T_i ratios.

This work is supported by the ITER Scientist Fellow Arrangement: Detlev Reiter_ ITER _ D _ YS6ZZZ, The ITER International Fusion Energy Organization, 13067 Saint-Paul-Jez-Durance, France.

Electron-driven molecular processes in the edge plasmas of fusion devices: new state-to-state cross sections and rate coefficients

J. Zs. Mezei[1,2], J. Boffelli[2], E. Djuissi[2], A. Abdoulanziz[2], N. Pop[3], F. Iacob[4], S. Niyonzima[5], M. D. Epée Epée [6], V. Laporta[7], K. Chakrabarti[8], O. Motapon[6], D. Reiter[9], J. Tennyson[10], and I. F. Schneider[2,11]

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Dissociative recombination, elastic scattering, (ro-)vibrational excitation, vibrational de-excitation and dissociative excitation [1]:

$$AB^+(N^+, v^+) + e^- \rightarrow AB^*, AB^{**} \rightarrow \begin{cases} A + B \\ AB^+(N'^+, v'^+) + e^- \\ A + B^+ + e^- \end{cases}, \quad (1)$$

are dominant elementary processes in numerous cold ionized gases. Here N^+/v^+ stand for the rotational/vibrational quantum numbers of the cation, AB^* for a bound excited (mostly Rydberg) state of the neutral, and AB^{**} for a dissociative (mostly doubly- or multiply-excited) state of the neutral.

The quantum interference between the direct mechanism - capture into the doubly-excited states AB^{**} - and the indirect one - temporary capture into a Rydberg state AB^* - induces resonances in the cross section.

The Multichannel Quantum Defect Theory (MQDT) [1, 2] is the most suitable approach for these processes, efficiently handling channels - open for the direct process and closed for the indirect one - and the corresponding channel mixing via electronic and vibronic interactions. We will provide new cross sections and rate coefficients for H_2^+, and isotopologues [3, 4, 5], BeH^+ and isotopologues [6, 7, 8], and N_2^+ [9].

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Collisional-Radiative Modelling of Tungsten Plasma

Authors: James Colgan[1]; Christopher J. Fontes[1]

[1]Los Alamos National Laboratory

The Los Alamos suite of atomic physics codes [1], combined with the plasma modelling code ATOMIC [2,3] has been successfully used in a number of applications to understand the properties of local thermodynamic equilibrium (LTE) and nonLTE plasmas. For example, in LTE, the codes have been used to produce opacity tables for the elements hydrogen through zinc for use in astrophysical modelling [4]. Opacity tables for heavier elements, including the lanthanide metals, have also been produced to assist in the interpretation of light curves from neutron star mergers that also produce gravitational wave signatures [5].

For nonLTE plasmas, ATOMIC has been used for many years to contribute to the series of nonLTE workshops [6], in which detailed comparisons have been made between the results from a variety of nonLTE modelling efforts. For example, ATOMIC was used to predict the ionization balance and radiative power loss from tungsten at temperatures of interest to fusion modelling [7]. ATOMIC has also been used to explore the nonLTE effects in tin plasmas of interest to EUV lithography [8].

In this presentation, we briefly describe the capabilities of ATOMIC, using the calculations performed for tungsten plasma modelling as a worked example. We describe the various types of atomic data that may be used in collisional-radiative modelling. We discuss the difficult problem of ensuring completeness with respect to the number of configurations included in a CR calculation. We also provide a short overview of the opacity-generating capabilities of ATOMIC that may be of interest to the opacity needs of vapor shielding modelling efforts.

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