International Atomic Energy Agency INDC(NDS)-450

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Technical Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (17th Meeting of the A+M Data Centres and ALADDIN Network)

6-7 October 2003, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared by: Denis Humbert

March 2004

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (17th Meeting of A+M Data Centres and ALADDIN Network), held on 6-7 October, 2003 in Vienna, Austria are briefly described. The meeting conclusions and recommendations on the priorities in A+M data compilation and evaluation, and on the technical aspects of data processing, exchange, and distribution are also presented.

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March 2004

Table of Contents

Appendices:

1. Introduction

On 6-7 October, 2003, the IAEA held the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing (17th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network)". The objectives are to review the progress in the A+M data related activities in the Data Centres, the methods and procedures applied in the data processing and exchange, developments in the ALADDIN system, and to coordinate the working plans for the next period. Thirteen participants attended the meeting from eleven Data Centres (see Appendix 1).

This year the committee members note with sadness the absence of two of their relevant data centre representatives, Dr. Shirai who died in September 2002 and Prof. Delcroix who died in May 2003. They were respectively replaced by Dr. Kubo and Dr. Bretagne who gave a short talk in their memories. The meeting organizers thanked them a last time for the very valuable contribution they provided to our community.

In the previous two-year period no new Data Centres have been added to the network. This year Dr. L. Machado (Universidade federal de Sao Carlos, Dpt de Fisica) was asked to attend the meeting as an observer. Dr. A. Godunov(TRINITI, A+M data Unit), Dr. V. Barabash (Efremov Institute, PMI Data Center) and Dr. S. Yongsheng (CRAAMD, Bejing) were unable to attend the meeting. Dr. Yuri Ralchenko (NIST), expert in data exchange and web databases tools, attended the meeting as a consultant.

2. Meeting Proceedings

The Meeting was opened by Dr. N. Ramamoorthy (Director, Division of Physical and Chemical Sciences, NAPC), R. E. H. Clark (Head, A+M Data Unit, Nuclear Data Section) and D. Humbert (Atomic Physicist, A+M Data Unit, Nuclear Data Section). They welcomed all participants and stressed the usefulness of this AGM to the Data Centre Network, and the new developments in this field that have occurred since the 16th AGM held in September 2001. The attendees had continual web access in the meeting room to all Data Centre sites, which was actively used in the presentations and demonstrations.

After adopting the Agenda (see Appendix 2), the meeting proceeded in four sessions:

1) Current Activities of the A+M Data Centres
2) Interfaces and web tools
3) Data Issues
4) Meeting Conclusions and Recommendations.

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

In Session 1, progress reports on the activities of individual Data Centres during the period September 2001-September 2003 were presented. These reports, which are reproduced in Appendix 3, describe the work of the Data Centres on A+M data compilation, evaluation and generation, WWW developments, Data Centre publications produced during the reporting period, and the status of ongoing Data Centre programmes and plans for future work. The presentations in this session indicate that the Data Centre activities effectively followed the recommendations of the previous Advisory Group Meeting, both in terms of content and mutual cooperation.

Dr. W. Wiese, NIST

Dr. W. Wiese discussed activities and trends at the NIST Data Centres in the last two years. He indicated that funding remained tight and there are needs for new manpower showing the actual Atomic Spectroscopic Data Center structure. He highlighted the new group "Database Design and Expansion" headed by Dr. Yu. Ralchenko. He reviewed the recent work on data compilations and gave a list of available databases at NIST (http://physics.nist.gov), focusing on the new online ones and new improvements as for:

New version of the Atomic Spectra Database (ASD) Version 2.0
Handbook of Basic Atomic Spectroscopic Data
The new database on Spectral Data for the Chandra X-ray Observatoty
Electron–Impact Ionization Cross Section Database

Dr. T. Kato, NIFS

Dr. T. Kato reported on recent work at the A+M Data Research Center, NIFS, consisting of compilation activities, research and collaboration programs, data publications, and future plans. She reviewed the NIFS website and services, the status of data records in the numerical databases (for electron impact ionisation, recombination and excitation, charge transfer cross sections) and bibliographic databases. These databases are accessed through a new WWW homepage (http://dbshino.nifs.ac.jp/) and require a simple user registration process.

Two new databases for molecular processes are now available online. Dr. T. Kato outlined the importance of such databases due to the data needs of the fusion community for processes like molecular collisions in divertor plasmas, formation of hydrocarbon molecules at surfaces and negative ion source. The first database, AMOL, is dedicated to electron impact cross sections and rate coefficients and covers a large number of processes. The second one, CMOL is for heavy particles collisions and gives cross sections, rate coefficients and branching ratio for various processes.

NIFS has a number of collaboration programs and research activities and it is emphasized that such collaborations are encouraged. She underlined collaboration with the KAERI to make a numerical database for satellite lines. NIFS will be hosting the ICAMDATA conference in October 2004.

Statistics showed the rapidly growing interest of the fusion community in the NIFS website activities.

NIFS publishes the NIFS-DATA series reports as the results of collaboration. A large amount of bibliographic data of electron and photon cross sections with atoms and molecules are now being published by Dr. M. Hayashi (NIFS-DATA-72(Ar), 74(Carbon Dioxide), 76(SF_6),77(N_2), 79(Xe), 80(Halogen molecules)). Cross section data at low impact energies for Ar^{q+} ions on Ar and Ne target are published in NIFS-DATA-75 by X. Ma et al. Population alignment collisional radiative model and atomic data are published in NIFS-DATA-78 by Iwamae et al.

Dr. D. R. Shultz, CFADC, ORNL

Dr. D. R. Schultz presented the recent activities of the Controlled Fusion Atomic Data Center (CFADC, http://www-cfadc.phy.ornl.gov/).

He described the Multicharged Ion research Facility (MIRF) and the benefits of its recent upgrades. MIRF is an electron cyclotron resonance (ECR) source method to study

atomic processes in plasmas and interactions of ions with materials. Studied processes are mainly ion-surface interactions, electron-ion and molecular ion collisions, ion-atom and molecule collisions. The MIRF upgrade gives an expanded range of energies and new capabilities and opportunities for all experiments.

For computational atomic physics for plasma edge modeling, a large amount of calculation and data compilation has recently been done (transport cross sections for cool hydrogen plasmas, inelastic collisions involving H_2 and H_2^+, Lithium studies, Beryllium wall studies, Krypton ionisation data).

Work for recommended charge transfer cross sections for C^{6+} + H and LTDSE calculations to address charge transfer data needs have been completed.

Dr. H. Kubo, JAERI

The whole DCN Committee expressed the great loss due to the death of Dr Shirai and Dr. Kubo reviewed his very valuable work for the fusion community. Then Dr. H. Kubo reported on the A+M activities at the Department of Fusion Plasma Research of the Japan Atomic Energy Research Institute (JAERI). A new structure of the data center is under discussion; the atomic and molecular data activities are now under the responsibilities of Drs. Kubo, Sataka and Ozeki.

Cross sections by electron impact for 138 processes have been compiled for different hydrocarbons (T. Shirai & al., ADNDT 80, 147 (2002). Total cross sections for single- and multiple-charge transfer by multi-charged Ne and Ar ions colliding with various hydrocarbons have been measured (T. Kusakabe et al., Nucl. Instrum. Meth., B205, 600 (2003). Dr. H. Kubo then presented the works in progress in data compilation and data production.

Data compilation:

i) Spectral data for Ga, W and Ar, in collaboration with NIST,
ii) Analytic cross sections for electron collisions with Nitrogen molecules in collaboration with Prof. Tabata of Osaka Prefecture University,
iii) Charge transfer cross sections in collaboration with Profs. Imanishi and Imai of Kyoto University.

Data production:

i) Differential cross sections for elastic scattering, vibrational excitation and electronic excitation of hydrocarbon molecules by electron impact from 1.5 to 100 eV, in collaboration with Prof. Tanaka of Sophia University,
ii) Cross sections for charge transfer by H, C, O, He, Ne, Ar, Kr, Xe ions colliding with hydrocarbons at keV energies, in collaboration with Dr. T. Kusakabe of Kinki University,
iii) Cross sections for charge transfer by Fe^+, $Ni^{+,2+}$, $Cr^{+,2+}$, $Be^{+,2+}$, B^+ colliding with He, Ne, Ar, Kr, H_2, N_2, CO, CO_2, CH_4, C_2H_6 and C_3H_8 at 30-600 eV/amu, in collaboration with Profs. Imanishi and Imai of Kyoto University,
iv) State-selective charge-transfer cross sections for C^{+4} and H(n=2) collisions and for B and Be ions in metastables states and H and He at energies below 25 keV/amu, in collaboration with Prof. Shimakura of Niigata University.

Dr. Yu. V. Martynenko, Kurchatov Institute

Dr. Yu. V. Martynenko discussed the data activities of the A+M Data Centre at the Scientific Research Centre "Kurchatov Institute" (Moscow). He first reported on new data

generation in Kurchatov Institute showing some published results or generated data in the context of IAEA CRPs and activities within their laboratory:

- Electron capture and ionization in slow collision of H and He with atoms and ions, M. Chibisov, CRP "A+M Data for Fusion Plasma Diagnostic".
- Enhanced dielectronic recombination (DR) rates in electric fields, L.A. Bureyeva, T. Kato, V.S. Lisitsa and C. Namba, Phys. Rev.A, 2002, V.65, P.032-702.
- Polarization radiation channel and electron recombination in plasma with heavy ions, V.A. Astapenko, L.A. Bureeva, V.S. Lisitsa, Phys.Rep., 2002, 28, 337.
- New simple method for calculating the cross section of impact ionization of neutral atoms, V.A. Astapenko, Laser Physics, Vol. 11, 1336 (2001).
- Production of H^+_3 Ions in Low- Energy Collision between Hydrogen Molecular ions, Plasma Phys. Reports, V.27, No. 10, 2002, p. 901 and V.27, No. 12, 2002, p. 1032, V. Belyaev, M. M. Dubrovin, A. A. Terent'ev, A. E. Trenin, G. V. Sholin.
- Subthreshold Sputtering at High Temperatures, JETP Letters V.77, p. 430 (2003).

Dr. Martynenko then talked about the Project "Complex computer modeling of modern tokamak plasma processes". The aim of this project is the integration of physical codes for tokamak plasma processes, as well as existing codes as new ones. Databases will also be included. This project contains three subtasks aimed to A+M data:

- Electron, atom and molecular collisions.

- Universal code for atomic kinetic and radiation loses.

- Material response on plasma effect in tokomaks.

In his conclusion Dr. Martynenko pointed out the needs for relevant data for specific conditions in fusion devices and the accuracy to include databases in plasma codes.

Dr L. Machado, Universidade Federal de Sao Paolo

Dr L. Machado attended the meeting as an observer. He has been invited on the recommendation from the DCN Committee, during last meeting held in Vienna on September 2001. He introduced himself as a representative of the Brazilian atomic and molecular Physics research, and presented different topics collected from different Brazilian labs, which may be of interest for the DCN activities. After some general words about Brazil, he gave a short description of each Brazilian laboratory that could be interested in joining the Data Centre Network in the near future.

<u>LNLS synchrotron, State University of Campinas (UniCamp)</u>:

LNLS is the only synchrotron facility in operation in the south hemisphere. It started working in December 1986. Scientists and engineers from Brazil and from several others countries of South America are the usual users of LNLS. Collaboration programs between LNLS and others synchrotrons both in America and Europe are well developed.

In the field of Atomic and Molecular Physics and Plasma Physics, Unicamp has at least three very active groups:

1) The group of Lasers and Spectroscopy do high resolution atomic and molecular spectroscopy for several systems in the visible region. In the infrared and far infrared regions of the spectrum, techniques such as photoacoustic spectroscopy, sub-Doppler spectroscopy and Stark and non-linear Hanle spectroscopy are also used.

2) The group of Plasma Physics develop both experimental and theoretical work. The main lines in experimental research are plasma processing, multiple-pass Thomson scattering; laser interferometry and spectroscopy of light elements. A small tokamak is in operation. On the theoretical side, studies on Magneto-hydro-dynamical equilibrium, stability and transport in plasmas, travelling wave current drive, dusty plasma and ball lightings are being carried out.

3) The group "Atomic and Molecular Collisions" focus on processes such as elastic electron (positron)-polyatomic molecule scattering and electronic excitation of polyatomic molecules by electron impact by calculating DCS, ICS and MTCS. Processes including positron annihilation are included in their initiative. Rotational and vibrational excitations of diatomic and selected polyatomic molecules are also studied. Studies on both bound-state and scattering proprieties of atoms embedded in finite-temperature plasmas environment are carried out.

UFSC, University of Flrianopolis, Santa Catarina:

The main interest of the research done in UFSC is on the inner-shell excitation processes in light molecules by electron impact. For a couple of years they have done both theoretical and experimental work on this theme. The target molecules they have considered include CO, N_2, CO_2, OCS, CS_2, N_2O, C_2N_2, among others. They have calculated and measured integral, differential and momentum-transfer cross sections, as well as singlet to triplet rations of both ICS and DCS. Presently, only the theoretical research is being kept active. Calculation of cross sections are done for elastic electron scattering by small radical as CNN, NCN, CCO, CCN, CNC.

Federal University of Rio de Janeiro (UFRJ)

One group is working in the area of ion collisions with atoms, molecules and solids. With the Pelletron device, some of the ions can be accelerated to one hundredth of light velocity. Theoretical work is done for the determination of ICS and DCS for light ion collisions with atoms. Calculations involving molecular targets are underway.

UFSCar

Collision physics at UFSCar includes the studies of elastic electron-molecule scattering, electronic, rotational and rovibrational excitation of molecules by electron impact and molecular photoionization. Some of the molecular systems of interest are light polyatomic molecules as H_2O, CH_4, C_2H_4, NH_3, N_2O. Dissociative processes induced by electron impact are also studied experimentally. Finally, in collaboration with LNLS, photodissociation is investigated in CF_3H.

State-owned USP, São Carlos

The Atomic and Molecular Physics group uses trapping devices to produce cold atoms. Magneto-optical traps (MOT) are usually used. Rubidium and Ceasium are the most commonly studied systems.

Dr J. Bretagne, GAPHYOR, LPGP

The whole DCN Committee notes with sadness the death of Prof. J.-L. Delcroix and Dr. Bretagne (LPGP, Orsay) reviewed his very valuable work for the French plasma community and his role in the creation and development of the GAPHYOR Database. GAPHYOR is now directed by a scientific council of 6 members from different French universities and institutions, headed by Prof. M. Fitaire. This council defines scientific and technical issues for the Data Centre. The GAPHYOR Data Centre is part of the LPGP and is under the

direction of Dr. J. Bretagne head of the laboratory. The data collection contribution of Prof. Delcroix was redistributed among the experts team, which consists of 18 members at the present time. GAPHYOR is still waiting for the replacement of Dr. D. Humbert, who left one year ago.

Dr. J. Bretagne reviewed the current data needs and data production at LPGP, mainly in low-temperature plasmas and discharge physics, fields of interest of the laboratory. He gave some examples for numerical codes, diagnostics of plasmas and discharge and plasmas surface interactions.

Numerical modelling:

- Microscopic approaches of charged particle transport (electron energy deposition including plasmas created by high energy e-beams, Boltzmann equation, production and transport of negative and positive hydrogen ions).
- Kinetics of plasma species for plasmas created in molecular gasesDiagnostics of plasmas and discharge:

- Use of Optical Emission & Absorption Spectroscopy (magnetron discharges, plasma thrusters…) and development of Collisional-Radiative Model including non-maxwellian eedf calculated through Boltzmann equation

Plasma surface interactions:

- Sputtering and deposition of materials in non-reactive and reactive conditions in low-pressure magnetized discharges: sputtering, sticking, coupling of gas phase processes with surfaces

Dr. Bretagne continued his talk on the interest of the plasma physicist French community in the plasma and A+M databases. After briefly describing some recent trends in low-temperature plasmas and in magnetic fusion, he presented new developments and data needs for inertial fusion and laser-matter interactions. There is a strong interest of the French academic plasma community in connection with Laser Mega Joule (LMJ) facility under construction with the recent creation of the 'Institut Laser Plasmas', which groups about 20 French laboratories. Some items concerned are:

- Particle transport and energy deposition: cross-sections for particle collisions, correlation effects in high density (non-ideal) plasmas, determination of stopping power, development of models: fluid, PIC…
- Radiation transport: identification of levels and lines of highly stripped ions, spectroscopic data (transition probabilities, radiative lifetimes…), effects of plasma density on atomic structure, interaction between free and bound electrons, spectral line shapes (widths, shifts), correlation effects, plasmas diagnostics, determination of opacity of dense plasmas and matter, X-ray lasers: development of models (CRM,…) for laser emission.

- Statistical physics: equation of state and transport coefficients of dense plasma and matter, ionization equilibrium between multiply charged ions, dynamical effects, validity of LTE approximation, …

Dr. Enzo Menapace, ENEA

Dr. E. Menapace reported on atomic and molecular data production activities and relevant needs at ENEA and other Italian research institutes. He reviewed:

- The most relevant results on A+M data production by the Italian research institutes, particularly within international collaborations.

- Atomic and molecular data needs in the Italian scientific community. Data needs have been expressed for fusion studies, but also for biomedical and environmental research fields:

    - Needs expressed by ENEA, CNR and Italian Universities in the frame work of the international projects on fusion, mainly for ITER, and related to Italian programs (FTU, IGNITOR and RFX)
    - Needs for radiotherapy and related to radiobiology
    - Data needs for environmental analyses

A detailed report on "Atomic and Molecular Data Production Activities and Relevant Needs at ENEA and other Italian Research Institutes" is attached to this document.

Dr. Yong Joo Rhee, KAERI

Dr. Yong Joo Rhee presented data centre activities at the Laboratory for Quantum Optics, KAERI, which supports several experimental and theoretical atomic, molecular, and optical (AMO) physics programs. Different experimental plants for data productions were presented as for designs for high resolution spectrometry and ultra-short lasers pulse and laser fusion. The applications are for nuclear safety around nuclear plants, environmental protection and inertial fusion energy.

The experimental program at KAERI includes transition line measurements, isotope shifts, and hyperfine structure. Theoretical work and results, using the BEB model, for total cross section for ionization of neutral Mo by electron impact were presented.

The accommodation of AMO data sources at AMODS (http://amods.kaeri.re.kr/) has expanded since 2001. Some useful improvements of the interface were done for database consultations and online calculations. A new online treatment of the spectroscopic database, Atomoc Spectral Lines (ASL), to get excitation paths of elements is available. The ASL will be connected in the near future to the IAEA search engine GENIE.

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

Dr. W. Eckstein presented a report of A+M data activities of the Max-Planck Institut fur Plasmaphysik. He showed new calculations of the sputtering yield, as a function of energy at normal incidence, and as a function of angle of incidence at a fixed projectile energy, using a new fit formula. For energy dependence of the sputtering, the new fit formula allows a better description at low energies near the threshold. For the angular dependence, the new fit formula allows a better description at low mass ratios (target atom mass/projectile atom mass) and low energies. The new sputtering threshold values determined with the new fit formula give more realistic threshold energies.

Dr. W. Eckstein also presented data tables of energy levels compiled some time ago by Prof. Fricke. The compilation comprises about 100,000 levels from elements Z=1 to Z=81. Dr. Wiese agreed to check the accuracy of this work.

Dr. R. E. H. Clark

Dr. R. E. H. Clark (IAEA, Vienna) presented a report of activities of the IAEA A+M Data Unit. The activities consisted of data evaluation and recommendation, WWW database

developments and others AMDIS services, Coordinated Research Projects, and A+M Data Centre Network coordination. Dr. Clark first reviewed the different running CRP:

- Data for molecular processes in edge plasma, 2001-2003, extended to 2004
- Atomic and Molecular Data for Fusion Diagnostics, 2001-2003, extended to 2004
- Tritium inventory in fusion reactors, 2002-2004

Plan is to add one new CRP in 2004 and one in 2005. This will results in 3 to 4 running CRPs depending on funding and policies:

- Atomic and molecular data for plasmas modelling
- Atomic data for heavy elements impurities in fusion reactors

There is a strong support from the Nuclear Data Section of the Division of Physical and Chemical Sciences in organizing workshops. Any proposal is very welcome. In September 2003 the A+M data unit successfully organized a workshop on "Atomic and Molecular Data for Fusion Energy Research" in Trieste, Italy.

The Technical meeting held approximately every 10 years on "Atomic and material interaction data for fusion science technology" was hosted by the Institut of Plasmaphysik Forschungzentrum in Juelich last October 2002.

APID volume 10 on charge exchange, APID volume 11 on radiated power, and APID volume 12 on mixed material are now available. The Bulletin, volume 62 is now in press.

GENIE and DANSE are two web search engines, which allow simultaneous retrieval of data from different web sites. GENIE, available online, is dedicated to numerical atomic data. DANSE, still in development, is dedicated to bibliographical atomic and molecular data. For codes on the web, the "Average approximation is online. Collaboration with Los Alamos is now in progress to access several atomic physics codes. Collaboration started with University of Bergen to make some ion-atom codes available online.

2.2. Session 2: Interfaces and Web Tools

Session 2 covered two topics. The first one was a presentation by Dr. Yuri Ralchenko on "Modern WWW databases and Tools". The second one was dedicated to Data Centers WWW and software presentations.

Dr. Yuri Ralchenko: "Modern WWW databases and Tools"

After an introduction on what a user should expect from an atomic database Yuri Ralchenko presented the two new databases on the Web, namely, SPECTR-W3 Database on spectral properties of atoms and ions and ATOMDB from the CHANDRA X-Ray Center.

He then gave a description of the new NIST Atomic Database Management System, based on MySQL database management system. The new version of the Atomic Spectra Database (ASD) was detailed.

Dr. Yuri Ralchenko outlined the necessity to get computer-readable format of the output data. A new exchange format (AMDML: Atomic and Molecular Data Markup Language, based on XML) could be an adapted version of XML to replace the outdated ALADDIN

format. His proposal is to create a working group to prepare a presentation of AMDML at the next ICAMDATA in Japan.

Data Centers WWW and software presentations

- **Denis Humbert**, GENIE + DANSE: GENIE and DANSE are two web search engines which allow simultaneous retrieval of data from different web sites. GENIE available online, is dedicated to numerical atomic data. DANSE, still in development is dedicated to bibliographical atomic and molecular data.

- **Bob Clark**, Codes on the AMD Unit Websites: Bob Clark demonstrated two running atomic physics codes through the WWW he implemented at the IAEA. The atomic physics data are generated from Los Alamos National Laboratory (LANL) codes that calculate electron impact excitation, ionization, photoionization, and autoionization, and inverse processes through detailed balance (AAEXCITE code), and for some atoms, effective rate coefficients (RATES). For "AAEXCITE", the on-line code employs the Cowan HF atomic structure package, the average approximation and a distorted wave approximation. Bob Clark demonstrates its usefulness in generating cross sections of reasonable accuracy when more accurate cross section data is not available. For "RATES coefficients", data are derived from a compilation of effective ionization and recombination rate coefficients calculated with atomic physics and plasma modeling codes from Los Alamos National Laboratory with the Los Alamos modeling codes. Bob Clark shows interpolations to obtain total radiated power, average ion charge, and relative ionization populations in a steady state plasma for Ne.

- **Yuri Ralchenko**, new NIST Databases: Yuri Ralchenko first demonstrated the two new Web databases SPECTR-W3 Database on spectral properties of atoms and ions and ATOMDB from the CHANDRA X-Ray Center. He then gave a demo of the next version of the Atomic Spectra Database (ASD version 3.0). In this version search of lines, transitions and levels may be done using a Grotrian graph. Version 3.0 will also include links between the numerical data and the bibliographic ones.

- **Yong Joo Rhee**, new AMO databases. Yong Joo Rhee presented the new improvements of AMODS (Atomic Molecular and Optical Database Systems). Yong Joo Rhee presented some new aspects of database "Atomic Spectral Lines" now available on the KAERI website, as well as the improvement in the electron impact excitation and ionisation cross section database. The interface allows easy data retrieval in a table format as well as graphs. The possibility to connect this database to the web search engine GENIE was also demonstrated.

- **Takako Kato**, Numerical databases at NIFS. Takako Kato gave a review of the available databases at NIFS. She showed different retrievals of data cross sections by electron impact for molecular processes. Data results presented on graphs allow comparison between different data sources. She also showed cross-linking between outputs from numerical searches and bibliographic databases.

2.3. Session 3: Data Issues (Chairman: W. Wiese)

Session 3 covered three topics:

- Priorities in A+M data compilation and evaluation for fusion
- DANSE Processes Classification
- Plan of DCN activities for the near future

The priorities in A+M data compilation and evaluation for fusion

The priorities in A+M data compilation and evaluation for fusion were reviewed using priority lists from the last DCN Meeting. The new list was generated by removing data needs that have been fulfilled, keeping those that have not been fulfilled, and adding new data requirements. There was also some agreed-upon merging and splitting of some collision categories and the elimination of some previous needs now deemed to be redundant or irrelevant. Suggested corrections and modifications have been collected and compiled by Denis Humbert. The adjusted and updated data priorities that were identified and discussed during Session 2 are summarized in Appendix 3 below.

DANSE Processes Classification

The purpose of this topic is to review the prepared document on "DANSE Processes Classification" (e.g. Appendix 4) and to define a "recommended" classification of processes to be used by DANSE.

DANSE is a web search engine for atomic and molecular bibliographical data. DANSE simultaneously retrieves data on collision processes, plasma-surface interactions and properties of atoms and molecules from the 3 well-known bibliographic databases:

- 1. AMBDAS at the IAEA: http://ripcrs01.iaea.or.at/AMBDAS/
- 2. GAPHYOR at LPGP: http://gaphyor.u-psud.fr/gaphyor/gaphyor.html
- 3. CFADC Biblio Search: http://www-cfadc.phy.ornl.gov/bibliography/search3.html

To make this search engine efficient, a classification of processes is needed. First all the processes for the three available databases have been reviewed and distributed into 5 majors categories (some categories like "macroscopic properties", "bibliographic data", are not considered in this first version of DANSE):

- Electron-Heavy Particle Interactions
- Heavy Particle-Heavy Particle Interactions
- Photon-Heavy Particle and Field-Heavy Particle Interactions
- Particle-Matter Interactions
- Structure and Spectra

A "recommended" classification is defined to fit as well as possible the databases overview and the A+M physics needs. From this "recommended" column, the DANSE values have been defined to fit as well as possible a general search on each database.

Discussions took place on the recommended classification of processes and some changes were applied. The DCN committee agreed on the classification for the 2 first categories (electron-heavy particle interactions and heavy particle-heavy particle interactions). A test version of DANSE on these 2 categories will be online soon.

Plan of DCN activities for the near future

D. Humbert pointed out the difficulties to organize the DCN meeting and to contact representatives. This is due to the fact that the DCN list is not up to date. The list has been reviewed and new memberships one from Brazil and one for molecular data have been discussed. For data centres represented to the meeting, no problem arose. The following actions were decided:

- CRAAMD, Institute of Applied Physics & Computational Mathematics, Beijing, China. Dr. T. Kato, mentioned that Dr. Sun Yongsheng is now retired and Dr. Jum Yan replaced him. D. Humbert will contact him.
- Weizmann Institute of Sciences, A+M Data Center. Dr. Yu. Ralchenko mentioned that there are probably no more A+M data activities at Weizmann Institute. He will contact the Institute for confirmation.

- Efremov Institute, PMI Data Center. Dr. W. Eckstein will contact the Institute for further information about A+M data activities.

- TRINITI A+M Data Unit. Dr. A. Godunov, representative of TRINITI, is no more in the Institute. Dr. Yu. Martynenko will contact him for further information.

The proposition of two new memberships was also discussed.

- Dr. L. Machado was invited this year as an observer. His talk showed strong A+M data activities in different institutes and universities in Brazil. Dr. L. Machado will make a proposal for a Brazilian contribution to the next DCN meeting.

- During Session 3 on "Data Priorities" the participation of a new member with a focus in molecular data needs for fusion has been advised. Dr. U. Fantz (Institut fuer Physik, Universitaet Augsburg), specialist in this domain, was proposed. D. Humbert will contact her.

3. Session 4: Meeting Conclusion and Recommendations

3.1. Status of Data Generation and Priorities in Data Compilation and Evaluation

- It was concluded that some of the data needs and priorities presented at the 17th TM were still valid. A number of the data needs have now been satisfied, and some new data priorities have been identified. The current list of data priorities is summarized in Appendix 3. This updated list is to be re-posted on the A+M Data Unit webserver following the 17th AGM.

- The IAEA experts' meetings, consultants' meetings, coordinated research programmes and individual consultants make a significant contribution to the data evaluation and quality control effort. Communication of data needs takes place through web pages posted on the A+M Data Centre website, and through representation at comprehensive meetings such as ICAMDATA. In the past two years, use of short-term consultants (several from within the Data Centre Network) in collaboration with the Data Unit has proven effective in tackling problems in some system and software (GENIE, AMBDAS). Additionally, cross-institutional collaborations have been very useful in establishing new data sets.

3.2. Data Processing and Exchange

All A+M Data Centres that maintain web presentations have been very effective at delivering their own data. As discussed in Dr. Ralchenko's presentation one way to improve this exchange is to create a new exchange format in XML: AMDML, which is supposed to be a development of the old ALADDIN format. A working group was created to present this

new format at the next ICAMDATA. This group is composed of: D. Humbert, T. Kato, Y.J. Rhee, Yu. Ralchenko and D. Schultz.

GENIE has been online for 2 years, and its method of multiple searches and comparison of data from different web sites will probably become more important as shown by the monthly statistics done on GENIE. The test version of DANSE will be soon online. A new XML data format (AMDML) will improve a lot the efficiency of such engines.

3.3. Recommended Actions

The Advisory Group recommended the following actions be taken by the IAEA A+M Data Unit:

- Continue the efforts on the co-ordination of data compilation, evaluation and recommendation by the Data Centre Network members. In particular, Dr. L. E Machado from Brazil is invited to participate to the next DCN Meeting with the view to welcome Brazil as a new member. The participation of a new member with a focus in molecular data needs for fusion should be taken into consideration.

- Continue the development of atomic and molecular database search engines. Make the test version of DANSE (search engine for A+M bibliographic data) available on-line. Modify GENIE to search the KAERI spectral online database AMOS. To improve the efficiency of these search engines, requests to the different databases should be done simultaneously instead of sequentially as at present time.

- AMDML: Cooperate in the initiative to create a new data format for the exchange of fusion data using XML. A working group has been recommended for this purpose. A presentation of AMDML should take place at the next ICAMDATA conference in 2004.

- Strengthen the communication of identified data priorities in fusion research to DCN Members and others in the fusion research community on the world-wide-web**.** In particular, a representative from ITER should be invited to attend and rotate through future DCN meetings.

- Continue efforts on the coordination of data generation projects through the Coordinated Research Projects in order to meet the evolving A+M and PSI data needs of the fusion research community. In particular, plan to add two new CRPs. “Atomic and Molecular Data for Plasma Modeling” in 2004 and “Atomic data for heavy element impurities in fusion reactors” in 2005.

Appendix 1

IAEA Technical Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(17th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

6-7 October 2003, IAEA Headquarters, Vienna

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Appendix 2

IAEA Technical Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(17th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

6-7 October 2003, IAEA Headquarters, Vienna

Meeting Agenda

Monday, October 6 **Meeting Room: F-0118**

09:30 - 09:45 Opening (N. Ramamoorthy, Director, Division of Physical and Chemical Sciences, NAPC, R.E.H. Clark, Head, A+M Data Unit)
Adoption of Agenda

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

Chairman: W. Eckstein

09:45 - 10:45 Reports from Data Centres:
W. Wiese (NIST), T. Kato (NIFS)

10:45 - 11:15 ***Coffee break***

11:15 - 12:15 Reports from Data Centres:
D.R. Schultz (ORNL), H. Kubo (JAERI)

12:15 - 13:45 ***Lunch***

Session 1. (Cont'd.)

Chairman: T. Kato

13:45 - 14:45 Reports from Data Centres:
Yu.V. Martynenko (Kurchatov Institute), L. Machado (Univ. de Sao Carlos)

14:45 - 15:15 ***Coffee break***

15:15 - 16:45 Reports from Data Centres:
J. Bretagne (GAPHYOR), E. Menapace (ENEA), Y. Rhee (KAERI)

Tuesday, October 7

Session 1.	(Cont'd.)
Chairman:	Y. Rhee
09:00 - 10:00	Reports from Data Centres: W. Eckstein (MPIP), R.E.H. Clark (IAEA)
Session 2.	Interfaces and web tools
10:00 - 10:30	Yu. Ralchenko (NIST) "New Databases Web Tools"
10:30 - 11:00	***Coffee break***
11:00 - 12:30	Data Centre WWW and software demonstrations
12:30 - 14:00	***Lunch***
Session 3.	Data Issues
Chairman:	W. Wiese
14:00 - 15:00	Priorities in A+M data compilation and evaluation (all participants)
15:00 - 15:30	DANSE processes classification
15:30 - 16:00	***Coffee break***
16:00 - 16:30	Plan of DCN activities for the near future (coordination: R.E.H. Clark and D. Humbert)
Session 4:	Meeting Conclusions and Recommendations
Chairman:	D. Humbert
16:30 - 17:00	Formulation of meeting conclusions and recommendations
17:00 -	***Adjourn of the Meeting***

Appendix 3

Priorities in Data Compilation, Evaluation and Generation for Fusion Research

Reviewed by Denis Humbert, 8 October 2003

The long-term priorities in A+M and PMI data compilation, evaluation and generation, were reviewed during the IAEA Technical Committee Meeting on "A+M Data for Fusion Reactor Technology" held in October 12-16, 1992 in Cadarache, France (IAEA Report **INDC(NDS)-277** and "Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion", R. K. Janev and H. W. Drawin, editors, Elsevier Science Publishers B.V., Amsterdam, 1993).

Data priorities were also identified and reviewed at four IAEA Advisory Group Meetings (now called Technical Meetings) held on 6-7 October 2003 (IAEA Report **INDC(NDS)-450**), on 11-12 September 2001 (IAEA Report **INDC(NDS)-430**), on 13-14 September 1999 (IAEA Report **INDC(NDS)-410**), on 21-22 July 1997 (IAEA Report **INDC(NDS)-377**) and, on 10-11 July 1995 (IAEA Report **INDC(NDS)-339**).

Atomic and Molecular Data

Spectroscopic Data

- Transition probabilities for neutral Be, B and their ions. Na, Mg, Si and S are done. Others are in the planning stage by NIST ASDC.

- Energy levels, wavelengths, transition probabilities for low-q metallic ions, high-Z impurities [V (no data), W (almost finished by NIST ASDC)] especially the low ions for divertor applications.

- Updating and compilation of spectroscopic databases for Be^{q+} and B^{q+} ions. Some work done and is in plans by NIST ASDC. Some work has been done for H- and He- like.

- Complete spectroscopic characterization of Ne and Ar ions, particularly the high ions of Ne. Ne almost done. Compilation of Xe desired and neatly done. Data for Kr ions are also desired.

- Spectroscopic characterization of H_2, H_2*, H_2^+, H_3^+ and isotopic variants. Impurity plasma edge molecules (CO, CO_2, CH_4, CH, CO and other hydrocarbons and radicals). The HITRAN database at Harvard CFA has some of this data. These are identified data needs that would require expanded capabilities for this DCN.

Collisional Data for Plasma Edge Studies

This section includes neutral particle transport modeling and diagnostics, H-recycling and He-exhaust. All the molecular data are needed for different hydrogen isotopes, including mixed molecules like DT.

- Elastic and momentum transfer ion-neutral and neutral-neutral collisions in the energy range 0.1 eV - 1 keV/amu, involving H, H^+, He, He^+, He^{2+}, H_2 and H_2^+. Some

combinations, e.g. He^{+} + $He^{2+\ +}$ on He, H2 still not done. Excited states and higher energies still need to be done.

- Ro-vibrational electronic excitation and attachment for D_2, T_2, DT

- Elastic collisions, charge transfer, inelastic collisions of H, H_2, H^+, H_2^+, H_3^+ with H_2 at low and intermediate energies (0 to 10 keV)

- Electronic excitation and ionization of vibrationally excited $H_2^*(v)$ and $H_2^+(v)$ in low-energy collisions with e (including dissociative processes and information on energy distribution of reaction products). Molecular Processes in Fusion Plasmas CRP (initiated in 2001) has produced initial work on cross sections for H_2^+. The rate coefficients for dissociation of H_2*(v) are calculated (NIFS-DATA-73).

- Electronic excitation and ionization of vibrationally excited $H_2^*(v)$ and $H_2^+(v)$ in low-energy collisions with H, H^+ and H_2^+ (including dissociative processes and information on energy distribution of reaction products). Molecular Processes in Fusion Plasmas (initiated in 2001) to address some of this. Work is going on with the excited ions and impinging H ions.

- Inelastic electronic collision processes of He, He^+, He^{2+} and excited states of H, He and H_2 at low energies. Molecular processes CRP (initiated in 2001) to address some of this.

- Inelastic collision processes of He, He^+ and He^{2+} with H, H^+, H_2, H_2^+ at low energies, including processes with excited H, He and H_2. Molecular processes CRP (initiated in 2001) to address some of this.

- Completion of collisional databases for Be, B and their ions (including collision processes of Be^{q+}, B^{q+} with electrons, and quasi-resonant processes of Be^{q+}, B^{q+} with H, He and H_2).

- Further development of the databases for hydrocarbons, H_2O and CO, and Be-, B-oxides and hydrides (including their ions). For hydrocarbons, all processes with electrons and protons should be considered including vibrational excitation and the effect of this excitation on the dissociation processes, as vibrational excitation might affect dissociation. Particle interchange reactions among primary species, C, O, metals and hydrocarbons. Data published for electronic collisions, CRP on "Molecular Processes" adding considerable data for hydrocarbons. NIFS and FZ Julich Reports on hydrocarbons.

- Collision processes of high-Z impurities in priority order (W, Mo, V, Ga) with e, H^+, H, H_2. IAEA AGM or CRP needed to establish data.

Collisional Data for neutral particle beam heating

- Data for collision processes of the ions H_2^+, H_3^+ with e, H, H^+, H_2, H_2^+, He^{2+}

- Data for collisional processes H^- on (H^-, e, H, H_2, H_2^+) in ion beam used (after neutralization) for plasma heating. (Pertinent energy range: from threshold to 15eV). Data needed for loss mechanisms in beams.

Radiative Plasma Cooling

Plasma core region

- Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (X = Ti, Ni, Cr, Fe, Mo, W, Ga, V) (Pertinent energy range: from a few keV to 30 keV). A large amount of data exists for Ti and Fe, but dielectronic recombination rate coefficients are not adequate for L-shell and M-shell ions even for Fe.

Plasma edge region

- Charge exchange collisions of X^{q+} (X as above) with H, H^+ and He^{2+} (Pertinent energy range: from 1 eV (or threshold) to 500 eV), particularly complete and consistent data sets. Collisions of X^{q+} (q >= 5, X as above) with H, He, H_2, including state- selective electron capture.

- All processes of Kr, Ne, Ar and Kr-ions with e, H, H^+, H_2, H_2^+, He^+, He^{2+} and H^- (for the proposed Kr, Ne, Ar radiative cooling scheme of divertors). Paper in preparation on N_2.

- Complete collisional database for N, N_2, Ne and Ar (for divertor radiation enhancement).

Plasma-Material Interaction

Disruption erosion

- Assessment of data needed for Be, carbon-based materials and medium- and high-Z materials (Ti, V, Mo, Nb, W, BeO). Data on sputtering yields of Ti, V, Mo and Yb? are partly available.

- Sputtered energy (to allow the determination of the mean energy of sputtered atoms).

Tritium retention and release in fusion materials and codeposited layers

- D/T permeability, diffusivity, solubility, desorption rate and surface reactions. Materials: tungsten, beryllium, BeO, Mo, new CFC's, deposited and codeposited layers of these materials. Data on traps in materials. IAEA CRP initiated in 2002 (Tritium Inventory in Fusion Reactors). Work underway in CRP on variety of materials

Molecular balance on surfaces

- Molecule (molecular ion) formation and destruction with identification of product charge and quantum state. Data for H^- formation on surfaces, particle sticking, pumping, gettering, and recycling.

- Mean range of impinging particles (and deposition profiles) would give information on the disturbed target region.

Material Properties

Data collection and generation needed

- Data for dust formation at disruption, C, Be, W, Mo.

Appendix 4

Classification of Processes
Version 1.2, 7 October 2003
Yuri Ralchenko and Denis Humbert

Categories

ORNL	IAEA	GAPHYOR	RECOMMENDED/DANSE
Heavy Particle-Heavy Particle Interactions	Heavy Particle Collisions	Atomic and Molecular Collisions	**Heavy Particle-Heavy Particle Interactions**
Interactions of Atomic Particles with Fields	Interactions of Atomic Particles with Fields		**Photon-Particle and Field-Particle Interactions**
Electron and Particle Penetration in Macroscopic Matter	Surface Interaction		**Particle-Matter Interactions**
Heavy Particle Interactions with Solid Surfaces	Surface Interaction		**Particle-Matter Interactions**
Electron-Heavy Particle Interactions	Electron Collisions	Collisions of Electrons	**Electron-Heavy Particle Interactions**
Photon Collisions with Electrons and Heavy Particles	Photon Collisions	Photonic Collisions	**Photon-Particle and Field-Particle Interactions**
Data Compilations	Data collection, bibliographic and progress report		**Data Compilations**
Reviews and Books			
Bibliographies	Data collection, bibliographic and progress report		**Bibliography**
	Structure and Spectra	Structures	**Structure and Spectra**
		Macroscopic Properties	
	Beam heating and fueling of plasmas		**Particle-Matter Interactions**
	Beam-Matter interaction		**Particle-Matter Interactions**
	Fusion research of general interest		
	Plasma diagnostics		
	Plasma composition, Impurities		
	Plasma heating, cooling, fueling		
	Plasma radiation and cooling		
	Plasma theory, models		

Electron-Heavy Particle Interactions
Recommended category code: **E**

SUBCATEGORY	IAEA	ORNL	GAPHYOR	DANSE	RECOMMENDED	PROCESS
General	GE	E01		**none**	**EGN**	
Angular Scattering	EG	E17	SC	**EAS**	**EAS**	
Bremsstrahlung	EB	E11	BS	**EBS**	**EBS**	$e+A \rightarrow e+A+h\nu$
Deexcitation	ED	E07	DX	**EDX**	**EDX**	$e+A^* \rightarrow e+A$
Elastic Scattering	EE	E02	EL	**EEL**	**EEL**	$e+A \rightarrow e+A$
Line Broadening, Shapes and Shifts	EL	E08		**ELB**	**ELB**	
Total Scattering	ES		SN	**ETS**	**ETS**	
Detachment	ET	E13	DT	**EDT**	**EDT**	$e+A^- \rightarrow A+2e$
Fluorescence	EU	E16	ER	**EFL**	**EFL**	
Excitation	EX	E03	EX	**EEX**	**EEX**	$e+A \rightarrow e+A^*$
Change of Excitation			XX	**See EEX**	**See EEX**	
Ionization	EZ	E05	IN	**EIN**	**EIN**	$e+A \rightarrow e+A^+ +e$
Multiple Ionization				**See EIN**	**EMI**	$e+A \rightarrow A^{+n}+(n+1)e$
Negative Ion Formation	EA	E09	AT	**ENI**	**ENI**	$e+A \rightarrow A^-$
Momentum Transfer		E19		**EMT**	**EMT**	
Transport CS's (momentum,…)			SM	**See EMT**	**See EMT**	
Unknown Products			PR	**none**	**EUP**	
Depolarization, Change of Polarization			DO	**EDP**	**EDP**	
Creation of an ion pair (positive-negative)			IM	**EIP**	**EIP**	$e+AB^+ \rightarrow A^-+B^-$
Recombination (general)	ER	E06	RC	**ERC**	**ERC**	$A^{+q}+e \rightarrow A^{+(q-1)}$
Radiative Recombination			RR	**See ERC**	**ERR**	$e+A^+ \rightarrow A+h\nu$
Dielectronic Recombination			RD	**See ERC**	**ERD**	$e+A^+ \rightarrow A^{**} \rightarrow A^*+h\nu$
3-body Recombination			RE	**See ERC**	**ERT**	$e+e+A^+ \rightarrow A+e$
e-i-o Recombination			RO	**See ERC**	**ERO**	$e+A^++B \rightarrow A+B$
Dielectronic Capture				**EDC**	**EDC**	$e+A^+ \rightarrow A^{**}$
Dissociation	EC	E04	DS	**EDS**	**EDS**	$e+AB \rightarrow e+A+B$
Dissociative Recombination			RS	**EDR**	**EDR**	$e+AB^+ \rightarrow A+B$
Dissociative Attachment	EA		AT	**EDA**	**EDA**	$e+AB \rightarrow A+B^-$
Dissociative Excitation				**EDE**	**EDE**	$e+AB \rightarrow A^*+B+e$
Dissociative Ionization				**EDI**	**EDI**	$e+AB \rightarrow A^+ +B+2e$

Photon-Particle and Field-Particle Interactions
Recommended Category Code: **P**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	DANSE	RECOMMENDED	PROCESS
General				**PGN**	**PGN**	
Total Absorption, Scattering	PA	H02		**PTS**	**PTS**	
Photodissociation	PD	H05	DS	**PDS**	**PDS**	$h\nu+AB \rightarrow A+B$
Elastic Scattering	PE	H03		**PES**	**PES**	$h\nu+A \rightarrow h\nu+A$
Multiphoton Absorption (excitation and ionization)	PM			**PMA**	**PMA**	$nh\nu+A \rightarrow A^*(A^+)$
Photodetachment	PT	H07	DT	**PDT**	**PDT**	$A+B \rightarrow AB+h\nu$
Fluorescence	PU	H08		**PFL**	**PFL**	
Photoexcitation	PX	H04	EX	**PEX**	**PEX**	$h\nu+A \rightarrow A^*$
Photoionization	PZ	H06	IN	**PIN**	**PIN**	$h\nu+A \rightarrow A^++e$
Free-Free Absorption or Inverse Bremsstrahlung	FF	H11	FF	**PFF**	**PFF**	$h\nu+e+A \rightarrow e+A$
Effective Absorption, Total Diffusion			SN	**PEA**	**PEA**	
True Absorption			AN	**PTA**	**PTA**	
Angular Diffusion (scattering)			SC	**PAD**	**PAD**	
Elastic Diffusion (Thomson, Rayleigh)			EL	**PED**	**PED**	
Depolarization, Change of Polarization			DO			
Non-linear Effects			NL	**PNL**	**PNL**	
Emission of Line			ER			
Change of Excitation			XX			
Zeeman Effect				**PZE**	**PZE**	
Stark Effect				**PSE**	**PSE**	
General Electromagnetic Field				**PGF**	**PGF**	
Interaction with Time-Varying Fields				**PTF**	**PTF**	
Creation of an Ion Pair (positive-negative)			IM			

Heavy Particle-Heavy Particle Interactions
Recommended Category Code: **H**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	DANSE	RECOMMENDED	PROCESS
General		A01			**HGN**	
Association	HA	A15	AS	**HAS**	**HAS**	$A+B \rightarrow AB$
Line Broadening, Shapes and Shifts	HB	A12		**HLB**	**HLB**	
Dissociation	HC	A04	DS	**HDS**	**HDS**	$A+BC \rightarrow A+B+C$
Deexcitation	HD	A11	DX	**HDX**	**HDX**	$A^*+B \rightarrow A+B$
Elastic Scattering	HE	A02	EL	**HES**	**HES**	$A+B \rightarrow A+B$
Charge Transfer	HF	A06	CX	**HCX**	**HCX**	$A^++B \rightarrow A+B^+$ $A^-+B \rightarrow A+B^-$
Unknown Products					**HUP**	
Angular Scattering	HG	A18	SC	**HAS**	**HAS**	
Interchange Reactions	HI	A14	IR	**HIR**	**HIR**	$A+BC \rightarrow AB+C$
Inelastic Energy Losses	HL			**HEL**	**HEL**	
Energy Transfer	HN	A10		**HET**	**HET**	
Interaction Potentials	HP	A17		**HIP**	**HIP**	
Recombination	HR	A09	RI	**HRC**	**HRC**	
Total Scattering	HS			**HTS**	**HTS**	
Detachment	HT	A16	DT	**HDT**	**HDT**	$A+B^- \rightarrow Abe$
Fluorescence	HU	A05		**HFL**	**HFL**	
Excitation	HX	A03	EX	**HEX**	**HEX**	$A+B \rightarrow A^*+B$
Ionization	HZ	A07	IN	**HIN**	**HIN**	$A+B \rightarrow A+B^++e$
Penning Ionization				**HPN**	**HPN**	$A^*+B \rightarrow A+B^++e$
Stripping (of projectile)		A08	SR	**HST**	**HST**	$A+B \rightarrow A^++B+e$
Attenuation		A20		**HAT**	**HAT**	
Excitation Transfer			TE	**HXT**	**HXT**	$A^*+B \rightarrow A+B^*$
Associative Interchange Reactions			IA	**HAI**	**HAI**	
Dissociative Interchange Reactions			ID	**HDI**	**HDI**	
Dissociative Charge Transfer			XD	**HDC**	**HDC**	$A^++BC \rightarrow A+B^++C$
Mutual Ion-Ion Neutralization				**HMN**	**HMN**	$A^++B^- \rightarrow A+B$

Structure and Spectra

Recommended Category Code: **S**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	RECOMMENDED	DANSE
General				**SGN**	**none**
Line Broadening, Shapes and Shifts	B	B01 E08 A12		**SLS**	**SLS**
Interatomic Potentials	I			**SIA**	**SIA**
Polarizabilities, Electric Moments	P		PE	**SPM**	**SPM**
Energy Levels and Wavelengths	S		EN	**SEW**	**SEW**
Transition Probabilities and Oscillator Strengths	T		TR	**STP**	**STP**
Potential Curves and Structure of Molecules		A17	VR	**SSM**	**SSM**
Dynamic Polarizability			PF	**SDP**	**SDP**
Infrared Spectra				**SIR**	**SIR**
Visible Spectra				**SVS**	**SVS**
UV/VUV/XUV Spectra				**SUV**	**SUV**
X-Ray Spectra				**SXR**	**SXR**
Rotational Spectra				**SRS**	**SRS**
Vibrational Spectra				**SVB**	**SVB**
Autoionization			IN	**SAI**	**SAI**
Autodetachment			DT	**SAD**	**SAD**
Autodissociation			DS	**SDS**	**SDS**
Dipolar Moments			DP		
Multipolar Moments			NP		
Magnetic Moments				**SMM**	**SMM**
Hyperfine Structure				**SHF**	**SHF**
Isoelectronic Sequences				**SIE**	**SIE**
Forbidden Transitions				**SFT**	**SFT**
QED Effects				**SQE**	**SQE**
Relaxation Processes				**SRP**	**SRP**
Ionization Potentials				**SIP**	**SIP**
Rydberg States				**SRY**	**SRY**
Energy of Isomerization			EI		

Particle-Matter Interactions

Recommended Category Code: **M**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	RECOMMENDED	DANSE
General				**MGN**	**none**
Accomodation	AC			**MAC**	**MAC**
Adsorption	AD		AD	**MAD**	**MAD**
Chemical Reactions	CR			**MCR**	**none**
Desorption	DE		DG	**MDE**	**MDE**
Surface Interactions	GM			**none**	**none**
Reemission	RE			**MRE**	**MRE**
Reflection	RF			**MRF**	**MRF**
Surface Damage	SD			**MSD**	**MSD**
Secondary Electron Emission	SE	D04	EE	**MSE**	**MSE**
Radiation Induced by Particle Impact on Surfaces		D12		**MIR**	**MIR**
Neutralization, Ionization, Dissociation	SI			**MNE**	**MNE**
Sputtering	SP		SP	**MSP**	**MSP**
Radiation-Enhanced Sublimation				**MRS**	**MRS**
Trapping, Detrapping	TD			**MTD**	**MTD**
Photoelectric Ejection of Electrons			EE	**MPE**	**MPE**
Energy Loss and Stopping Power		C02	SP	**MEL**	**MEL**
Particle Range		C04		**MPR**	**MPR**
Multiple Scattering		C05		**MMS**	**MMS**
Charge State Population		C06		**MCP**	**MCP**
Excited State Population		C07		**MEP**	**MEP**
Reflection of Heavy Particles from Surfaces				**MRH**	**MRH**
Reflection of Electrons from Surfaces		D07		**MRL**	**MRL**

Data Compilations

Recommended Category Code: **D**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	RECOMMENDED
General				**DGN**
Electron-Heavy Particle Interactions		J02		**DEH**
Heavy Particle-Heavy Particle Interactions		J03		**DHH**
Photon-Particle and Field-Particle Interactions		J01		**DPF**
Structure and Spectra		J04		**DSS**
Transport Properties		J05		**DTP**
Particle-Matter Interactions		J06		**DPM**

Bibliography

Recommended Category Code: **B**

SUBCATEGORIES	IAEA	ORNL	GAPHYOR	RECOMMENDED
General				**BGN**
Electron-Heavy Particle Interactions		L02		**BEH**
Heavy Particle-Heavy Particle Interactions		L03		**BHH**
Photon-Particle and Field-Particle Interactions		L01		**BPF**
Structure and Spectra		L04		**BSS**
Transport Properties		L05		**BTP**
Particle-Matter Interactions		L06		**BPM**

Appendix 5

Data Centre Reports of Activities

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usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL.
NDSONL for FTP access to files sent to NDIS “open” area.
Web: http://www-nds.iaea.org