International Atomic Energy Agency

INDC(NDS)-294

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (12th Meeting of the A+M Data Centres and ALADDIN Network)

20-21 September 1993, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared By J. Botero

January, 1994

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (12th Meeting of A+M Data Centres and ALADDIN Network)", held on September 20-21, 1993, in Vienna is briefly described. The meeting conclusions and recommendations on the priorities in A+M data compilation, evaluation and generation and on the technical aspects of data processing and exchange are also presented.

Reproduced by the **IAEA** in Austria
January, 1994
94-00411

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1 Introduction

On September 20-21, 1993, the IAEA organized the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing (12th 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, the developings in the ALADDIN system, and to co-ordinate the working plans for the next period. The meeting was attended by 16 participants and one observer from 15 data centres (**see Appendix 1**). The participant form the Belfast Queen's University A+M Data Centre (Prof. F. J. Smith) was not able to attend the meeting, but sent a report of activities of the data centre. The Max-Plank-Institute für Plasmaphysik (Garching) and the D.V. Efremov Institute of Electrophysical Apparatus (St. Petersburg) were represented for the first time at this series of Advisory Group Meetings.

2 Meeting Proceedings

The Meeting was opened by **Dr. C. L. Dunford**, Head of the Nuclear Data Section. He stressed the importance of having ALADDIN as the international format for data exchange and the convenience, mainly due to financial considerations, of the Data Centre Network (DCN) to address A+M data needs outside fusion related projects. After adopting the Agenda (**see Appendix 2**), the meeting proceeded in four sessions:

1. Current activities of the A+M data centres,
2. Priorities in A+M data compilation and evaluation,
3. Data processing and exchange,
4. Meeting conclusions and recommendations.

2.1 Session 1: Current Activities of the A+M Data Centres (Chairmen: Drs. Abramov, Wiese, Tawara)

In Session 1, progress reports on the activities of individual data centres during the period June 1992 - September 1993 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, the data centres publications during the reporting period, the status of ongoing programmes and the plans for immediate future work in this area. The presentations in this session have demonstrated that the data centre activities closely follow the recommendations of the previous Advisory Group Meeting, both in terms of content and mutual co-operation.

The session started with the presentations of **Dr. W. L. Wiese** (NIST) and **Dr. A. Ya. Faenov** (VNIIFTRI), who described the ongoing work on establishing spectroscopic data bases in their respective centres. **Dr. Wiese** reported recent work on compilation and evaluation of data for wavelengths of OII, S, V and Cr; for energy levels of OII, S, V, Cr and Ge; and transition probabilities of the ions of C, N and O. Work in progress in his data centre includes data compilation and evaluation for the wavelengths of SiI, NeI and Mn; the energy levels fo SiI, Mn, Zn and Kr; and the transition probabilities of additional (not covered above) ions of C, N and O and extension to Li, Be and B. **Dr. Faenov** described the ongoing spectroscopic data compilation, evaluation and generation work at VINIITFRI (and collaborating institutions), and the structure and scope of the data base SPEKTR. About 340,000 records are contained in the data base, including now about 6000 A+M collisional data for electron impact processes (excitation, ionization and dielectronic recombination). Recent work on high performance X-ray spectroscopy of plasma microsources was also reported, as well as recent A+M data compilation and ALADDIN formatting.

The session continued with the presentation of **Dr. C. Havenner** from ORNL, CFADC. He reported on the continued bibliographic data compilation, the generation of elastic heavy-particle cross sections, the preparation of the Vol. 2 of the Red Book Series (in collaboration with JILA and NIST) and the progress towards establishing on-line access to the bibliographic data base and ALADDIN formatted numerical A+M data bases. The CFADC will in the near future install a HP 755 UNIX workstation, using INGRES as the data base management system. The interface developed by J. T. Broad at JILA will be used. **Dr. Tawara** from NIFS, Nagoya, reported on the recent A+M data compilation, evaluation and recommendation activities, which include: differential and total cross sections for scattering of electrons by helium atoms, cross sections for impurity (C^{q+}, O^{q+} Be^{q+}, B^{q+}) ions, data compilation for molecular species relevant to edge plasmas, new data for hydrocarbon molecules, electron impact excitation of N atoms and N-like ions, and on-going work on a collisional radiative model for highly excited species. **Dr. E. Menapace** (ENEA NDC Data Unit, Bologna) reported on evaluation of molecular spectroscopic data obtained with algebraic methods, such as the Vibron Model, and on comparison with other *ab initio* methods and experimental results. Specific results were reported for the triatomic molecules HCO and DCO. Results of a calculation of particle and energy reflection coefficients of slow protons with an iron surface were also reported.

New developments on the GAPHIOR data base were reported by **Dr. J.L. Delcroix** (GAPHIOR, Orsey). The data base is being moved to a UNIX workstation, using the ADABAS software. Several new features and descriptors were reported, such as: new format of the GAPHIOR UPDATE, new descriptors for gas(plasma)-surface interactions, expanded field of authors (up to 10), and others. The data activity of the A+M data centre at the Kurchatov Institute, Moscow, was presented by **Dr. V. A. Abramov**. The main activities reported are: collection of the A+M bibliography from Russian publications, compilation of cross sections for processes involving Ga, Be, C and B ions, calculations of the radiative cooling rates for Be-seeded plasmas, evaluation of excitation cross sections for different metallic ions, electron impact excitation cross sections of Be ions and hydrogen retention and release in carbon graphite materials. The progress report on the A+M activities at the Chinese Nuclear Data Centre (Beijing) was presented by **Dr. Jinzhang**

Yao. This activities include the evaluation and compilation of physical sputtering data of plasma facing materials by light projectiles H^+, D^+, T^+ and He^+, and the generation and evaluation of particle reflection coefficients from solid surfaces using the PANDA-U code.

The Max-Plank Institute für Plasmaphysik was represented for the first time in a A+M Data Centre Network meetings. **Dr. W. Eckstein** reported on data production, collection and evaluation at MPIPP. The main area of the data activities at MPIPP are kinetic reflection and sputtering. Both types of data are investigated experimentally and by computer simulation. Particle and energy reflection coefficients for a large number of projectile-target combinations over a wide rage of energies and angles were reported. Sputtering yield data for a large number of target-projectile combinations for normal and oblique incidence were also reported. A new analytical fit, the revised Bohdansky formula with the Yamamura formula for oblique incidence, was shown to give accurate sputtering yields over a wide range of energies. **Dr. J. T. Broad** reported on the A+M activities at the Atomic Collision Data Center (JILA, Boulder). The main ongoing projects at the data center are: modification of the gas laser database, critical review of atomic data for the argon reference gas discharge cell, collisional alignment and orientation of atomic outer shells and the red book on electron-impact excitation and ionization (in collaboration with the ORNL data centre and the NIST Standard Reference data Programme). Dr. Broad described the newly developed data base interface used at the data centre, a user-friendly, menu-driven interface using the INGRES software. **Dr. Sun Yongsheng** presented the progress report of the A+M data activities at CRAAMD, Beijing. Compilation and ALADDIN formatting of collision strengths for electron impact excitation of Ne-like Ti, Fe, Se, Cu and Ge ions and F-like (Z=22-92) ions was reported. The CRAAMD group has also incorporated material properties in the ALADDIN structure. These are the Rosseland radiative opacities and the electron conductive opacities.

The session continued with the presentation of **Dr. K. Katsomis**, who reported ongoing work at the unit of Atomic Physics of Fusion Plasmas (PAPF) of the Laboratory of Gases and Plasma Physics (LPGP). A+M data activities include the evaluation of ion-atom collision cross sections of interest to fusion, total for ionization and partial (n,l resolved) for excitation, and generation of cross sections using the Classical Trajectory Monte Carlo (CTMC) method . A new data storage system is being developed at PAPF, which can be directly translated into ALADDIN format. The data available in this system, the software implementation necessary for its storage and retrieval were presented. The report of the A+M activities at the Nuclear data center of the Japan Atomic Energy Research Institute was presented by **Dr. T. Shirai**. Ongoing work on the preparation of the 4th edition of the Evaluated Atomic and Molecular Data Library (JEAMDL-4) was reported. This includes analytical least squares fits to the recommended cross sections of the ORNL Red Book Vol. 1 for total and partial electron capture collisions of H, H_2, He and Li atoms and ions with atoms and molecules, the compilation of measured cross sections for single-, double-, and triple-electron capture for carbon ions passing through different gases, and critical evaluation of spectroscopic data of interest to fusion. **Dr. V. R. Barabash** presented the report of the computer data base for fusion materials at the D. V. Efremov Institute of Electrophysical Apparatus (St. Petersburg). This was the first time that this data centre was present at a Data Centre Network meeting. Dr. Barabash presented the main objectives of the centre, and its data activities related to material properties for fusion reactor materials. A new interface for ALADDIN is being developed (in collaboration with the IAEA), the main features of which were presented at the meeting. These include a user-friendly, menu-driven system to search and open files , graphical capabilities and a tree-type structure of hierarchical labels. A set of hierarchical and boolean labels for material properties was presented as well as a preliminary data base for beryllium.

At the end of this session **Dr. J. Botero** (IAEA, A+M Data Unit) presented the report of activities of the IAEA A+M Data Unit. The activities were divided into three areas: data base development, data evaluation and recommendation and co-ordinated research projects. In the first area, the establishment of AMDIS (Atomic and Molecular Data Information System) was reported. AMDIS currently contains an on-line service for ALADDIN, with a new interface being developed for a more efficient and simple handling of data files by remote users. It is envisaged that AMDIS will contain in the near future the IAEA Bibliographic Data Base and a A+M and PSI Computer Code Library. The efforts of the IAEA A+M Data Unit on data base development have been concentrated mainly on AMDIS. In the data evaluation and recommendation area, the final handbooks for "Cross sections for collision processes of hydrogen atoms with electrons, protons, and multiply charged ions" and "An evaluated data base for sputtering" were presented. Ongoing work on the He- and Li-beam penetration, Be and B, particle interchange reactions, material properties, and plasma-surface interaction induced erosion data bases were reported. Finally a summary of the current and planned co-ordinated research programmes on A+M, PSI and material properties data was presented.

2.2 Session 2: Priorities in A+M, PSI and Materials Data Compilation and Evaluation (Chairman: Dr. Barabash)

Session 2 was dedicated to discussing the priorities in A+M, PSI and material properties data compilation and evaluation. The session started with a short presentation by **Dr. R. L. Langley** (IAEA A+M Data Unit), who presented a summary of the priorities of materials data generation and evaluation and the actions being taken by the IAEA A+M Data Unit in those regards. It included the recommendations of recent IAEA meetings on the co-ordinated research programmes: "Plasma-Interaction Induced Erosion of Fusion Reactor Materials", "Collection and Evaluation of Reference Data on Thermomechanical Properties of Fusion Reactor Plasma Facing Materials" and "Tritium Retention in Fusion Reactor Plasma Facing Components". **Dr. R. K. Janev** (IAEA A+M Data Unit) presented a report on the status of A+M data for ITER, which summarized the conclusions and recommendations of the IAEA Technical Committee Meeting on "Atomic and Molecular Data Needs for Fusion Reactor Technology", Cadarache, France, October 12-16, 1992 (see **Appendix 4**). It included the ITER EDA status, ITER divertor concept selection, particle and power control issues, and A+M data for disruption erosion modelling and

ITER diagnostics. After some discussion, the advisory group arrived at the conclusions and recommendations presented in Section 3.3.

2.3 Session 3: Data Processing and Exchange (Chairman: Dr. Delcroix)

This Session was devoted to a discussion on the ALADDIN implementation, developments and future DCN activities. A list of points for discussion was distributed to all participants (see **Appendix 5**). There were open discussions on all points, with contributions from all meeting participants. There was a consensus regarding the yearly frequency of the DCN meetings, especially for the following years, since many data centres are developing new systems and the ITER data needs are evolving rapidly. The ALADDIN data format is recognized as the internationally accepted format for atomic, molecular, particle-surface interaction and material properties data exchange among data centres themselves and among data centres and the fusion community. The on-line service now available at the IAEA was regarded as very important, and it was agreed that efforts of the IAEA A+M Data Unit regarding data base management should be concentrated on this service. Since most of the data centres are now moving to workstations, the need for a new PC version of ALADDIN is not as severe. Nonetheless, the IAEA A+M Data Unit is committed to have the C-interface finished in collaboration with Dr. Yushko from the Efremov Institute (St. Petersburg). Dr. Havener (ORNL) proposed having an electronic bulletin board with the latest news on data production and requirements. The IAEA A+M Data Unit agreed upon having such a bulletin board on AMDIS, available on-line and distributed by e-mail to all data centres and other interested parties.

The importance of the ALADDIN format for collaboration among different data centers was also stressed. These collaborative projects consist mainly of data processing, data distribution, and the preparation of special-purpose data bases. It was agreed that a quarterly report from all data centres will be circulated by e-mail among all data centres to improve the communication and make collaboration easier. The discussion ended with comments from different data centres regarding the possibilities of extending the areas of collaboration and data exchange of the DCN to non-fusion areas. Several data centres pointed out that, mainly due to financial constraints in the local fusion programme, they had already expanded their areas of work to environmental and health related applications. All data centres agreed on investigating the possibilities for such an extension.

It was also agreed that an editorial board for the International Bulletin on Atomic and Molecular Data for Fusion should be created, in order to oversee the publication of the bulletin.

3 Meeting Conclusion and Recommendations

The presentations and discussions at the Advisory Group meeting regarding the A+M, PSI and material properties data related activities in the A+M Data Centre Network and the IAEA A+M Data Unit, the data processing, management and exchange methodology, the ALADDIN system implementation and development, as well as regarding the priorities in A+M data compilation and evaluation work, have resulted in the following sets of conclusions and recommendations:

3.1 Conclusions

3.2 Status of Data Compilation and Evaluation Activities

1. The present level of A+M data compilation activity in the areas of spectroscopic and A+M collisional data has to be extended to satisfy the increasing and evolving data needs of ITER. The insufficient manpower and the scarcity of funds may hinder this activity. On the other hand, apart from the members of the A+M Data Centre Network, this activity is being carried out also by individual experts in relation with Agency organized meetings on specific topics, as well as within two ongoing Agency's Co-ordinated Research Programmes. The PSI and material properties data compilation efforts are currently still being done mainly in the fusion laboratories. With the participation of the IPP-Garching group (PSI data) and the Efremov Institute (material properties data), the DCN has strengthen itself to cover this important areas.

2. The Advisory Group is of the opinion that the present level of the data evaluation effort in all areas, A+M collisional, PSI iand material properties, data, is insufficient to respond to the growing needs of fusion research and reactor design work. The main reason for this is the lack of manpower and consultancy funds in the A+M Data Centre Network for data evaluation purposes. The IAEA experts' meetings, co-ordinated research programmes and individual consultants make a significant contribution to the data evaluation effort, but the size of this effort which is limited by the available Agency's resources, appears to be insufficient to change the situation. A stronger collaboration between the data centres should be beneficial in this respect. Enhancement of the evaluation activity, both in the A+M data centres and through the IAEA, is essential for meeting the A+M and PSI data needs of ITER EDA. Closer collaboration with the fusion community for identification of most urgently required data would also help in minimizing and better focussing the evaluation efforts.

3. The Advisory Group observes an increase of data generation activities in the A+M Data Centre Network. The strengthening of this effort, which strictly follows the demands of fusion researchers for A+M and PSI data, is highly encouraged.

3.3 Data Processing and Exchange (ALADDIN)

1. The implementation of ALADDIN in the data exchange among the A+M data centres can now be considered as well established. As for data base management, it seems more appropriate that each data centre develops its own system, depending on the hardware and software available. Compatibility is guaranteed by the fact that all data centres have an interface of their own system to ALADDIN formatted data. A good example is the system established at JILA by J. T. Broad using the INGRES software.
2. The development of the on-line version of ALADDIN is to be continued and finalized with a more user-friendly interface, as well as more information on the data available. The development of a graphical interface shell for ALADDIN, initiated by the IAEA, is to be finalized as soon as possible. These, and other recent developments of the ALADDIN structure (e.g. the sections on particle-surface interaction and material properties data), have to be included in the new version of ALADDIN Manual, to be prepared by the IAEA during 1994.
3. A bulletin board (on-line in AMDIS and distributed by e-mail) should be developed by the IAEA A+M Data Unit.
4. In order to improve the communication and data exchange among data centres, a quarterly report on the data related activities from all data centres will be circulated by e-mail.
5. An editorial board should be created among members of the DCN in order to oversee the publication of the International Bulletin on Atomic and Molecular Data for Fusion.

3.4 Priorities in Data Compilation, Evaluation and Generation

The long-term priorities in A+M and PMI data compilation, evaluation and generation, were throughout reviewed during the IAEA Technical Committee Meeting on "A+M Data for Fusion Reactor Technology" held in October 12-16, 1992 in Cadarache, France (see 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). Based on this review, the Advisory Group adopted the following priorities in the A+M, PMI and material properties data compilation, evaluation and generation:

1. Atomic and Molecular
   (a) Spectroscopic Data
      i. Transition probabilities for the He-, Li-, Be-, B-like isoelectronic ions.
      ii. Energy levels, wavelengths, transition probabilities for low-q metallic ions, high-Z impurities (Ga, V, Mo W) and for Kr, Si and Xe.

iii. Updating and compilation of spectroscopic data bases for Be^{q+} and B^{q+} ions (including publication in the ORNL "Red book" series).

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

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

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

iii. Electronic excitation and ionization of vibrationally excited $H_2^*(v)$ and $H_2^+(v)$ in low-energy collisions with e, H and H^+ (including dissociative processes and information on energy distribution of reaction products).

iv. 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.

v. 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).

vi. 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).

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

viii. Three-body processes among primary species and impurities.

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

(c) Radiative Plasma Cooling

i. Plasma core region

A. Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (Ti, Ni, Cr, Fe, Mo, W, Ga, V) (Pertinent energy range: from a few keV to 30 keV).

B. Charge exchange collisions of A^{q+} (A as above) with H, H^+ and He_2^+ (Pertinent energy range: from 1 eV (or threshold) to 500 eV).

ii. Plasma edge region

A. Electron impact processes involving low-, medium- and high-Z impurities in low charge states ($q \geq 5$). The most important low-Z impurities are Be and B. (For C and O the data base is in good shape).

B. Collisions of A^{q+} ($q \geq 5$) with H, He, H_2, including state- selective electron capture

C. All processes of Kr and Kr-ions with e, H, H^+, H_2, H_2^+, He, He^+, He_2^+ (for the proposed Kr^- radiative cooling scheme of divertors).

2. Plasma-Material Interaction
   (a) Physical sputtering: Data needed for: the threshold regime for self-sputtering, for grazing angles vs. surface roughness and surface composition changes, and for self-sputtering of Be and Li.
   (b) Chemical Sputtering in carbon-based materials: Data needed for yield dependence on flux, energy of molecules and surface composition.
   (c) Radiation enhanced sublimation (for carbon-based materials): Data needed for flux dependence and for the description of the loss of dopant at high temperature.
   (d) Thermal evaporation: Assessment of data needed for Be, carbon-based materials and medium- and high-Z materials (Ti, V, Mo, Nb, W)
   (e) 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).
3. Material Properties
   (a) Data generation
      i. Physico-mechanical properties of the new carbon fiber composites are needed.
      ii. Mechanical and post-irradiation physico-mechanical properties of Be and other plasma-facing components candidates are needed.
      iii. Physico-mechanical properties of new classes of materials, such as Ti-doped graphite, are needed.
      iv. Data on the effects on the physico-mechanical properties of material after neutron irradiation is essential.
   (b) Data evaluation and compilation
   Data evaluation and compilation is very important for new materials, such as CFC and Ti-doped materials. Existing databases need throughout evaluation.
4. The Advisory Group recommended that all data centers, including the IAEA Data Unit, investigated the possibilities of expanding the coverage of data compilation and evaluation to other nuclear, non-energy applications, such as human health, environmental and industrial. Some of the data centres (NIST, JAERI, ENEA) already have programmes in these areas.

3.5 Recommended Actions

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

1. Continue the efforts on the co-ordination of data compilation, evaluation and recommendation by the data centre network along the lines presented in the conclusions of this meeting (see previous section).
2. Strengthen its efforts on the coordination of data generation projects through its Co-ordinated Research Programmes in order to meet the evolving A+M, PSI and material properties data needs of the fusion community, specially of ITER.
3. Continue the maintenance and development of ALADDIN, including the on-line system AMDIS as well as the PC version. This includes the final version of the ALADDIN manual for the two versions and the formatting of new data files.
4. Implement an electronic bulletin board and an electronic newsletter to be circulated among the data centres. These should include information on new data bases, IAEA meetings and reports, and any changes or additions in the A+M, PSI and material properties data needs.
5. Co-ordinate the circulation (via e-mail) of a quarterly informal report of all members of the DCN among themselves.
6. Investigate the possibility of extending the scope of the Unit to include non-fusion applications of A+M data. Suggested areas are human health, environmental iand industrial applications.

Appendix 1

IAEA Advisory Group Meeting on

"Technical Aspects of Atomic and Molecular Data Processing and Exchange (12th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

20-21 September 1993, IAEA Headquarters, Vienna, Austria

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Appendix 2

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange (12th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

20-21 September 1993, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

Monday, September 20 — Room: A-07-42

09:30 - 09:45	- Opening (C.L. Dunford, Head NDS) - Adoption of Agenda
Session 1.	Current Activities of the A+M Data Centres
Chairman:	Abramov
09:45 - 10:45	Reports from Data Centres: Wiese (NIST), Faenov (VNIIFTRI)
10:45 - 11:00	**Coffee break**
11:00 - 12:30	Reports from Data Centres: Havener (ORNL), Tawara (NIFS), Menapace (ENEA)
12:30 - 14:00	**Lunch**
Session 1.	(Cont'd.)
Chairman:	Wiese
14:00 - 16:00	Reports from Data Centres: Delcroix (GAPHYOR), Abramov (Kurchatov Institute), Yao Jinzhang (IAE, Beijing)
16:00 - 16:15	**Coffee break**
16:15 - 17:45	Reports from Data Centres: Eckstein (Max-Planck, Garching), Broad (JILA), Sun Yongsheng (IAPCM, Beijing)

Tuesday, September 21

Session 1.	(Cont'd.)
Chairman:	Tawara
09:00 - 11:00	Reports from Data Centres: Katsonis (LPGP-Orsay), Shirai (JAERI), Barabash (Efremov Institute), Botero (IAEA)
11:00 - 11:15	**Coffee break**
Session 2.	Priorities in A+M, PSI and Materials Data Compilation and Evaluation
Chairman:	Barabash
11:15 - 11:35	PSI and Materials Data Base at IAEA (Langley)
11:35 - 12:00	Priorities in A+M Data Compilation and Evaluation Related to ITER, and other Possible Areas of Interest (Janev)
12:00 - 12:30	Demonstration of Software (Faenov, Botero)
12:30 - 14:00	**Lunch**
Session 3.	Data Processing and Exchange
Chairman:	Delcroix
14:00 - 15:30	ALADDIN Implementation and Developments; Possibilities for Technical Improvements: Comments from all Data Centres (all participants)
15:30 - 16:00	Plan of DCN Activities for the Near Future (Botero)
16:00 - 16:30	**Coffee break**
Session 4:	Meeting Conclusions and Recommendations
Chairman:	Botero
16:30 - 17:00	Formulation of Meeting Conclusions and Recommendations
17:00 -	**Adjourn of the Meeting**

Appendix 3

Data Centres Report of Activities

Activities of the Atomic Spectroscopy Data Centers at the National Institute of Standards and Technology (NIST)

1992/93

W.L. Wiese

	Data Center	Director	Workforce
1.	Atomic Energy Levels and Wavelengths	W.C. Martin	$2^1/_2$ Professionals
2.	Atomic Transition Probabilities	W.L. Wiese	2 Professionals
3.	Spectral Line Shapes and Shifts	W.L. Wiese	Occasional contractors, guests

Work Areas on Data Compilations

	Recent work	In Progress
Wavelengths:	OII, S, V, Cr	SiI, NeI, Mn
Energy Levels:	OII, S, V, Cr, Ge	SiI, Mn, Zn, Kr
Transition Probabilities:	Ions of C, N, O	Additional ions of C,N, O Extensions to Li, Be, B

Database work

1. Bibliographic databases (annotated):

   Energy levels and wavelengths, since 1985 Transition Probabilities since 1980

   Lineshapes, since 1978

   (ORACLE software, lineshapes accessible on Internet)

2. Numerical databases:

   General database with wavelengths, energy levels and transition probabilities (ORACLE software) developed and many data loaded into it.

   Also, another userfriendly database is developed for PC users. First edition in 1994 (?)

New NIST data publications (1992/93)

1. Wavelengths and Energy levels of SI through SXVI, JPCRD 22, 279 (1993)
2. Wavelengths and Energy levels of OI, JPCRD 22,1179 (1993)
3. Energy Levels of GeI through Ge XXXII, JPCRD 22, 1213 (1993)
4. Energy Levels of ZnI through Zn XXX, JPCRD (in press)
5. Tables of Spectra for H, C, N and O CRC Press, 336 pp. (1993)
6. Bibliography on Atomic Line Shapes and Shifts, NIST Spec. Publ. 366, Suppl. 4
7. Spectral Data and grotrian Diagrams for V (JPCRD 21, 273 (1992), for Cr (JPCRD 22, 1279 (1993) and Mn (in preparation) with JAERI

Progress Report On The A+M Data Researches

FOR 1992 / 93

Jinzhang Yao

Chinese Nuclear Data Center

China Institute of Atomic Energy

(1) Data on physical sputtering for light projectiles

We will completed the evaluation and compilation of physical sputtering data of light projectiles H^+,D^+,T^+,$He^+$and $^4He^+$onto certain impurities on candidate plasma facing component materials. We use the Bohdansky formula for the evaluated calculation of sputtering yields from threshold energies to 100 KeV. The sputter ing data of Carbon and Nickel targets by H^+,$D^+$and $^4He^+$projectiles have been shown in Figs 1–6. Our evaluated results compared with experimental measurement, Monte Carlo calculation by J.P.Biersack and W.Eckstein and calculation of bipartition model of PANDA–SP code by Zhengming Luo et al.

(2) particle reflection from solid surfaces

Particle and energy reflection of projectiles H^+,D^+,T^+, $^3He^+$and $^4He^+$onto Be,B,C,Al,Si,Ti,Fe,Ni,Cu,Mo,W and Au solid surfaces have been evaluated and compiled under incident angle region of $0 < \alpha < 60$ degrees and impact energies from 10 eV to 100 KeV in CNDC / A+M Unit

It has long been recognized that particle and energy reflection coefficients are decreased monotonically as projectile energy increase and approach to unity at very low incident energy. The computational results to take account of surface binding energy using a PANDA–U code by Z. Luo are shown that the reflection coefficients decrease again when the incident energy less than 100 eV. Our evaluation results have been illustrated the same tendency. The reflection coefficients from ALADDIN have been put into Micro–VAX–II.

Recent publications

1) Communication of Nuclear Data Progress No.7 (1992) 67;″ A Database on ion–atom collision processes″; Jinzhang Yao, Shaohong Fang

2) Communication of Nuclear Data Progress No.7(1992) 68;" Evaluation of trapping and desorption data"; Zhang Di, Li Yexiang
3) Chinese Journal of Atomic and Molecular Physics Vol.9 No.2(1992) 2295; " Approximate calculation of ionization cross section by electron impact"; Qing Yang, Jinzhang Yao
4) Communication of Nuclear Data Progress No.8 (1992) 70; " Reflection of $H^+$and D^+plasma particles from solid surfaces"; Jinzhang Yao, Shaohong Fang and Hongwei Yu
5) Proceeding of Sixth Chinese Atomic and Molecular Physics Conference (1992) P 279 Changzheng,China;" Reflection of particles from plasma edge", Jinzhang Yao and Shaohong Fang
6) Chinese Journal of Nuclear Physics Vol.15, No.2 (1993) 179–184 "Radiation Damage in the surface of materials created by Hydrogen and Deuterium ions"; Zhengming Luo and Qi Zhu

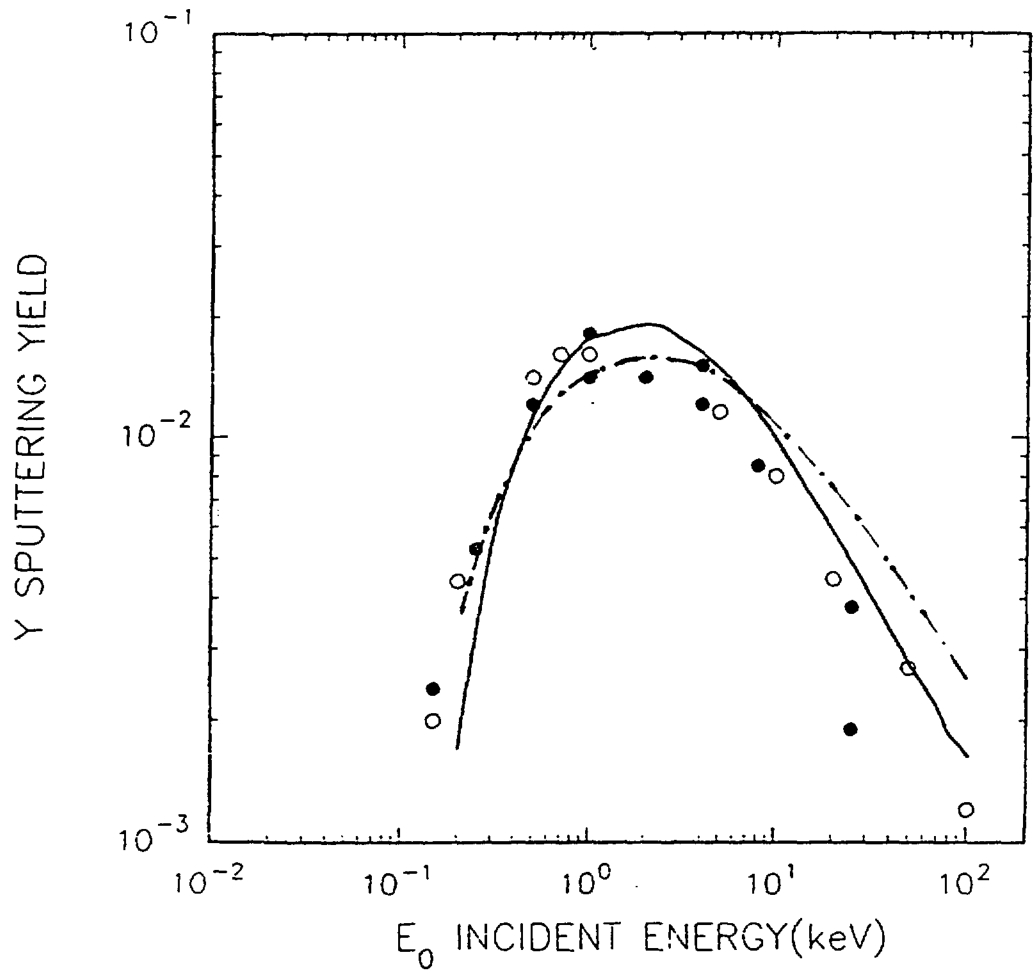

Fig.1 Sputtering yields of Ni surface by H+ projectile at normal incidence

● Exp. ○ Monte Carlo

——— Luo —·—·· Present work

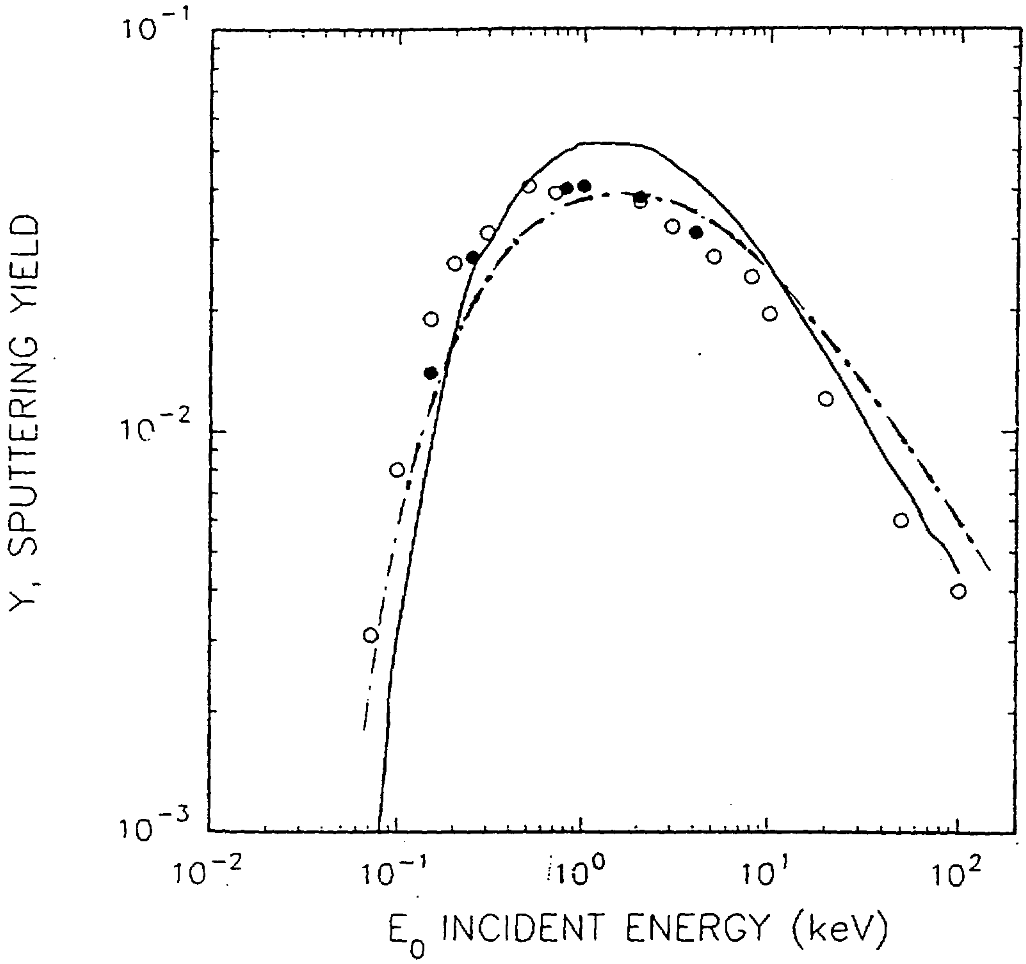

Fig.2 Sputtering yields of Ni surface by D+ projectile at normal incidence

● Exp. ○ Monte Carlo

——— Luo —·—·· Present work

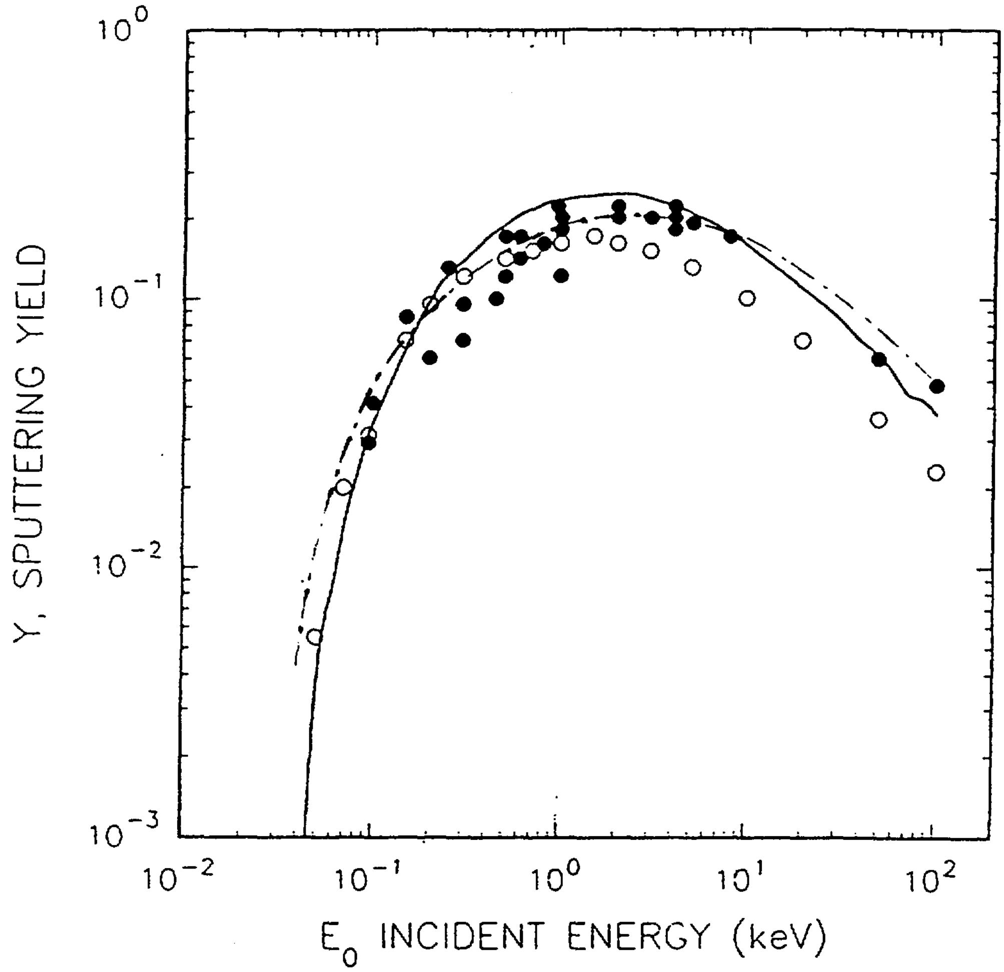

Fig.3 Sputtering yields of Ni surface by He4+ projectile at normal incidence

● Exp. ○ Monte Carlo

——— Luo —·—·· Present work

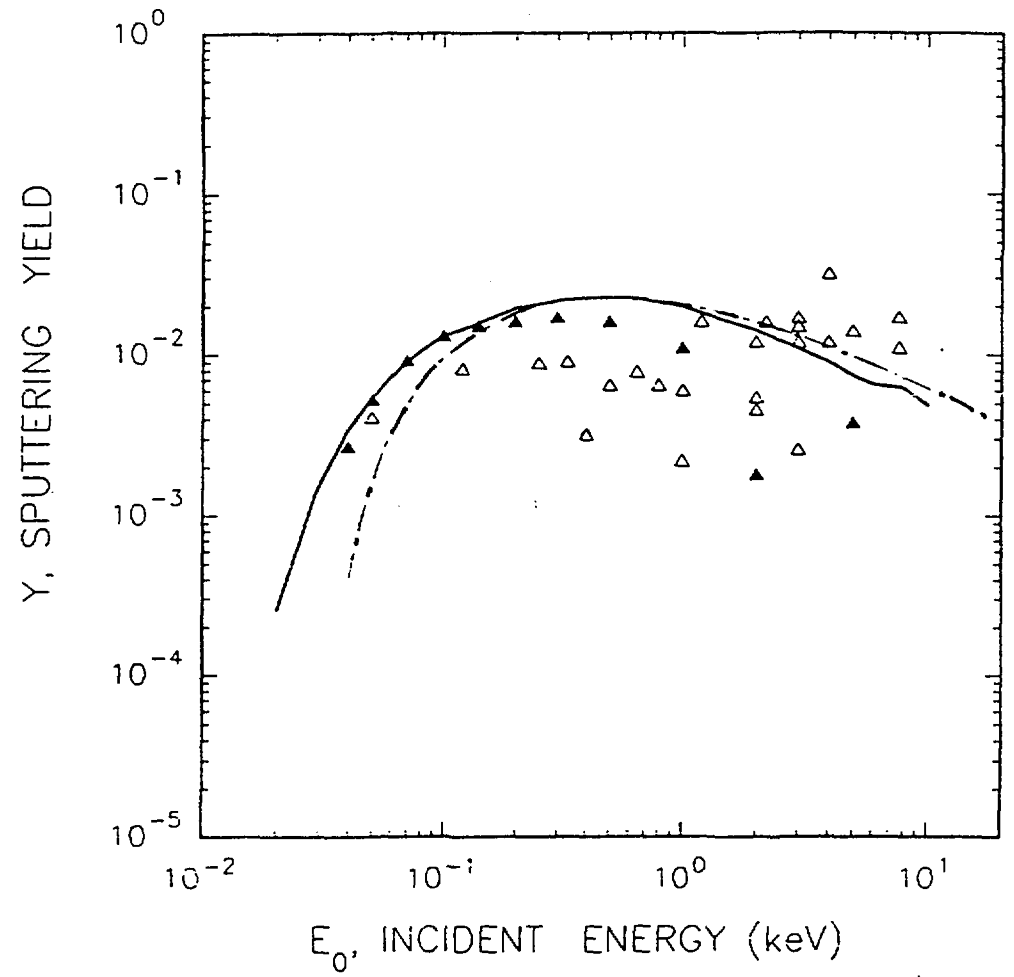

Fig.4 Sputtering yields of C surface by H+ projectile at normal incidence

△ Exp. ▲ Monte Carlo

——— Luo —·—·· Present work

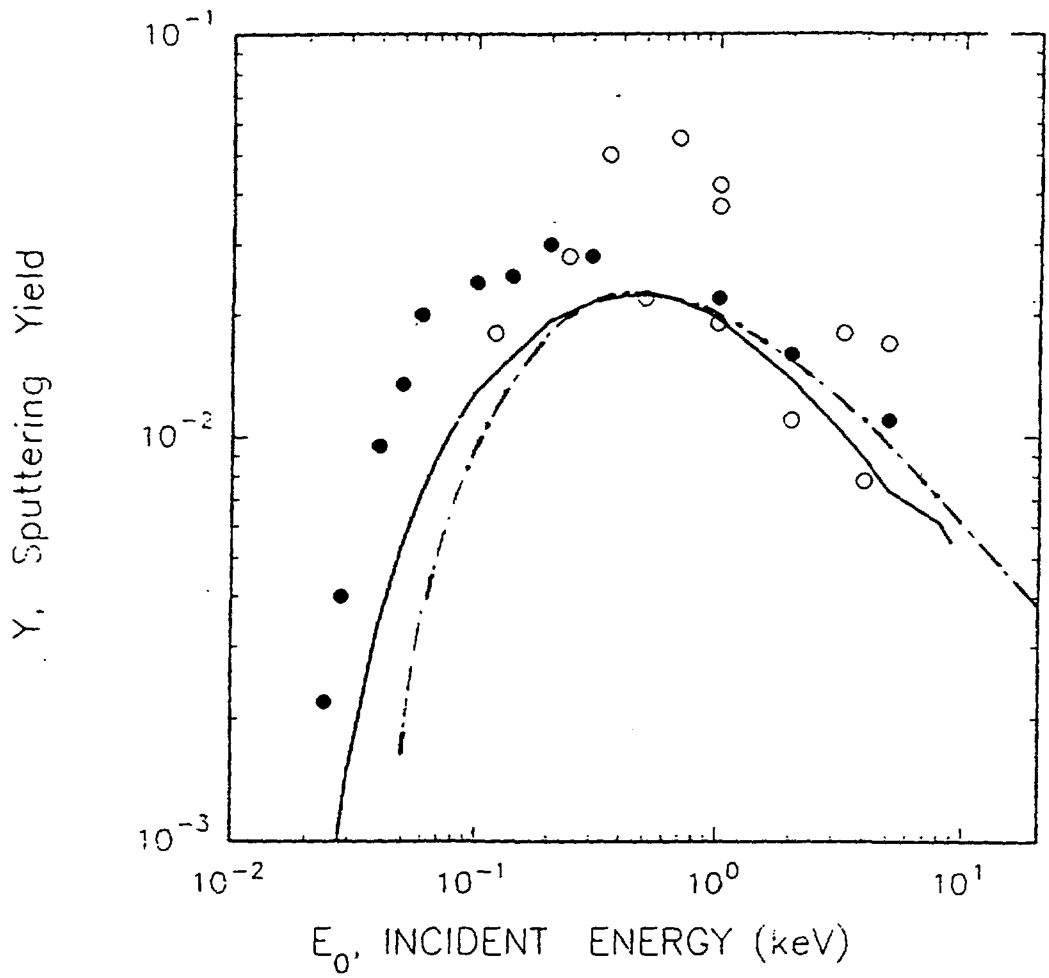

Fig.5 Sputtering yields of C surface by D+ projectile at normal incidence

o Exp. ● Monte Carlo

——— Luo —·—·· Present work

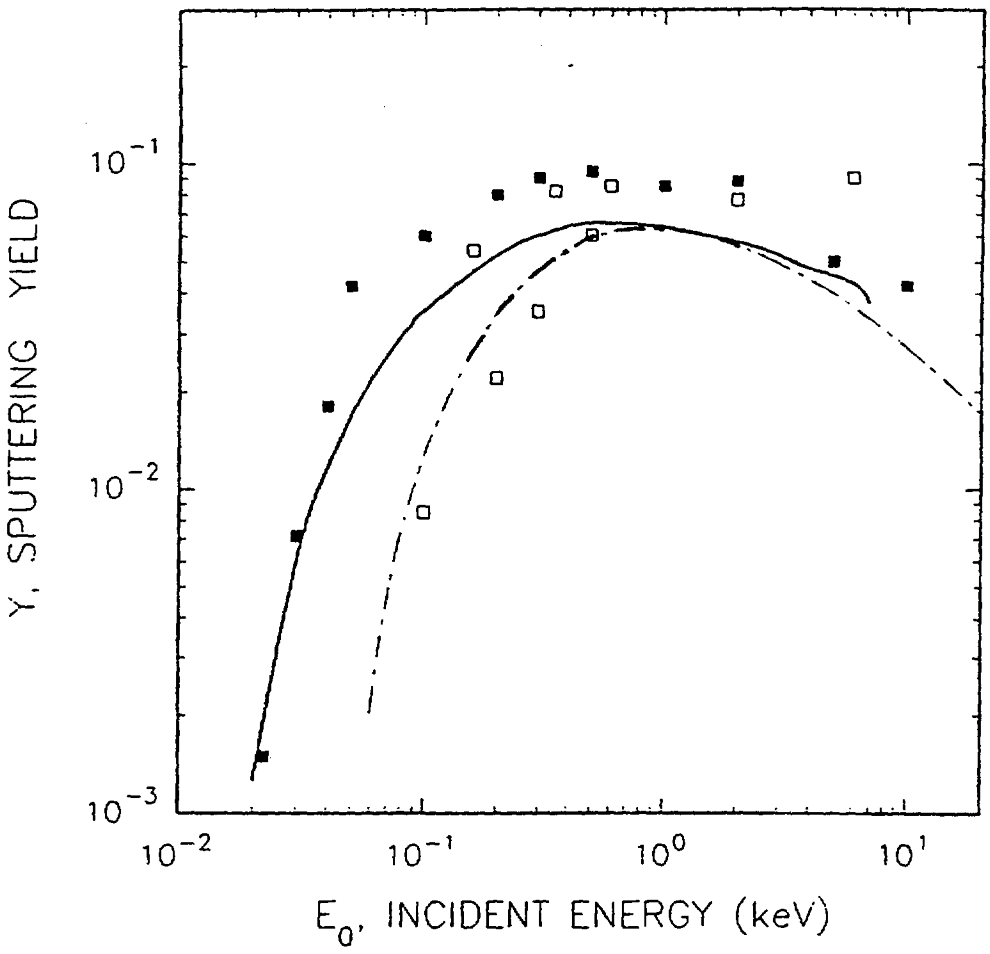

Fig.6 Sputtering yields of C surface by He4+ projectile at normal incidence

□ Exp. ■ Monte Carlo

——— Luo —·—·· Present work

Activity report at the Russian Scientific Centre "Kurchatov Institute" 1992/1993

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The present activities on the field of collection,dissimination and evaluation of (A+M) data for fusion performed in the Institute of Nuclear Fusion of the Russian Scientific Centre "Kurchatov Institute" are connected both the present tokamak research and the ITER design study and the DEMO design study.As previously,the Russian bibliography on (A+M) data for fusion are collected.The corresponding collection is submitted to the "International Bulletin on Atomic and Molecular Data for Fusion".

Because of the interest to the innovation schemes of the liquid-metal limiter the data about the cross-sections and rates of different elementary processes involving Ga -ions have been compiled and reported.The new model to describe the interaction of fast monoatomic beams with fusion plasmas is developed by Dr. V.S.Lisitsa et al.In the frame of the quasistationary model the method for the calculation of the population of excited levels of non-hydrogenic atoms is proposed.It is hybrid model combined the analytical approach by I.Beigman for the highly-excited levels and the numerical calculation the populations for low levels.The numerical code is developed .The problem of the penetration of the diagnostic Li-beam in fusion plasmas is considered in detail.Because of the large interest to regimes in tokamak with Be-limiter (or with Be -coated inner surfaces) the data for ionization,excitation,recombination and charge exchange cross-sections and rates for different Be-ions have been compiled and partly evaluated (G.I.Krotova ,Preprint Institute of Nuclear Fusion-5568/6,1992).Some data for C-ions and B-ions are included in this document.

The calculations of the radiative cooling rates for Be-seeded plasmas with taking into account the charge-exchange between different Be-ions and neutral hydrogen atoms have been performed by V.A.Abramov during his stay in the NIFS,Nagoya,Japan.The results of these calculations are included in the contribured paper presented by V.A.Abramov and D.Kh.Morozov at the Plasma Edge Theory Workshop(Varenna,4-6 October 1993).The detailed analysis of the radiative cooling rates gives the possibility to explain the different thresholds for MARFE creation at the JET experiments.

The group headed by Dr. V.A.Belyaev have terminated the experimental investigation of the molecular hydrogen ions dissociation due to self-collision at low energies (5-20 eV).It is shown that the experimental results are smaller than the results predicted by theoretically (L.I.Menshikov).The preparation of the experimental equipment to measure the ionization cross-sections of Ga-ions(q=1-3) by electron impact (E < 100 eV) is performed.The ion soyrce must provide the next currents of Ga-ions:Ga^{+}-10 mA,Ga^{+2}-500 μA, Ga^{+3}-100 μA, Ga^{+4} -3 μA.In principle,there is possibility to measure the charge exchange cross-sections for the collision of different Ga -ions with the neutral hydrogen atoms at low energies.

The activities in the field of the plasma-surface interactions are carried out in the laboratory headed by Prof.M.I.Guseva.The study of the accumulation ,kinetics of releasing and other topics at the interaction of the hydrogen isotopes with carbon-graphyte materials have been performed.Also,the sputtering of W by light ions at the near-threshold energies have been investigated.

On-going and future activities:

1) Data compilation related impurities such as carbon-hydrogen molecules

2) Calculation of the radiative cooling rates gor B-seeded plasmas

3) Evaluation of the excitation cross-sections (rates) for different metallic ions.

4) Evaluation of the excitation cross-sections(rates) of Be-ions by electron impact for transitions which have not been included in the data presented at the IAEA meeting on data for Be and B, June 11-13 ,1991,Vienna.

Data Collection at MPIPP

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EURATOM-Association

The main data produced and collected at MPIPP are those of kinetic reflection and sputtering. Both types of data are investigated experimentally and by computer simulation. In the following no further attention is given by which method the data are gained. The two fields are discussed separately.

Reflection

Particle and energy reflection coefficients for a large number of projectile-target combinations have been determined. A survey of these available data is given in table 1. The data also cover a wide range of incident energies and angles. Most reflection coefficients at normal incidence have been fitted [1] by a formula using six parameters applicable to some mass ratio range. At high energies two and for self-reflection three additional parameters are used to describe the behaviour at low projectile energies.

The ratio of the energy and particle reflection coefficient gives the mean energy of reflected projectiles. But this is not always sufficient for the characterization of the energy distribution. In this case the method of inverse cummulative distributions can be used [2].

From the simulated distribution $f(E_0, \alpha; E, \beta, \varphi) dE \sin\beta \, d\beta \, d\varphi$, three one-dimensional distributions f^i are determined :

$$f^1_{E,\alpha}(E) = \int_0^{2\pi} \int_0^{\pi/2} f(E_0, \alpha; E', \beta, \varphi) \sin\beta \, d\beta \, d\varphi$$

With a given energy E', β' is obtained from

$$f^2_{E,\alpha;E'}(\beta) = \int_0^{2\pi} f(E_0, \alpha; E', \beta, \varphi) \, d\varphi$$

Finally, with the chosen values E' and β', φ' is selected from the distribution

$$f^3_{E,\alpha;E',\beta'}(\varphi) = f(E_0, \alpha; E', \beta', \varphi) \quad .$$

Suppose that $F^1(\xi), F^2(\eta,\xi)$ and $F^3(\zeta,\eta,\xi)$ are the inverse cumulative distributions of f^1, f^2 and f^3, respectively. Choose three random numbers, ω_1, ω_2 and ω_3, between 0 and 1. Then the corresponding energy is $F^1(\omega_1)$, the polar emission angle is $F^2(\omega_2,\omega_1)$ and the azimuthal emission angle is $F^3(\omega_3,\omega_2,\omega_1)$. The inverse distributions F^i have been tabulated for $\omega = 0.1, 0.3, 0.5, 0.7, 0.9$, which leads to five values for F^1, 25 values for F^2 and 125 values for F^3 [3]. Other values may be approximated by linear interpolation. Twelve incident energies E_0 and seven incidence angles α were used leading to 84 datasets for each projectile target combination. This method has been applied for some projectile-target combinations [3,4], see table 2. Another possibility is the reconstruction of the energy distribution from the moments of the distribution.

Sputtering

As for reflection sputtering yield data are produced for a large number of projectile-target combinations, which are summarized in table 3 for normal incidence and in table 4 for oblique incidence. Most of these data are given in [5], where fits to these data at normal incidence are made with a revised Bohdansky formula and at oblique incidence with the Yamamura formula [6]. The Yamamura is not a good description of the available data at low mass ratios (target mass to projectile mass) and low energies.

Again as for the reflected projectiles the same methods can be applied for the energy distribution of the sputtered atoms. But the energy distribution of sputtered atoms is well described by the Thompson formula [7]; an energy E can be easily picked by a random number r between zero and one.

$$E = \frac{E_s}{\left(1 + \frac{1}{a}\right) r^{-1/2} - 1} \quad ,$$

where $a = \gamma E_0 / E_s$ is the upper limit of the distribution. E_0 is the projectile energy, γ the maximum energy transfer in an elastic collision, and E_s is the surface binding energy.

Analogously, a polar emission angle β of the cosine distribution of sputtered atoms can be determined by a random number

$$\beta = \pm \sin^{-1}(r^{1/2})$$

Both formulae are not valid for oblique incidence but can be used as approximations.

There are many cases which cannot simply described by sputtering yields. Multicomponent targets usually change their surface composition due to bombardment and the yield depends therefore on fluence. This will happen even with a monoatomic target bombarded with a nonvolatile projectile species [8]. In these cases single case studies have to be performed.

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6 Y.Yamamura, Y.Itikawa, N.Itoh: IPPJ-AM-26, Nagoya (1983)

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8 W.Eckstein, J.Roth: Nucl. Instrum. Methods B **53**, 279 (1991)

Table 1 : Reflection data for the following ion-target combinations

elements	H	D	T	^3He	^4He	C	O	$self$	Ne	Ar	Kr	Xe	Hg	Rn
Li		x	x					x						
Be	x	x	x		x		x	x	x	x				
B		x					x	x						
C	x	x	x		x	x	x	x		x		x		
Al		x			x			x	x	x				
Si	x	x			x				x	x	x	x		
Ti		x			x			x	x					
V		x						x						
Fe	x	x			x			x						
Ni	x	x		x	x			x	x	x	x	x		
Cu	x	x			x			x		x		x		
Ga		x	x					x					x	
Ge										x				
Zr												x		
Nb		x												
Mo		x	x	x	x		x	x		x	x		x	
Pd					x							x		
Ag					x					x		x		
In		x	x					x						
Sm											x			
Ta	x													
W		x	x			x	x	x		x		x		
Pt														
Au		x			x			x		x		x		
Hg											x			
U	x				x			x	x	x	x	x		x
B_4C	x	x			x				x					
BeO							x							
$USB15$		x					x							
WC					x									

Table 2 : Datasets for energy and angular distributions of reflected projectiles

elements	H	D	T	^4He
C	x	x	x	x
Fe	x	x	x	x
W		x		x

Table 3 : Sputtering data at normal incidence for the following ion-target combinations

elements	H	D	T	^3He	^4He	C	O	$self$	Ne	Ar	Kr	Xe	Hg	Rn
Li		x	x					x						
Be	x	x	x		x		x	x	x	x				
B		x			x		x	x						
C	x	x	x		x	x	x	x	x	x	x	x		
Al	x	x			x			x	x	x				
Si	x	x		x	x			x	x	x	x	x		
Ti	x	x			x			x	x					
V		x						x						
Fe	x	x			x			x						
Ni	x	x		x	x		x	x	x	x	x	x		
Cu	x	x			x			x		x		x		
Ga		x	x					x					x	
Ge										x				
Zr		x			x							x		
Nb		x												
Mo	x	x	x	x	x		x	x	x	x	x		x	
Pd					x							x		
Ag	x	x			x					x		x		
In		x	x					x						
Sm											x			
Ta	x	x			x				x	x	x	x		
W	x	x	x		x	x	x	x	x	x	x	x		
Pt					x							x		
Au	x	x		x	x			x		x		x		
Hg											x			
U					x			x	x	x	x	x		x
Al_2O_3	x	x			x									
B_4C	x	x			x	x	x		x					
Be_4B	x	x			x									
BeO	x	x			x		x							
SiC	x	x			x		x		x					
SiO_2	x	x			x									
TaC	x	x			x									
Ta_2O_5	x	x			x									
TiB_2	x	x			x									
TiC	x	x			x		x		x					
WC	x	x			x									
ZrC	x	x			x									
$Inconel$	x	x			x									
$SS316$	x	x			x		x							
$USB15$		x												

Table 4: Sputtering data at oblique incidence for the following ion-target combinations

targets	H	D	T	^4He	C	O	$self$	Na	K	Ne	Ar	Kr	Xe
Li			x				x						
B		x					x						
Be		x	x	x	x		x						
C	x	x	x	x	x		x						x
Si				x									
Ti				x						x			
Fe	x												
Ni	x	x		x			x						
Cu	x	x					x				x		
Ga							x						
Mo	x	x		x			x				x		
Ag		x						x	x				
In	x						x						
Ta	x												
W	x					x	x						
Au	x	x						x	x				
U	x											x	
B_4C		x		x	x								
BeO						x							
SiC	x	x		x									
TiC	x	x		x									
$USB15$		x											

Atomic Collisions Data Center
Joint Institute for Laboratory Astrophysics
University of Colorado
National Institute of Standards and Technology
Standard Reference Data

Personnel:

- John Broad jtb@jiladc.colorado.edu
- Stephen Krog skrog@jiladc.colorado.edu

Equipment:

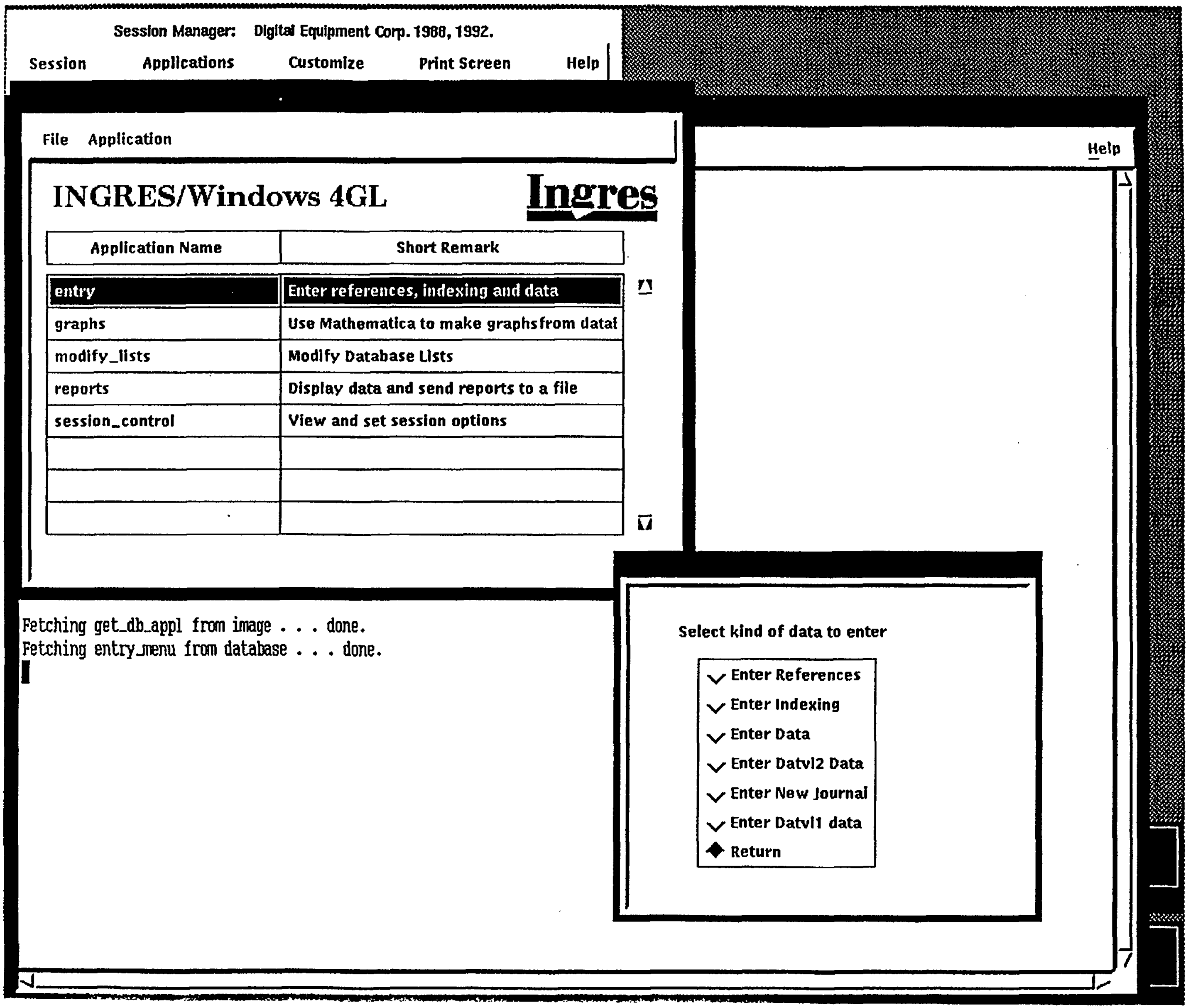
- DEC 5000/200 UNIX Workstation with 32MB RAM and 1.5GB hard disk with INGRES Database Management System and Mathematica
- 486 DX2 PC with 8MB RAM and CLARION Database Developer

Databases:

- Atomic Collisions Database on DEC Workstation under INGRES with 20,000 bibliographic entries and 20MB of collision data. Repository for data used in generating scientific reviews.
- Gas Laser Database on PC in CLARION. Gas Laser wavelength/transition tables with bibliography from Vol II and Supplement 1 of the *Handbook of Laser Science and Technology*, Marvin Weber, ed. CRC Press.

Projects in Progress:

- Modification of Gas Laser Database and distribution for sale.
- Critical review of atomic data for the Argon Reference Gas Discharge Cell, with Zoran Petrović.
- *Collisional Alignment and Orientation of Atomic Outer Shells, II. Quasi-molecular Excitation and Beyond.*, with N. O. Andersen, E. Campbell, J. W. Gallagher, and I. V. Hertel
- *Collisional Alignment and Orientation of Atomic Outer Shells, III. Spin-dependent Effects*, with N. O. Andersen and K. Bartschat.
- Redbook on Electron-Impact Excitation and Ionization, with D. Schultz and J. W. Gallagher. Data will be managed under INGRES on UNIX workstation in Oak Ridge. One output format will be traditional redbook typset with LaTeX. On-line query over INTERNET will be possible.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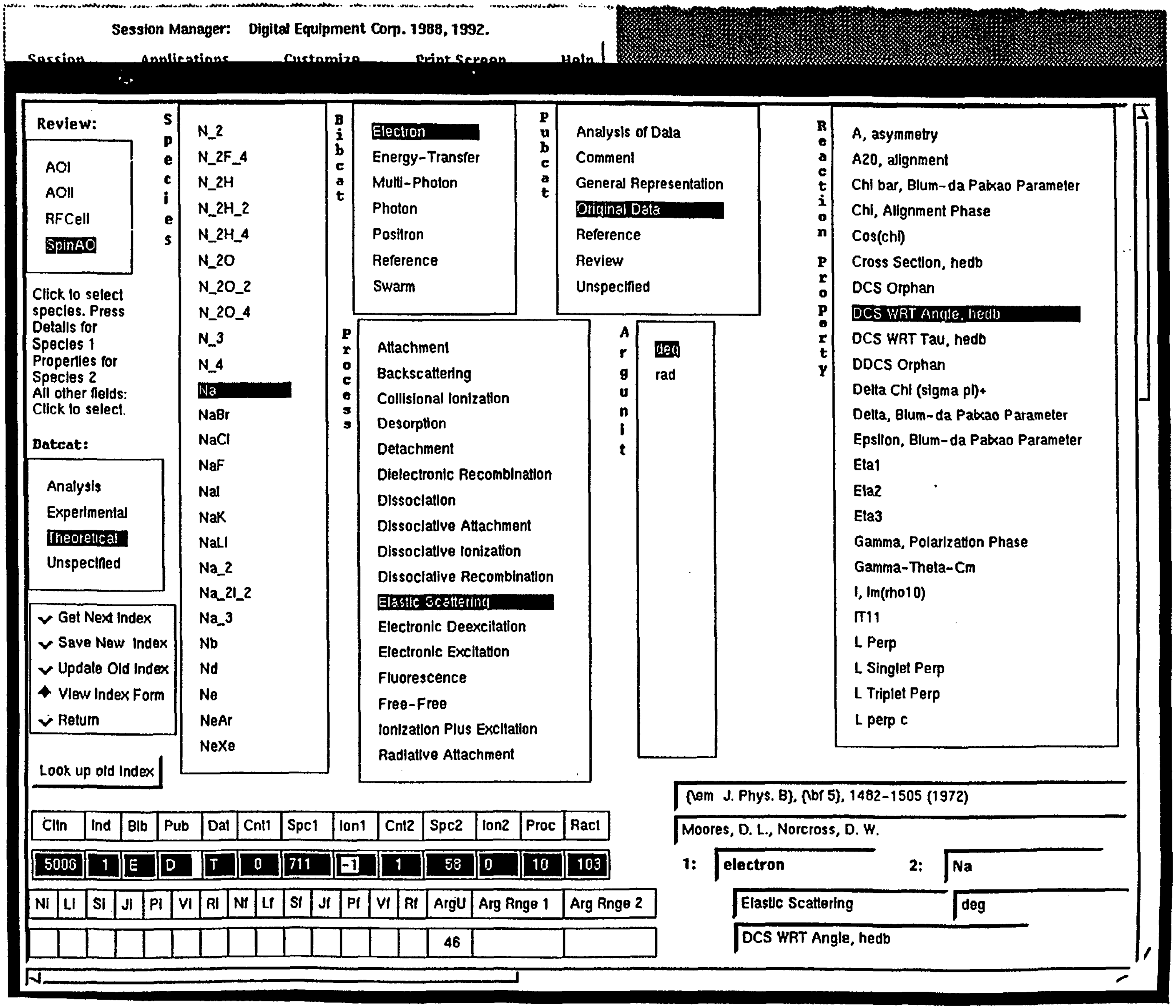
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Detachment
Dielectronic Recombination
Dissociation
Dissociative Attachment
Dissociative Ionization
Dissociative Recombination
Elastic Scattering
Electronic Deexcitation
Electronic Excitation
Fluorescence
Free-Free
Ionization Plus Excitation
Radiative Attachment
Pubcat
Analysis of Data
Comment
General Representation
Original Data
Reference
Review
Unspecified
Argunit
deg
rad
Reaction Property
A, asymmetry
A20, alignment
Chi bar, Blum-da Paixao Parameter
Chi, Alignment Phase
Cos(chi)
Cross Section, hedb
DCS Orphan
DCS WRT Angle, hedb
DCS WRT Tau, hedb
DDCS Orphan
Delta Chi (sigma pi)+
Delta, Blum-da Paixao Parameter
Epsilon, Blum-da Paixao Parameter
Eta1
Eta2
Eta3
Gamma, Polarization Phase
Gamma-Theta-Cm
I, Im(rho10)
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L Perp
L Singlet Perp
L Triplet Perp
L perp c
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Nl Ll Sl Jl Pl Vl Rl Nf Lf Sf Jf Pf Vf Rf ArgU Arg Rnge 1 Arg Rnge 2
46
{\em J. Phys. B}, {\bf 5}, 1482-1505 (1972)
Moores, D. L., Norcross, D. W.
1: electron
2: Na
Elastic Scattering
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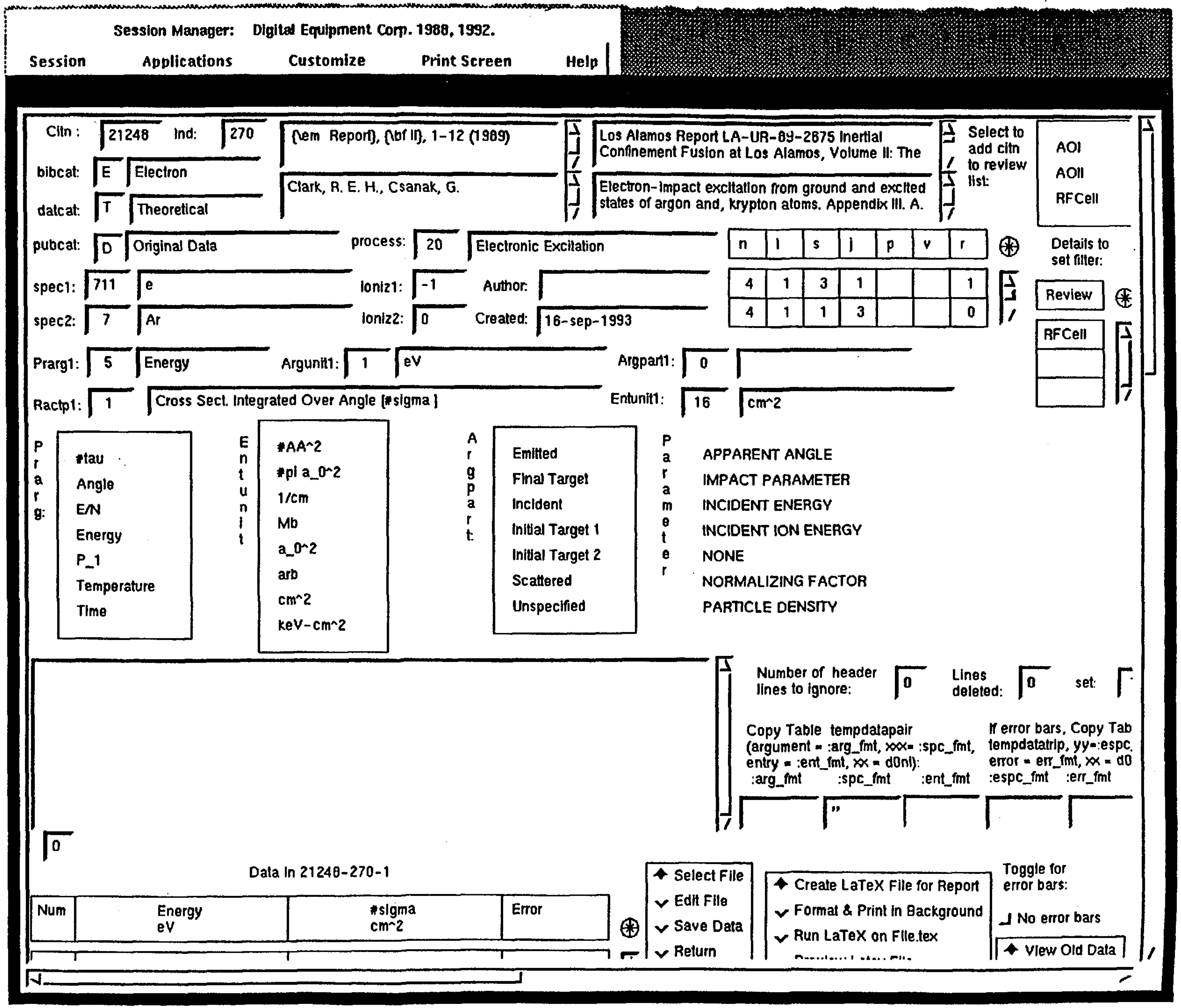
DCS WRT Angle, hedb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Num	Energy eV	#sigma cm^2	Error

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Num	Energy eV	#sigma cm^2	Error
1	7.4268773e-002	1.9846192e-015	
2	9.4211844e-002	7.0547597e-015	
3	1.1951015e-001	9.1537472e-015	
4	1.5160169e-001	1.1579329e-014	
5	1.9231064e-001	1.3630920e-014	
6	2.4395098e-001	1.3909924e-014	
7	3.0945808e-001	1.2302085e-014	
8	3.9255552e-001	9.9079775e-015	
9	4.9796676e-001	7.6365255e-015	
10	6.3168363e-001	5.8006475e-015	
11	8.0130690e-001	4.4144030e-015	
12	1.0164784e+000	3.4193005e-015	
13	1.2894289e+000	2.7287277e-015	
14	1.6356737e+000	2.2191705e-015	
15	2.0748941e+000	1.7625221e-015	
16	2.6320584e+000	1.2895290e-015	
17	3.3388312e+000	8.1776370e-016	
18	4.2353931e+000	4.4217759e-016	
	0.0000000e+001	0.0000000e+001	0.000e+001

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- Select File
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- Create LaTeX File for Report
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Num	Comment
2	auxiliary table sent by author
1	$4s^3P_0 #rightarrow 4s^1P_1$

Code	Parameter	Value	Unit Name	Unit
505	THRESHOLD	7.3533439e-002	eV	1

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11th ICPIG
12th Informal Conf. Photochem.
18th Annual Gaseous Electronics Conference
20th EGAS Abstracts, Eur. Group for At. Spectrosc.
33rd Annual Gaseous Electronics Conference
3rd Summer Colloq. Electronic Transition Lasers
4th Intl. Conf. Infrared #& Millimeter Waves
5th Intl. Conf. Gas Discharges
6th Intl. Swarm Seminar
8e Colloq. Phys. Coll. At. Mol.
ACS Symp. Ser.
AIAA J.
Abh. Braunschw. Wiss. Ges.
Acc. Chem. Res.
Acta Astronaut.

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Review Article

SpinAO

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References by Moores%

Citn Num	Year	Journal	Vol	Pagef	Pagel	First Auth
16346	1979	EMPMC1	00000	00003	00013	Moores
4074	1970	JPAMA4	00003	00161	00172	Moores
4636	1972	JPAMA4	00005	00286	00298	Moores
5006	1972	JPAMA4	00005	01482	01505	Moores
5987	1974	JPAMA4	00007	00371	00375	Moores
8271	1976	JPAMA4	00009	01329	01349	Moores
12717	1978	JPAMA4	00011	0L403	0L405	Moores
15743	1979	JPAMA4	00012	04171	04178	Moores
17186	1980	JPAMA4	00013	00385	00395	Moores

J. Phys. B 5, 1482 (1972)

Moores, D. L., Norcross, D. W.

The Scattering of Electrons by Sodium Atoms

Session Manager: Digital Equipment Corp. 1988, 1992.

Session | Applications | Customize | Print Screen | Help

Data Indexing for e -1 with Na 0

Citn	Ind	Set	Process	Process Argument	Argument Unit	Reaction Property	Entry Unit
17431	3	1	Elastic Scattering	Energy	eV	Cross Sect. Integrated Over Angle	cm^2
21258	1	1	Elastic Scattering	Angle	deg	SA, Spin Asymmetry	unitless
21258	1	2	Elastic Scattering	Angle	deg	Target Spin Asymmetry	unitless
21258	1	3	Elastic Scattering	Angle	deg	Parallel Spin Asymmetry	unitless
21258	1	4	Elastic Scattering	Angle	deg	Perpendicular Spin Asymmetry	unitless
21258	7	1	Elastic Scattering	Angle	deg	DCS WRT Angle, hedb	a_0^2/sr
21272	1	2	Elastic Scattering	Angle	deg	Perpendicular Spin Asymmetry	unitless
21272	1	3	Elastic Scattering	Angle	deg	SA, Spin Asymmetry	unitless
19286	1	1	Electronic Deexcitation	Angle	deg	Spin Polarization	arb
19286	1	2	Electronic Deexcitation	Angle	deg	Spin Polarization	arb

J. Phys. B 24, 4815 (1991)

Authors

Bartschat, K.

Data in datvi1 for 21258-1-4

#	Angle (deg)	S_#perp (unitless)	Error
1	1.650e-001	6.383e-002	
2	5.591e+000	7.177e-002	
3	1.058e+001	7.282e-002	
4	1.495e+001	7.437e-002	
5	1.910e+001	7.248e-002	
6	2.343e+001	6.281e-002	
7	2.764e+001	4.702e-002	
8	3.118e+001	2.451e-002	
9	3.473e+001	-5.430e-003	
10	3.868e+001	-4.847e-002	
11	4.184e+001	-9.158e-002	

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Spin-dependent effects in elastic and inelastic low-energy
electron scattering from sodium atoms

Figure 1, dot-dash

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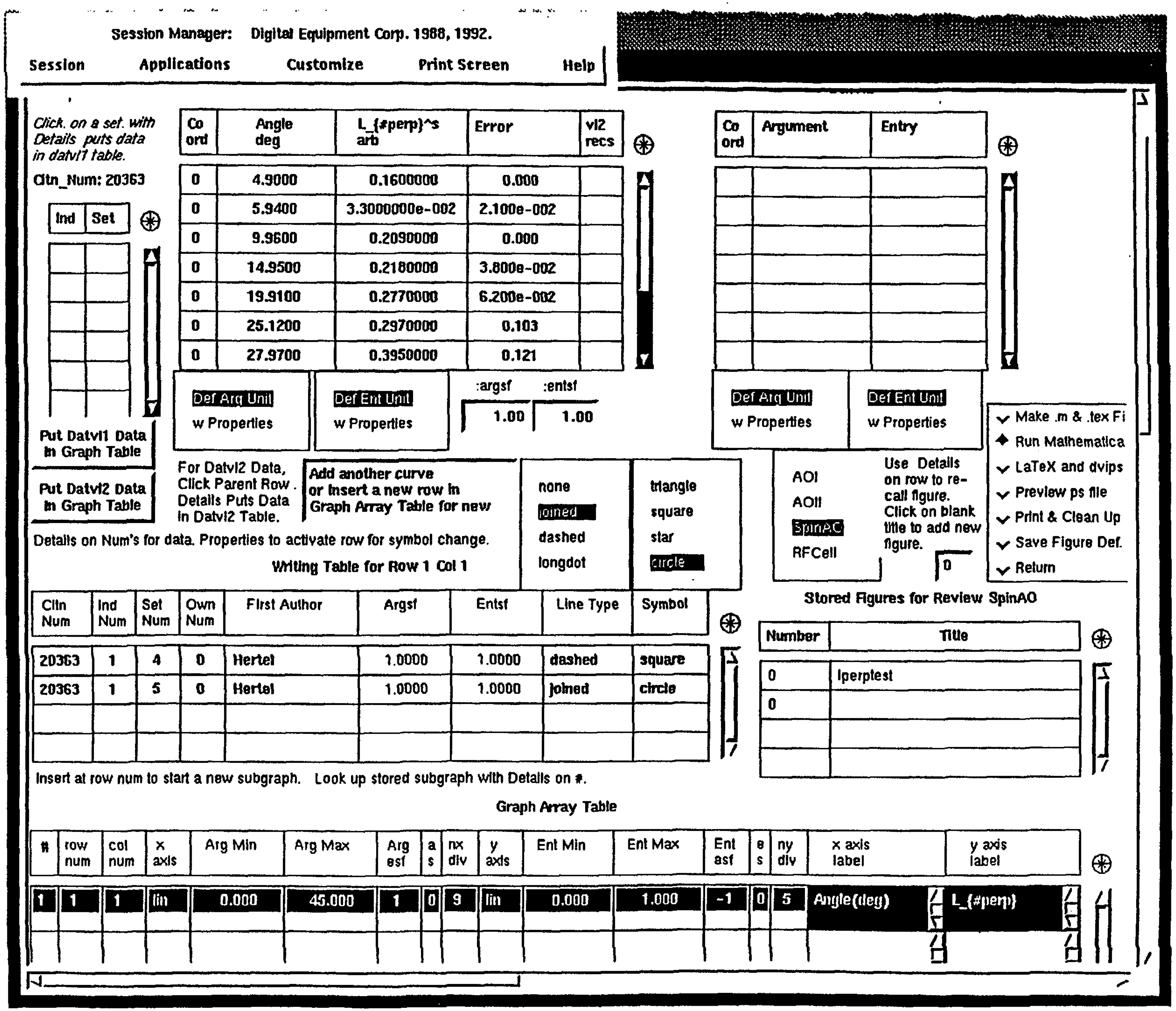

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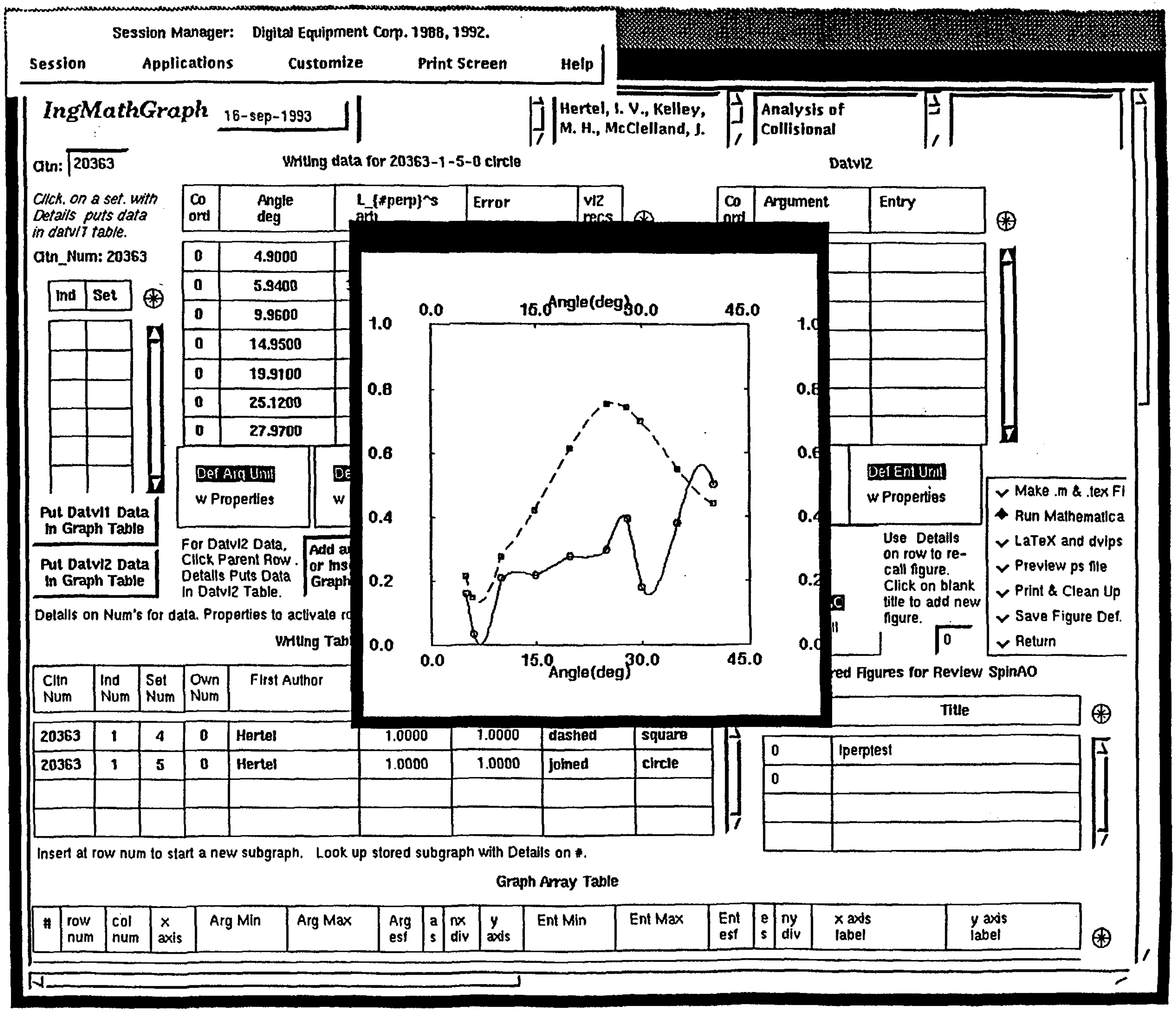
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Caption for Graph with source of data

16-sep-1993 Atomic Collisions Data Center at JILA
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From Review Article SpinAO Figure

No	Row	Col	Axis	Min	Max	Esf	Div	Label
1	1	1	x: lin	0	45	1	3	*Angle(deg)*
			y: lin	0.0	1.0	-1	5	$L_\perp$

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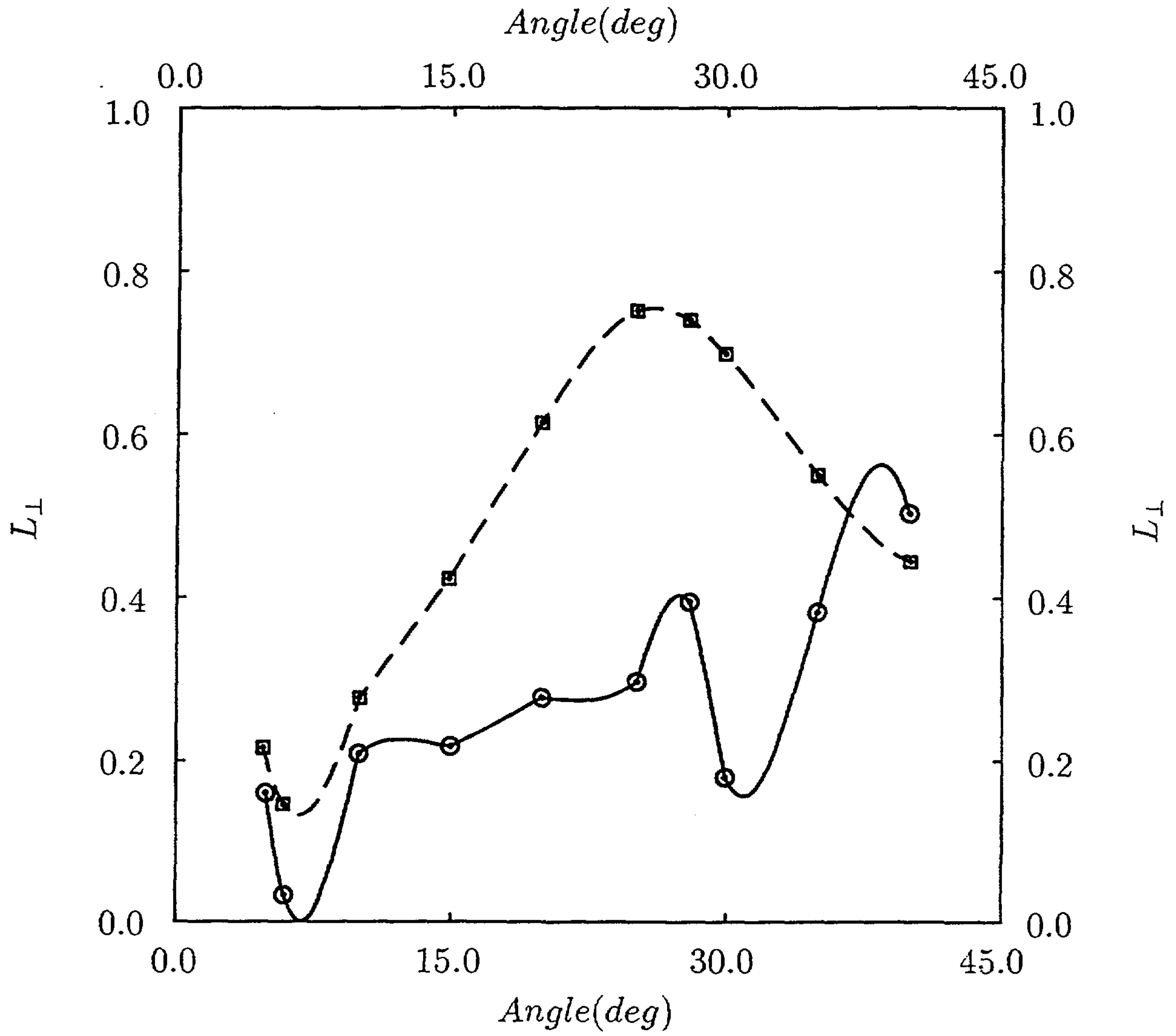
1	1	1	square	dashed	20363	1	4	0	Hertel	1.000	1.000
1	1	1	circle	joined	20363	1	5	0	Hertel	1.000	1.000

Sample Graph made with
Mathematica and LaTeX



Progress Report for 1992–1993 at CRAAMD

Sun Yongsheng

During the past year, we have done the following tasks:

A. Data Compilation and Evaluation

1. The collision strengths for the electron impact excitation of Ne–like(Ti, Fe, Se, Cu and Ge) ions and of F–like (Z = 22–92) ions have been compiled in ALADDIN system.
2. The ALADDIN structure have been extended to incorporate data on material properties. These data are the Rosseland radiative opacities and the electron conductive opacities. They were calculated by our own code recently.

B. Related Publications

1. H.Y.Yang, Y.H.Qiu, S.C.Li and Y.S.Sun
"Dielectronic Recombination for F–like and Ne–like Ge ions"
J.Phys.B, 25(1992)791–798.
2. Y.H.Qiu, S.C.Li and Y.S.Sun
"DR into Excited Levels of Ne–like Ti from F– like Low– lying States"
Physica Scripta, Vol.47,(1993)192–195
3. Y.H.Qiu, S.C.Li and Y.S.Sun
"Dielectronic Spectra for Ne–like Ti from F– like Low–lying States"
At. Data. Nucl. Data Tables(1993)(in Press)
4. In addition, there are about our 10 papers published in the Chinese periodicals.

C.Internal Reports

- **Theory**

1. Wang Yansen, Hu Wei, Fang Dufei and Yang Fujia
   "Theoretical Calculation of Electron Impact Ionization Cross Sections for H– and He–like Ions"(O, F,Mg,Al,Si,S,Cl,Cu)
   Reports:"CRAAMD–AM–4" No.2(1993)30
2. Qiu Yubo and Long Yanqiu
   "Charge Transfer in A^{q+}+H Collisions"
   Reports:"CRAAMD–AM–5" No.3(1993)(in press)
3. Chen Gouxin and Sun Yongsheng
   "Theoretical Calculation for Oscillator Strength and Excited Level Lifetime of CI–VI Ions"
   Reports:"CRAAMD–AM–5" No.3(1993)(in press)

- **Experiments**

1. Zhou Yuqing, Zhang Baohan, Yang Guohong and Lei Anle
   "Study of X–ray spectra of Highly stripped ions from laser–induced plasmas"
   Reports:"CRAAMD–AM–3", No.1(1993)31
2. Wang Youde, Wang Xinglin, Ma Xinwen, Xu Qian, Yang Zhihu, Liu Huiping and Zhao Mengchun
   "The Studies of Low Energy Beam–Foil Spectra and Highly Charged Ions Collisions"
   Reports:"CRAAMD–AM–3", No.1(1993)1

Next year (1993–1994), we want to

1. Compile and evaluate the dielectronic recombination rates of C,O,Mg, Ar, Fe, Se, Mo ions and the collision strengths for the electron impact excitation of W ions.
2. Continue to compile the material property data.
3. Calculate the cross sections of electron impact ionization, from the excited states, for H–, He– and Li–like (O, F, Mg, Al, Si, S, Cl, Fe, Cu and so on)

PROGRESS ON A+M DATA ACTIVITIES AT ENEA (ITALY).

By E. Menapace(*).

A. Evaluation of molecular spectroscopic data.

(A. Mengoni* in cooperation with T. Shirai in the frame of a stage at JAERI within the Science and Technology Fellowship Programme by the EC)

The activity concerned the development of techniques and methods for the calculation of the vibrational spectra of polyatomic molecules using algebraic models.

In this frame the Vibron Model was investigated and applied to the calculation of the vibrational spectra of two bent triatomic molecules; such as

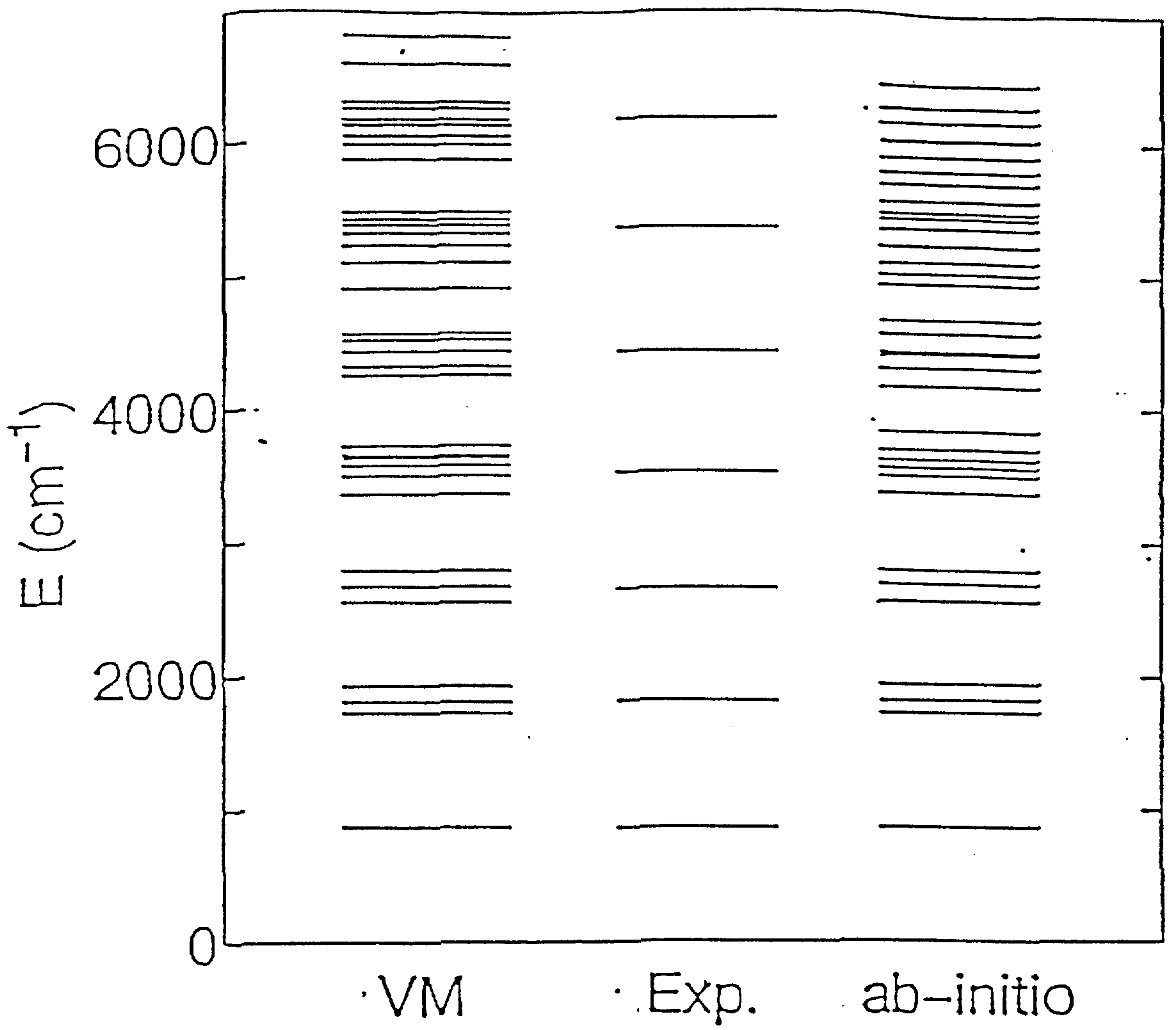
HCO and DCO,

and the results were well compared both with the experimental data and with those obtained with "ab initio" calculations, showing a comparable accuracy, at least for the low vibrational modes.

Only in the upper part of the spectrum the two computational physics approaches show different results, then a detailed analysis in the two sets of calculated spectra has been initiated in order to determine the influence of the Majorana operator in the results of the Vibron Model calculations.

The results for the complete spectrum (up to 6500 cm^{-1}) are shown for the purpose of comparison in Tables 1.2.3 and in Fig. 1 as follows.

(*) Dept. for Advanced Technologies-Nuclear Data and Codes Laboratory



J. Mol. Spectr. A. Mengoni and T. Shirai : Fig. 1

Note: - spare experimental levels; more data needed (*)
- agreement by VM with "abinitio" calc. at lower vibrational model;
- for discrepancies at higher part of the spectrum see work on the influence of majorana operator (*)

FIG. 1

All the parameters, except for N_i, are in cm^{-1}:

$N_1 = 6$	$N_2 = 95$	$N_3 = 41$
$A_1 = -35.125$	$A_2 = -0.25$	$A_3 = .1375$
$A_{12} = -2.75$	$A_{13} = -3.375$	$A_{23} = -1.25$
$\lambda_{12} = -0.1766$[a]	$\lambda_{13} = 0.6835$[a]	$\lambda_{23} = 0.0155$[a]

v_1 = H–C stretch, v_2 = HCO bend, v_3 = CO stretch

v_1 v_2 v_3	E^{exp} (cm^{-1})	E^{calc} (cm^{-1})		ΔE
	Ref. 7	case 1	case 2	
0 1 0	1089.0	1076.0	1081.5	7.5
0 0 1	1871.0	1869.0	1868.5	2.4
1 0 0	2444.0	2423.5	2434.9	9.1
0 2 0	2129.0	2126.0	2137.0	-8.0
0 1 1	2936.0	2935.0	2940.0	-4.0
1 1 0	3468.0	3472.5	3488.0	-20.0
0 0 2	3702.0	3704.0	3703.1	-1.1
1 0 1	4275.0	4270.5	4281.7	-6.7
0 2 1	3984.0	3975.0	3985.5	-1.5
1 2 0	4533.0	4495.0	4515.1	17.9
0 1 2	4767.0	4760.0	4764.5	2.5
δ (cm^{-1})		14.1	9.5	

[a] Fitted parameter in case 2.

Table 1

All the parameters, except for N_1 and N_2, are in cm^{-1}:

$N_1 = 8$ $\quad$ $N_2 = 105$

$A_{12} = -2.75$

$A_1 = -38.75$ $\quad$ $A_2 = -1.75$

VM analysis of HCO

$A_1 = -41.45$[1] $\quad$ $A_2 = -1.78$[1]

$\lambda = -0.2458$[1]

v_1 = H–C stretch, $\quad$ v_2 = HCO bend, $\quad$ v_3 = C–O stretch

$v_1\ v_2\ v_3$	$E^{exp}(cm^{-1})$	$E^{calc}(cm^{-1})$		ΔE	$E^{ab\text{-}initio}(cm^{-1})$
	Ref. 7	case 1	case 2		Ref. 8
0 1 0	1089.0	1130.0	1078.1	10.9	1104.0
0 0 1	1871.0	1865.0	1874.2	−3.2	1885.0
0 2 0	2129.0	2240.0	2144.4	−15.4	2184.0
1 0 0	2444.0	2370.0	2427.4	16.6	2448.0
0 1 1	2936.0	2975.0	2932.8	3.2	2996.0
0 3 0	----	3330.0	3198.5	–	3234.0
1 1 0	3468.0	3480.0	3481.8	−13.8	3503.0
0 0 2	3702.0	3696.0	3714.2	−12.2	3753.0
0 2 1	3984.0	4065.0	3979.6	4.4	4074.0
0 4 0	----	4400.0	4240.0	–	4254.0
1 0 1	4275.0	4215.0	4281.9	−6.9	4326.0
2 0 0	----	4410.0	4501.3	–	4484.0
1 2 0	4533.0	4570.0	4528.8	4.2	4563.0
0 1 2	4767.0	4786.0	4753.4	13.6	4871.0
δ (cm^{-1})		54.9	10.7		55.0

[1] Fitted parameter in case 2.

Table 2

All the parameters, except for N_1 and N_2, are in cm^{-1}:

$N_1 = 13$ $N_2 = 108$

$A_{12} = -1.635$

$A_1 = -20.935^a$ $A_2 = -2.334^a$ VM analysis of DCO

$\lambda = 0.3433^a$

$v_1 \equiv$ D–C stretch, $v_2 \equiv$ DCO bend, $v_3 \equiv$ CO stretch

v_1 v_2 v_3	E^{exp} (cm^{-1})	E^{calc} (cm^{-1})	ΔE
	Ref. 7		
0 1 0	863.0	870.7	−7.7
0 2 0	1715.0[b]	1719.9	−4.9
0 0 1	1807.0	1802.8	4.2
1 0 0	1930.0[b]	1921.3	8.7
0 3 0	2548.0[b]	2548.0	0.0
0 1 1	2637.0	2660.3	−23.3
1 1 0	2779.0[b]	2782.3	−3.3
0 4 0	3362.0[b]	3355.5	−6.5
0 2 1	3515.0	3496.0	19.0
1 3 0	4428.0	4433.3	−5.3
δ (cm^{-1})		10.8	

[a] Fitted parameter. (LS procedure).

[b] ab-initio value from Ref. (8).

Table 3

B. Progress in the calculation of the matrix elements of dipole transition operators in the cross section evaluation for the electron-molecule collision processes.

(A. Mengoni* in cooperation with T. Shirai in the frame of the above mentioned stage at JAERI).

The activity is in progress according to the algebraic-eikonal approach and description of the molecular rotational and vibrational degrees of freedom within the framework of the Vibron Model by F. Iachello.
This approach is extended to include the vibrationally inelastic processes, and the quadrupole interaction, in addition to the dominant dipole, has been included in order to improve the descriptionn of the collision process dynamics, particularly at large scattering angles.

In the following Fig. 2 differential cross sections for electron scattering on HF molecule at 2 eV(a) and 3 eV(b) are presented. The dotted lines refer to algebraic-eikonal approach with dipole interactions; only the solid line results are calculated including the quadrupole interaction.

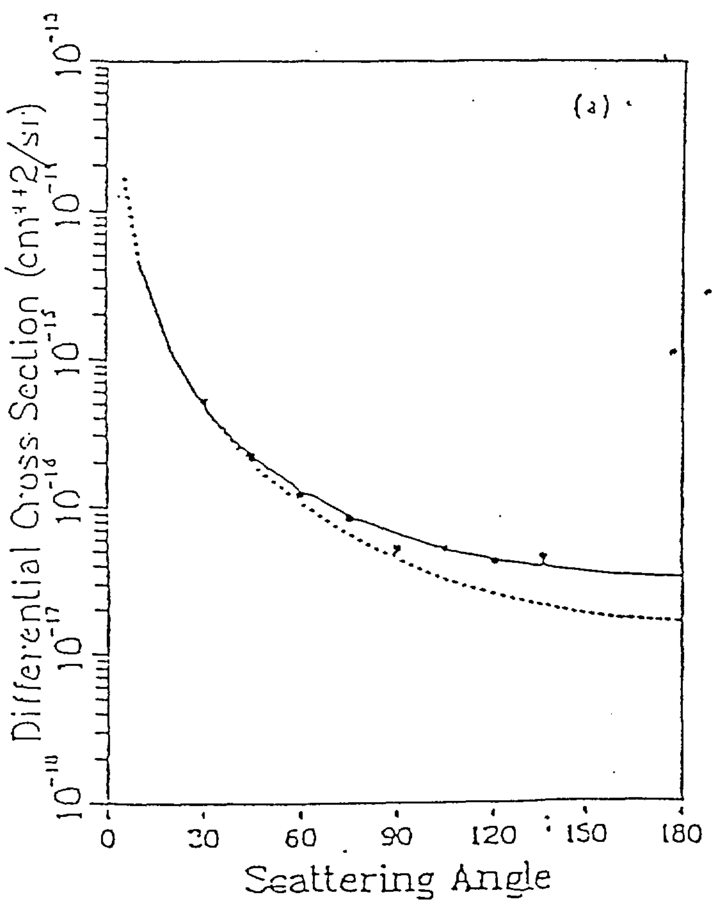


fig. 2.a

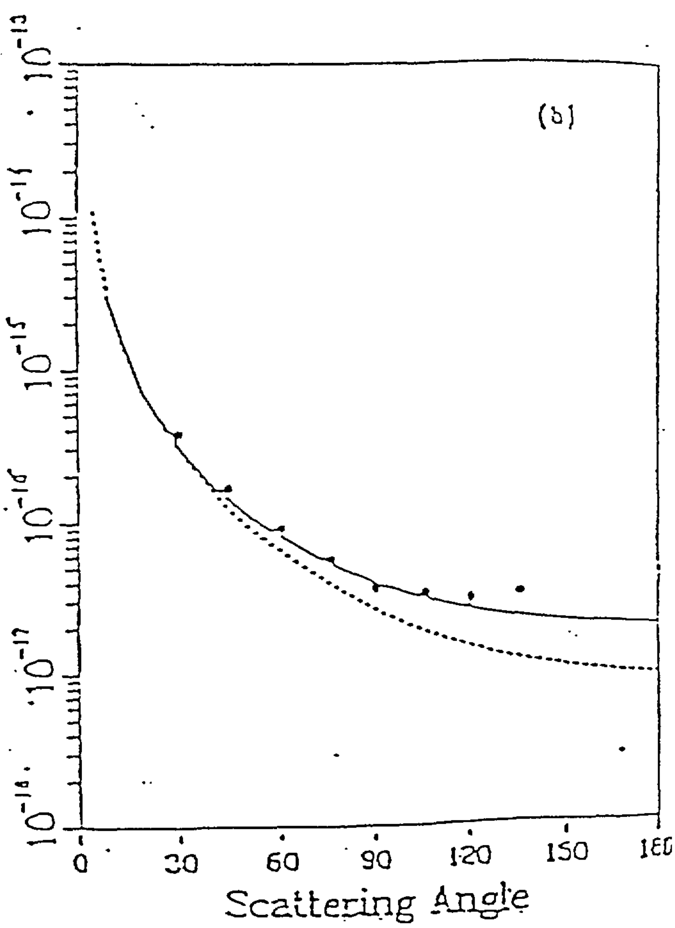


fig. 2. b

The calculated data are available to the international A+M community in the frame of the IAEA coordinated network.

Both the inclusion of other reaction mechanisms and the extension to the scattering processes on polyatomic molecules are investigated and in progress at present.

The "Hybrid Approach" by Bijker et al., i.e. coupled-channel calculations for "low" partial-waves and the algebraic-eikonal approach for "high" partial-waves (in a partial-wave expansion of the scattering amplitudes) and the more recent rotating-frame approximation have been considered as the appropriate basis for the progress on treatment of electron collision processes with polyatomic molecules, where short-range interactions play the key role.

C. Calculation of most relevant data for the interaction of slow protons with an iron surface.

V. Rosato and A. Ventura (**)

Particle and energy reflection coefficients were estimated and a detailed evaluation of the different contributions (elastic and inelastic) to the energy loss of the reflected particles was performed.

(**) Dept. for Innovative Technologies

It is well known that these data are requested for particle-material interaction (tipycally particles at the cold plasma edges in the, energy range O.1-100 eV) estimate, of interest as the main cause of embrittlement and swelling phenomena.

Following a previous analogous computer experiment devoted to the interaction of the ions on Ni surface, molecular dynamics (MD) simulation has been performed on proton interaction with a Fe surface, with particular regard to estimate the relevance of the inelastic energy loss (IEL) of the projectiles in comparison with the elastic one (EEL) at low energies.

With respect to analogous approach from the previous literature, the model has been improved by introducing a microscopic friction coefficient depending on the instantaneous electron density experienced by the projectile.

MD simulations have been carried out for protons incident at right angles to the {100} iron surface with energies 1,5,10 and 50 eV.

At higher energies the results have been compared with the simpler and faster binary collision approximation (BCA) and the agreement turns out to be good at 10 eV and slightly worse at 50 eV, probably because of increasing IEL, this contribution being greater in the present model.

At lower energies (1-10 eV) the pure BCA is not a good approximation and MD has been adopted as on almost unique tool for reliable calculations of data regarding ion absorption and scattering by metal surfaces.

Work submitted for publication in view of the availability of the results to the A+M data community under IAEA coordination.

Electron-ion collision excitation data.
P.L. Ottaviani(*), G.C. Panini (*) and M. Frisoni (*)

The conversion was completed of electron-ion excitation data for Iron (critically selected and compiled at ENEA-Bologna) from a strictly domestic structure into ALADDIN format according to agreed standardization rules for retrieval and distribution.

The FORTRAN code EXC, designed for a mainframe to selectively tabulate one or more excitation functions, was modified accordingly. Unlikely the EXC code cannot be compiled by Personal Computer FORTRAN compiler, because of the size of the main. This code generates, among others, one output file that can be put directly as input to the PLOTTAB code.

Both EXC code and the selected data (compiled at ENEA Bologna) in ALADDIN format were sent on diskette to IAEA, Atomic and Molecular Data Unit, for the purposes of distibution and exchange.

D. Atomic data requested for spectroscopic analises on FTU and general requirements at ENEA - Fusion Department (°)

i) For estimating the radiative emission rates and the transport of intrinsic or injected impurities in FTU plasma, atomic data of interest are:

- Ionisation coefficients;

- Radiative recombination coefficients;
- Energy levels, transition wave lenghts (λ< 7000 Å), Landé factors;

- Transition probabilitie

Data are required for the folowing elements:

Al, Cr, Fe, Ni, Mo, Mn, Ti, Cu Ag, Au;

Li, B, C, O;

Na, Mg

F, Cl

ii) For elements such as Ti, Fe, Mo, W, Si, at all ionisation states, required data are:

- Ionisation rate coefficients as a function of Te and Ne (in approximation formulas) or coefficients in Lotz formula, namely binding energy of the electrons and number of equivalent electrons in the i-th subshell, and fitting constants in Lotz formula.

(°) By Drs. R. De Angelis, M. Ciotti, G. Mazzitelli, G. Maddalumo, F. Romanelli, R. Zagorsky.

- For dielectronic recombination determination in every transition, the oscillator strenght and the transition energy in eV.

- For line radiation and cooling rate estimate, to define, for every ion, lines to be considered and calculate, for every line, excitation rate coefficient, as a function of Te, and excitation potential.

- Self-sputtering yield for Mo (particularly in TZM), W (mainly for Inconel 600 and 625) and Ni.

- Reflection coefficient, as a function of the particle energy, for H, D, He on the same elements (as in the previous point) at low energies (tens of eV) and different incident angles.

- Electron impact ionisation cross sections, especially at low energies (tens of eV) on Ni, Mo, W impurities.

E. Molecular Data Needs for Radiation Transport in the Atmsphere (°°).

In the Monte Carlo code development for electromagnetic transport simulation in the atmosphere, one has to face with diffusion and absorption reactions with molecules and aerosols.

As regard radiation-molecule interaction, the knowledge of line and continuum contributions to absorption coefficient is of primary interest (scattering coefficient can be obtained through the well-known Rayleigh formula).

The radiation wave length of interest is in the range of 0.2-300 μm.

Typical molecules are:

H_2O; O_2; O_3;

CO; CO_2; CH_4;

N_2; NO; N_2O; NO_2;

NH_3, HNO_3;

SO_2.

Spectroscopic molecular data both for rotational and vibrational bands are requested accordinghy.

(°°)By Dr. E. Cupini - Dept. for Advanced Technologies.

GAPHYOR Atomic and Molecular Data Centre

Activities during year 1993

J.L.Delcroix,D.Humbert, C.Leprince

Science Experts Group : P.Archirel, M.Aubès, J.P.Booth, M.Capitelli, J.L.Delcroix, A.M.Diamy, F.Emard-Katsonis, A.Faenov, V.Hrachova, K.Katsonis, C.Lalo, M.Magulov, J.Masanet, A.Ricard, B.Veyret, M.Yousfi

Data production and evaluation group : K. Katsonis

Centre de Données GAPHYOR, Université de Paris-Sud, Bat. 212
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presented at the 12th Atomic and Molecular
Data Centre Network Meeting
IAEA, Vienna, 20-21 September 1993
Rapport GA-.....

1. SOME STATISTICS.

As of the 15th of September 1993, the total number of entries in the files was about 278,000 distributed as shown in Table 1 and in more detail for each process in Table 2.

Table 1: Number of entries by sections and number of elements (15th-September-93)

	SECTION 1	SECTION 2	SECTION 3	SECTION 4	SECTION 5	TOTALS
	Structure	Photon. Coll.	Electron. Coll.	Atom.,Mol.Coll	Macro.Pro.	
1 ELEMENT	49412	7829	16905	7956	5056	**84458**
2 ELEMENTS	60266	6247	5222	36564	7970	**118269**
3 ELEMENTS	28876	2901	988	24342	3176	**60283**
4 ELEMENTS	6067	561	125	7165	943	**14861**
TOTAUX	**144621**	**17538**	**20540**	**78027**	**17145**	**277871**

Table 2: Number of entries by process in each section (15th-September-93)
(the process code has been published in [1] and recent developments in [2]) .

SECTION 1 Structure		SECTION 2 Photon.Coll..		SECTION 3 Electron. Coll		SECTION 4 Atom.,Mol.Coll.		SECTION 5 Macro.Prop	
EN	80839	AN	2062	SN	1156	SN	1169	PV	1269
CP	271	SN	496	SC	512	SP	249	FT	2045
DP	3782	SC	331	EL	1794	SC	697	VR	159
NP	952	EL	210	EX	5269	EL	830	ZT	135
PE	2957	FF	84	ER	582	EN	4107	CO	139
VR	37444	EX	1858	DX	205	EX	2790	DN	663
TR	13619	ER	419	XX	466	ER	1272	VI	767
IN	1152	DX	110	DO	46	DX	8439	CT	966
DT	276	XX	68	IN	5545	XX	2396	TD	336
DS	2035	DO	99	RC	220	DO	310	PE	307
XX	94	IN	6879	RR	208	TE	2237	EN	2901
EA	1135	DT	563	RE	104	IN	7806	DM	66
PF	20	DS	3904	RO	71	TI	35	RN	937
EI	33	NL	149	RD	577	DT	1027	FE	423
DG	12	PR	306	RS	658	IO	4331	CE	417
		EE	0	AT	1793	O-	272	ME	654
				DT	62	I-	2	DE	185
				DS	939	IM	367	PI	501
				BS	225	RI	494	AT	457
				PR	108	XD	747	DT	70
				EE	0	CX	3806	PC	68
				PU	0	CI	1371	FI	38
				DG	0	CA	297	MI	926
						SI	668	DI	194
						SR	160	DA	47
						IR	17645	RC	97
						IH	0	RR	85
						IA	108	RE	21
						ID	814	RO	7
						AS	5170	RD	7
						AH	0	RS	0
						DS	3461	RI	6
						DH	0	PD	0
						KE	804	LA	1003
						AD	22	MD	107
						PR	4107	ST	1142
						EE	0		
						PU	11		
						DG	6		
Σ	144621	Σ	17538	Σ	20540	Σ	78027	Σ	17145

[1] J.L. DELCROIX Gas-phase chemical database (Elsevier 1988)]
[2] GAPHYOR UPDATE 1993-2

2 CHANGES IN CLASSIFICATION SCHEME

In the new format GAPHYOR-93 we introduce two kind of changes in the classification scheme :

-New descriptors mainly for gas(plasma)-surface interactions : they are shown in boxes of Table 2. Their meaning are :

PF Dynamic polarizability (a function of frequency)
EI Energy of isomerization of a molecule
EE Emission of electrons or ions by a solid
PU Sputtering (emission of neutrals)
DG Desorption of an adsorbed molecule (or atom)

-Simplified descriptors for some domains (charge transfer, recombination, wave functions). This is obtained by cancelling some descriptors and grouping with some others. The cancelled descriptors are shown with shaded characters in Table 2.

3 GAPHYOR 73-93 MUTATION

We are presently working on a Program we call Mutation GAPHYOR 73-93. It was initially imposed to us by the closure at the end of 1993 of the main frame computer on which GAPHYOR is installed. This decision is due to the large changes in Computer Technology that occured since 1973, the beginning year of GAPHYOR.

But we also decided to introduce a new GAPHYOR format to take into account the new developments in some fields of atomic and molecular Physics (spectroscopy of internal shells in atoms, multi-charged ions, clusters, interactions gas/plasma-walls, ...). Finally we know better the needs and the requirements of users for an easier consultation, and we introduce also those in the conception of the new format that we call GAPHYOR-93.The Mutation Program GAPHYOR 73-93 includes then essentially three parts :

-Transfer of GAPHYOR from a main frame computer to a **Work Station** (Sun XXX). We shall for continuity still use ADABAS SGDB but in a new version implemented on this Work Station.

-**Direct entry** of the Data by our Science Experts on their personal computer using Micosoft EXCEL. This was discussed during our last meeting.

-A **new format** for the Data using natural physico-chemical language at every step of the production and use of the Database. This new GAPHYOR-93 format is compared to the former GAPHYOR-93 internal language format in Table 3. The main features of the new format are as follows :

The atoms, molecules, clusters, multi-charged ions, solids, adsorbed atoms or molecules, isoelectronic series and homonuclear sequences are described in a **natural physico-chemical language** which is totally explicit.

The new descriptor s **(internal structure)** describes the electronic structure of internal shells of an atom with for exemple :

s=K1L1 => one hole in K shell and one hole in L shell
s=H1 => one unspecified hole
s=MU1 => one electron replaced by a μ meson

It is also used to specify coarsely the structure of a wall with for exemple :

s=G => amorphous solid (glass)
s=M => mono-crystal
s=P => poly-crystalline solid
s=L => liquid

The new descriptor **n (multiplicity)** is used to describe multi-photon and multi-electron processes. It can be used also when in the final state their are several identical reactants (for exemple, energy of atomization of a molecule).

Energies are now described more accurately. We still use the values L, J, H of descriptor INFO to specify a class of energies (low, medium, high), but we use now the descriptor **ENER** to specify the limit values of energy.

The new descriptor **VAL (Values)** allows us to enter a numerical value. GAPHYOR is still essentially a factual and bibliographical Database. But in many simple cases the information is only a single number (life-time, probability, reaction rate and/or cross section at a given temperature or energy, ...). In those cases the descriptor VAL (free text) gives this value.

The new descriptors **AU1, ... AU10 (authors)** give now the full list of authors (up to 10 authors !). The site of the research is still is still described by NASTCI and is the one of the laboratory of the first author.

The new descriptor **REM (Remarks)** is used for special informations (remarks on the process, spectroscopic notation to specify a level,...). Exceptionnally, it can be used to specify authors 11, 12, ... when there is a (reasonable) number of authors larger than ten.

The descriptor REF **(Reference counter)** is only for internal use by GAPHYOR team.

GAPHYOR-73			GAPHYOR-93			Remarks
	Descripteurs	Exemples		Descripteurs	Exemples	
FA,FB,FC,FD	Mendeleev families					cancelled
AA,BB,CC,DD	Elements					cancelled
SE	Section	1, 2, 3, 4, 5	SE	Section	1, 2, 3, 4, 5	same
M1(f1 i1 x1)	Initial state (molecule 1)		M1(f1 i1 x1 s1 n1)	Initial state (molecule 1)		improved
f1	Formula	1124, e, P, 00	f1	Formula	Si1Ge1Cl2Br4, e, hν, (M)	improved
	cluster	complex code		cluster	(H1)+(C1O2)5	simpler
	clusters sequence	complex code		clusters sequence	(H1)+(C1O2)5-12	simpler
	stoechiometric solid	11 0W		stoechiometric solid	(Na1Cl1)s	simpler
	alloy	ABC 0W		alloy	(Fe-Ni-Co)s	simpler
	adsorbed molecule			adsorbed molecule	(N2)a(Fe-Ni-Co)s	simpler
	isoelectronic series	complex code		isoelectronic series	Aa(He)	simpler
i1	Ionization	0, 1, 6, complex code	i1	Ionization	0, +, -, 12+	simpler
	isoelectronic series	complex code		isoelectronic series	Z(2-10)	simpler
	homonuclear sequence	complex code		homonuclear sequence	n+(1-8)	simpler
x1	Excitation	0, 1, 2, ... (code)	x1	Excitation	0, srv***myn	improved
			s1	Internal structure	K2L1M1, H1, MU1	NEW
				solids	G, M, P, L	NEW
			n1	Multiplicity	21	NEW
M2(f2 i2 x2)	Initial state (molecule 2)	cf. M1	M2(f2 i2 x2 s2 n2)	Initial state (molecule 2)	cf. M1	improved
M3(f3 i3 x3)	Initial state (molecule 3)	cf. M1	M3(f3 i3 x3 s3 n3)	Initial state (molecule 3)	cf. M1	improved
PR	Processus	DS	PR	Processus	DS	same
M4(f4 i4 x4)	Final state (molecule 4)	cf. M1	M4(f4 i4 x4 s4 n4)	Final state (molecule 4)	cf. M1	improved
M5(f5 i5 x5)	Final state (molecule 5)	cf. M1	M5(f5 i5 x5 s5 n5)	Final state (molecule 5)	cf. M1	improved
M6(f6 i6 x6)	Final state (molecule 6)	cf. M1	M6(f6 i6 x6 s6 n6)	Final state (molecule 6)	cf. M1	improved
INFO	Informations	SWKUP<RETDXLJH23BI5M47	INFO	Class of datas, energies, ...	SWKUP<RETDXLJH23BI5M47	same
			ENER	Limits of energy	1-4 keV	NEW
			VAL	Data values	(free text)	NEW
AN	Publication year	92	AN	Annee de publication	92	same
JO	Journal	pr/a	JO	Journal	pr/a	same
VO	Volume	46.5	VO.n	Volume and number	46.5	improved
PAGE	Page	2592	PAGE	Page	2592	same
AU1	Author 1	Cederquist H	AU1	Author 1	Cederquist H	same
			AU2	Author 2	Andersson H	NEW
			AU3	Author 3	Beebe E	NEW
			AU4	Author 4	Biedermann C	NEW
			AU5	Author 5	Broström L	NEW
			AU6	Author 6	Engström Å	NEW
			AU7	Author 7	Gao H	NEW
			AU8	Author 8	Hutton R	NEW
			AU9	Author 9	Levin J C	NEW
			AU10	Author 10	Liljeby L	NEW
NASTCI	Site (laboratory of AU1)	sdstst	NASTCI	Site (laboratory of AU1)	sdstst	same
			REM	Remarks (optional)	(free text) (levels, ...	NEW
REF	Reference counter	1	REF	Reference counter	1	NEW
NB	Entry number	397452	NB	Entry number	397452	same

Progress Report :

A&M Data Activities at NIFS 1992/1993

1993.9.21 H.Tawara

I) Data compilation/evaluation

1) Critical compilation/recommendation of electron scattering cross sections by helium atoms : We have compiled and critically evaluated the elastic and inelastic (for 25 excited states) electron scattering cross sections from the ground state He atoms, differential in scattering angle and/or electron energy (DCS). A number of the iterations are necessary to get the final recommendation data which must be consistent in all DCS and total cross sections. The final results with about 200 figures will be published soon in NIFS-DATA report.[1]

2) Compilation and recommendation of cross sections data for impurity (C^{q+}, O^{q+}, Be^{q+}, B^{q+}) ions : Following a previous compilation,[2] this topics has been discussed at IAEA CRP meeting and a review on the present status of data for these species has recently been published.[3]

3) Compilation of molecular species relevant to edge plasma : Data for hydrocarbon have been published recently[4] and also those for common impurities (H_2O, CO, CO_2) have been reported.[5] It is noted that significant discrepancies still exist among these data, in particular for data for photon emissions and dissociation processes.

4) New data for hydrocarbon molecules[6] : In a previous report it is pointed out that there are still significant discrepancies of electron collision data for hydrocarbon. To improve the situations, we have remeasured the cross sections for total scattering cross sections and total ionization cross sections, using a carefully designed apparatus, for typical hydrocarbon molecules (CH_4, C_2H_6, C_2H_4, C_3H_8, C_3H_6 etc.), which may be present and play an important role in plasma devices with graphites. This systematic investigation has revealed some close correlation between total ionization cross sections and polarizabilities and total number of electrons in molecules.

5) Recommendation for electron impact excitation cross sections by N atoms and N-like ions : The present situation has been reviewed and recommended for the excitation cross sections for N atoms and N-like ions (up Fe XX)[7] (the survey has been made up to Kr XXX). The effective collision strengths for

Maxwellian distributions are fitted to an analytical expression, based on the assumed collision strength formula. These effective collision strengths and the fitted parameters are given for ions up to Fe XX ions.

References
1) M.Hayashi et al., to be published in NIFS-DATA-21 (1993)
2) H.Tawara, NIFS-DATA-12 (1991)
3) ref. III-2)
4) ref. III-1)
5) Ref. II-2)
6) H.Nishimura and H.Tawara, submitted to J. Phys. D (1993)
7) ref. II-1)

II) Internal Reports

1) T.Kato, NIFS-DATA-18 (Sept., 1992)
Electron impact excitation cross sections and effective collision strengths of N atoms and N-like ions - a review of available data and recommendation
2) H.Tawara, NIFS-DATA-19 (Sept., 1992)
Atomic and molecular data for H_2O, CO and CO_2 relevant to edge plasma impurities
3) H.Tawara, NIFS-DATA-20 (Apr., 1993)
Bibliography on electron transfer in ion-ion/atom/molecule collisions

III) Related publications

1) H.Tawara, Y.Itikawa, H.Nishimura, H.Tanaka and Y.Nakamura, Suppl. Nucl. Fusion Vol.2 (1992) 41
Cross sections for collisions of electrons with hydrocarbon molecules
2) T.Kato and R.K.Janev, Suppl. Nucl. Fusion vol.3 (1992) 33
Parametric representation of electron impact excitation and ionization cross sections for helium atoms
3) R.A.Phaneuf, R.K.Janev, H.Tawara, M.Kimura, P.S.Krstic, G.Peach and M.A.Mazing, Suppl. Nucl. Fusion vol.3 (1992)
Status and critical assessment of the database for collisions of Be^{q+} and B^{q+} ions with, H, H_2 and He

IV) On-going programs

1) Collisional radiative model for highly excited species

A working group has been organized to develop a new CR model which allows us to treat highly excited states of ions. At present, this group is concentrating on the following issues :

a) to find asymptotic form for the collisional excitation and ionization at high energy limit (GOS multiplying with a structure factor),

b) to compile radiative and dielectronic recombination rates (mainly for Fe ions),

c) to find suitable fitting formula for cross sections and rate as a function of energy and temperature,

d) to develop computational code to calculate l-changing processes,

e) to make substantial models.

They can generate the cross sections necessary for ions up to the n=20 states. They are also trying to treat non-hydrogenic ions.

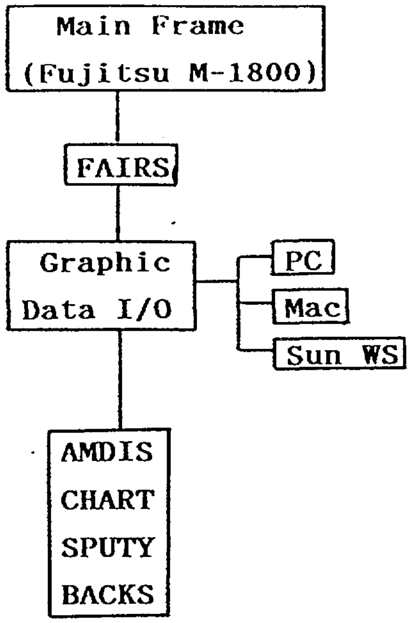
2) Compilation/empirical formulas of sputtering data :
Systematic updating of previous compilations (in collaboration with Y.Yamamura) including more data of graphites
At. Data & Nucl. Data Tables 31 (1984) [IPPJ-AM-32 (1983)] ; NIFS-DATA-1 (1990)

3) Compilation of atomic and molecular data involving excited species (mainly of H^* and H_2^*) (in collaboration with K.Onda et al.) : It is well known that many species, including molecules, are probably in the excited states near divertor regions, meanwhile the collision data strongly depend upon the electronic states of (atomic as well as) molecular species.

V) International collaboration

Dr.V.A.Abramov stayed at NIFS under the support of JSPS over 3 months and worked out instabilities of Be and B ion-seeded plasmas in tokamaks.

Data Handling at NIFS



Aladdin DB
(see Cadarache Report p.60)

Ionization :
  cross section/rate coefficient
   (Belfast, Lotz)
Excitation :
  cross section/rate for
   He atoms, He-like ions, O^{q+} ions
Molecular data (planned) :

access to NIFS database via internet :
     telnet msp.nifs.ac.jp

(you need to register as NIFS collaborator)

any inquiries should addressed to
     kato@nifs.ac.jp

Activities of the Multicharged Ions Spectra Data Center (MISDC) at the National Scientific and Research Institute for Physical-technical and Radio-technical Measurements (VNIIFTRI).

A.Ya. Faenov, Head of MISDC

During last year (June 1992 - September 1993) the major activity at MISDC has been connected with the following subjects:

I. Theoretical and experimental investigations of atoms and ions spectra (Measurements and calculations of different spectra; developing special software for database; collecting, evaluating data on electron impact excitation, ionization, dielectronic recombination, energy levels, wavelengths, transition probabilities, ionization potentials).

II. X-ray Spectra Excitation Features (Intensities and Line Shapes) and Plasma Diagnostics.

III. Creation of different x-ray spectroscopic equipment. Achieved main results.

I. a) According with agreement between LLNL and MISDC during last year we continue to develop the software for our database "SPECTR" operated at MISDC and LLNL on IBM PS/2 computer. Now we have some additional possibilities allowed, for example, to present DB "SPECTR" data in graphic form.

b) We continue inputing information on spectroscopic characteristics of ions to DB "SPECTR". Apart from new published data, during last year some unpublished results obtained at LLNL, LANL and some institutes of RF for satellite lines, caused by transitions in multicharged Li-, Be-, B-, C-, N-, O-, F-, Na-like ions, were inputed, and now our database is working with 346 985 records.

c) We continue collecting, evaluating data on atomic collisional processes. (See Appendix 1).

d) Together with LLNL (DR. J. Nilsen). We carried out the experimental and theoretical investigations of the satellites to resonance transitions of Ne-like selenium excited in laser-produced plasma. About of 300 features in spectra observed were identified as radiative transitions in Na-like selenium. Their wavelengths were determined with an experimental accuracy $\pm 5 \cdot 10^{-4}$ Å. A good agreement between the model satellite structure calculation and experimental results showed the usefulness of these spectra for high-temperature plasma diagnostic applications.

e) We analized the emission spectra of CO_2-laser produced plasma in the vicinity of the He-like ion resonance lines of Mg, Al, Si, P, S. Comparison the experimental results with theoretical ones allowed to identify about 120 spectral lines, caused by radiative transitions from doublyexcited levels of Be-, B-, C-, N-, O- and F-like ions. The discrepancy between theoretical and experimental wavelength values were usually $\pm 0.0005 \div 0.001$ Å.

f) Together with Max-Pnanck-Institute (Dr. P. Nickles, Berlin). We investigated the interaction of intensive (flux density up to 10^{18} W/cm^2) picosecond laser pulse with solid magnesium target. Spectrometers with flat CsAP crystal and spherically bent mica crystal were used to record the line emission spectra of H-, He-, Li- and Be-like magnesium ions. The unique luminosity and spectral resolution of mica spherical crystal spectrometer ($\lambda/\Delta\lambda$ up to 10^4) allowed to observe and identify the number of X-ray spectral lines, caused by $1s2l2l'3l'' \rightarrow 1s^2 2l'3l''$ transition in Mg IX. (calculations of wavelengths, energy levels and transition probabilities for such transitions were done by J. Abdallah. and R. Clark, LANL).

g) Together with Cornell University (Prof. D. Hummer) and P.N. Lebedev Physical Institute (Dr. S. Pikuz). We continue studying emission X-ray spectra of superdence X-pinch plasma. In this plasma we observed self-absorption effects for satellites to resonance line of He-like Mg XI ion and for the first time observed forbidden satellite transition $2p^2\ {}^1D_2 \rightarrow 1s2p\ {}^3P$.

h) Together with LLNL (Dr. J. Nilsen). Some experiments has been carried out in the field of short wavelengths lasers. It were the precise measurements of the coincidence of H-like Mg XII L_α-doublet (pumping line) and 3p-2s transition of Ne-like Ge XXIII near 8.42 Å. It was shown, that the defect of resonance for these lines is about 0.0016 Å. It means, that the spectral distance between these lines are smaller than its widths and Mg XII L_α radiation can be used for effective photo excitation of 2s-3p transition in Ge XXIII.

Appendix 1.

MISDC ACTIVITY ON STORING ELECTRON-ION COLLISION DATA.

The MISDC have compiled in ALADDIN format the data for following collision processes in plasma:

(i) Electron impact excitation (cross sections and rate coefficients) for:
H-like ions BeIV and CVI taken from ref. [1];
He-like ions LiII, CV, AlXII, CaXIX from refs. [2,3];
Li-like ions BeII, CIV, AlXI, CaXVIII from ref. [4];
Be-like ions CIII, OV, Si XI, Fe XXIII, Mo XXXIX from refs. [5,6] and Be atom from ref. [7].

(ii) Electron impact ionization (cross sections and rate coefficients) for:
H-like ions CVI and FeXXVI from ref. [8,9].

(iii) Dielectronic recombination rate coefficients for:
H-like ions BeIII, CVI, AlXIII, CaXX from ref. [10];
Multicharged O and Fe ions from ref. [11].

These data have been added to the DB "SPECTR" in MISDC together with data from refs. [12-16] which we received from the Atomic and Molecular data Unit of IAEA in ALADDIN format. Nowadays DB "SPECTR" contains about 6000 records for collision processes data for various energy levels. The software of DB enables to search and represent data in table and graphic forms and we continue to enhance it.

References.

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2. A.V. Borovsky et al., Preprint No. 223, Institute of General Physics, Moscow, 1987.
3. A.V. Borovsky et al., Preprint No. 49, Institute of General Physics, Moscow, 1988.
4. A.V. Borovsky et al., Preprint No. 85, Institute of General Physics, Moscow, 1989.
5. A.V. Borovsky et al., Preprint No. 48, Institute of General Physics, Moscow, 1990.
6. U.I. Safronova et al., Physica Scripta, V. 46, 409 (1992).
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10. A.V. Borovsky, and O.I. Zatsarinniy, Preprint No. 78, Institute of General Physics, Moscow, 1989.
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12. C. Bottcher, et al., Special Supplement to Nuclear Fusion, 1987.
13. R.A. Phaneuf et al., Atomic Data for Fusion, Vol 5. Report ORNL-6090/V, February, 1987.
14. Y. Itikawa, et al., Atom. Data and Nucl. Data Tabl., V.33, 149 (1985).
15. T. Kato, and S. Nakazaki, At. Data and Nucl. Data Tabl., V.42, 313 (1989).
16. C.F. Barnett, Atomic Data for Fusion, Vol 1, Report ORNL-6086/VI, July, 1990.

DB SPECTR version 3.03

The total number of records ≃ 340 000

(IBM PS/2, 4 MB RAM, 386/387 processor)

Query	Search time	The number of records selected
1. Lines of copper ions in wavelength region (10,1 ÷ 10,11) Å.	5 s	10
2. Lines of silver ions in wavelength region (10 ÷ 15) Å.	35 s	94
3. Lines of H-like and He-like silicon.	25 s	3083
4. 3d-2p transitions in Ne-like and Na-like silver.	12 s	316
5. $1s2p\ {}^1P_1 - 1s^2\ {}^1S_0$ transition in He-like uranium.	16 s	3
6. $2s2p^6 3p - 2s^2 2p^6$ transitions in Ne-like ions.	13 s	387
7. Lines of OI atom.	4 s	401
8. Lines of O-like and N-like iron.	24 s	986

The Oak Ridge National Laboratory

Controlled Fusion Atomic Data Center:

Progress Report, 1993

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Mission and Continuing Activities

⋆ The mission of the ORNL CFADC is to identify, compile, evaluate, and recommend atomic and molecular collision data of interest to fusion energy research and development.

- Maintain a PC-based bibliographic database of categorized references.
- Answer individual requests for bibliographic or numerical atomic data (1-2 per week typically).
- Publish data compilations and recommendations through the series *Atomic Data for Fusion* ("Redbooks") and other topical reports.
- Develop and implement the internationally accepted data exchange format ALADDIN.
- Identify data needs and assess status of existing data for fusion applications. Deduce scaling laws and parameterizations of this data to facilitate its use.
- Coordinate activities and collaborate with the International Atomic and Molecular Data Center Network.

The CFADC Bibliographic Database

<u>1978-present</u>

- PC-based, utilizing dBaseIII
- Currently 25,435 entries
- Approximately 1000-1500 entries added per year
- About 120 journals searched by consultants (Gilbody, McDaniel, Pindzola, Thomas, Morgan) and staff (Havener, Meyer) who index entries by reaction category, energy range, etc. (see example).
- The CFADC bibliography is electronically transmitted to several data centers internationally (IAEA, NIFS, Geissen) and with the contributions from other data centers, forms the basis for the IAEA publications *International Bulletin on Atomic and Molecular Data for Fusion* and *CIAMDA 87*.

<u>circa 1950 - 1977</u>

- Periodic bibliographies were published since the inception of the data center in 1958.
- Archival tapes and hardcopy outputs still exist. The old CFADC bibliographic publications may be searched by hand.
- CFADC bibliographic information is contained in the *CIAMDA 80* IAEA publication.

REACTION CATEGORIES WITH CODES

Code	**Reaction Description**
A01	Heavy Particle - Heavy Particle: GENERAL
A02	Heavy Particle - Heavy Particle: ELASTIC SCATTERING COLLISIONS
A03	Heavy Particle - Heavy Particle: EXCITATION
A04	Heavy Particle - Heavy Particle: DISSOCIATION
A05	Heavy Particle - Heavy Particle: FLUORESCENCE
A06	Heavy Particle - Heavy Particle: ELECTRON CAPTURE
A07	Heavy Particle - Heavy Particle: IONIZATION
A08	Heavy Particle - Heavy Particle: STRIPPING
A09	Heavy Particle - Heavy Particle: RECOMBINATION OR MUTUAL NEUTRALIZATION LEADING TO NEUTRAL PRODUCTS (ION-ION)
A10	Heavy Particle - Heavy Particle: ENERGY TRANSFER - VIB, ROTATIONAL, ELECTRONIC
A11	Heavy Particle - Heavy Particle: COLLISIONAL DE-EXCITATION
A12	Heavy Particle - Heavy Particle: COLLISIONAL LINE BROADENING
A14	Heavy Particle - Heavy Particle: INTERCHANGE INVOLVING H OR He
A15	Heavy Particle - Heavy Particle: ASSOCIATIVE REACTIONS
A16	Heavy Particle - Heavy Particle: ELECTRON DETACHMENT FROM NEG IONS ->CONTINUUM
A17	Heavy Particle - Heavy Particle: INTERACTION POTENTIALS
A18	Heavy Particle - Heavy Particle: ANGULAR SCATTERING
A20	Heavy Particle - Heavy Particle: ATTENUATION
B01	INTERACTION OF INDIVIDUAL ATOMS OR MOLECULES WITH EXTERNAL FIELDS
B07	COLLISIONS IN PRESENCE OF STATIC OR TIME VARYING FIELDS
C01	Particle Penetration in Macroscopic Matter: GENERAL
C02	Particle Penetration in Macroscopic Matter: ENERGY LOSS AND STOPPING POWER
C04	Particle Penetration in Macroscopic Matter: PARTICLE RANGE
C05	Particle Penetration in Macroscopic Matter: MULTIPLE SCATTERING
C06	Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION
C07	Particle Penetration in Macroscopic Matter: EXCITED STATE POPULATION
D01	Particle Interactions with Solid Surfaces: GENERAL
D02	Particle Interactions with Solid Surfaces: SPUTTERING BY ELECTRONS, NEUTRONS, H
D03	Particle Interactions with Solid Surfaces: SPUT PART CHARGE AND QUANTUM DIST
D04	Particle Interactions with Solid Surfaces: SEC ELECTRON EJECTION BY HEAVY PARTICLE AND ELECTRONS
D05	Particle Interactions with Solid Surfaces: PHOTOELECTRIC EJECTION OF ELECTRONS
D06	Particle Interactions with Solid Surfaces: REFLECTION OF ELECTRONS FROM SURFACE
D07	Particle Interactions with Solid Surfaces: REFLECTION OF HEAVY PARTICLES FROM SURFACES
D08	Particle Interactions with Solid Surfaces: CHARGE AND QUANTUM STATE DISTRIBUTION OF REFLECTED HEAVY PARTICLES
D09	Part Inter w/ Solid Surf: DE-EXCITATION, NEUTRALIZATION, IONIZATION, OR DISSOCIATION OF PARTICLES INTERACTING WITH SURFACES
D11	Part Inter w/ Solid Surf: STICKING COEFF, THERMAL ENERGIES AND ADSORPTION

Code	Reaction Description
D12	Part Inter w/ Solid Surf: ELECTMAGNETIC RADIATION INDUCED BY ELECTRON OR HEAVY PARTICAL IMPACT ON SURFACES
D13	Part Inter w/ Solid Surf: DESORPTION OF GASES FROM SURFACES
D17	Part Inter w/ Solid Surf: ELECTRON, ION AND PHOTON INDUCED CHEMICAL CHANGES TO SURFACES
D18	Part Inter w/ Solid Surf: TRAPPING AND REEMISSION OF HYDROGEN AND HELIUM
E01	Electron - Particle Interaction: GENERAL
E02	Electron - Particle Interaction: ELASTIC COLLISIONS
E03	Electron - Particle Interaction: EXCITATION
E04	Electron - Particle Interaction: DISSOCIATION
E05	Electron - Particle Interaction: IONIZATION
E06	Electron - Particle Interaction: RECOMBINATION (ELECTRON-ION)
E07	Electron - Particle Interaction: COLLISIONAL DE-EXCITATION
E08	Electron - Particle Interaction: COLLISIONAL LINE BROADENING
E09	Electron - Particle Interaction: NEGATIVE ION FORMATION
E11	Electron - Particle Interaction: FREE-FREE TRANSITIONS (BREMSSTRAHLUNG)
E13	Electron - Particle Interaction: ELECTRON DETACHMENT FROM NEGATIVE IONS
E16	Electron - Particle Interaction: FLUORESCENCE
E17	Electron - Particle Interaction: ANGULAR SCATTERING
E19	Electron - Particle Interaction: MOMENTUM TRANSFER
H01	Photon Collisions w/H.P. and Elec: GENERAL
H02	Photon Collisions w/H.P. and Elec: TOTAL ABSORPTION
H03	Photon Collisions w/H.P. and Elec: ELASTIC SCATTERING
H04	Photon Collisions w/H.P. and Elec: EXCITATION
H05	Photon Collisions w/H.P. and Elec: DISSOCIATION
H06	Photon Collisions w/H.P. and Elec: IONIZATION
H07	Photon Collisions w/H.P. and Elec: PHOTODETACHMENT
H08	Photon Collisions w/H.P. and Elec: FLUORESCENCE
H11	Photon Collisions w/H.P. and Elec: FREE-FREE ABSORPTION OR INVERSE BREMSSTRAHLUNG
J01	Data Compilation: HEAVY PARTICLE
J02	Data Compilation: ELECTRONS
J03	Data Compilation: PHOTONS
J04	Data Compilation: PARTICLES ON SURFACES AND SOLIDS
J05	Data Compilation: TRANSPORT
J06	Data Compilation: STRUCTURE
K01	Reviews and Books: HEAVY PARTICLE
K02	Reviews and Books: ELECTRONS
K03	Reviews and Books: PHOTONS
K04	Reviews and Books: PARTICLES ON SURFACES AND SOLIDS
K05	Reviews and Books: TRANSPORT
K06	Reviews and Books: STRUCTURE
K07	Reviews and Books: GENERAL
K08	Reviews and Books: USE OF ATOMIC DATE FOR PLASMA STUDIES
L01	Bibliographies: HEAVY PARTICLE
L02	Bibliographies: ELECTRONS
L03	Bibliographies: PHOTONS
L04	Bibliographies: PARTICLES ON SURFACES AND SOLIDS
L05	Bibliographies: TRANSPORT
L06	Bibliographies: STRUCTURE

REF. NO. = 6388
(E03)EXCITATION: e + Fe^{6+}; e + Fe^{7+}; e + Fe^{8+}
(E03)EXCITATION: e + Fe^{9+}; e + Fe^{10+}; e + Fe^{11+}
(E03)EXCITATION: e + Fe^{12+}; e + Fe^{13+}; e + Fe^{14+}
(E03)EXCITATION: e + Fe^{15+}; e + Fe^{16+}; e + Fe^{17+}
(E03)EXCITATION: e + Fe^{18+}; e + Fe^{19+}; e + Fe^{20+}
(E03)EXCITATION: e + Fe^{21+}; e + Fe^{22+}; e + Fe^{23+}
(E03)EXCITATION: e + Fe^{24+}; e + Ca^{17+}; e + Ca^{18+}
(E03)EXCITATION: e + Ca^{19+}; ;
(E05)IONIZATION: e + Fe^{6+}; e + Fe^{7+}; e + Fe^{8+}
(E05)IONIZATION: e + Fe^{9+}; e + Fe^{10+}; e + Fe^{11+}
(E05)IONIZATION: e + Fe^{12+}; e + Fe^{13+}; e + Fe^{14+}
(E05)IONIZATION: e + Fe^{15+}; e + Fe^{16+}; e + Fe^{17+}
(E05)IONIZATION: e + Fe^{18+}; e + Fe^{19+}; e + Fe^{20+}
(E05)IONIZATION: e + Fe^{21+}; e + Fe^{22+}; e + Fe^{23+}
(E05)IONIZATION: e + Fe^{24+}; e + Ca^{17+}; e + Ca^{18+}
(E05)IONIZATION: e + Ca^{19+}; ;
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{6+}; e + Fe^{7+}; e + Fe^{8+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{9+}; e + Fe^{10+}; e + Fe^{11+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{12+}; e + Fe^{13+}; e + Fe^{14+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{15+}; e + Fe^{16+}; e + Fe^{17+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{18+}; e + Fe^{19+}; e + Fe^{20+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{21+}; e + Fe^{22+}; e + Fe^{23+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{24+}; e + Ca^{17+}; e + Ca^{18+}
(E06)RECOMBINATION (ELECTRON-ION): e + Ca^{19+}; ;
THEORETICAL ENERGY RANGE: 10^8 K
Mewe, R.; Schrijver, J.; Sylwester, J.
Analysis of x-ray line spectra from a transient plasma under solar flare conditions: II. Rate coefficients.
Astron. Astrophys., Suppl. Ser. **40**, 323 (1980) The Netherlands

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REF. NO. = 10686
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{+}; e + Fe^{2+}; e + Fe^{3+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{4+}; e + Fe^{5+}; e + Fe^{6+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{7+}; e + Fe^{8+}; e + Fe^{9+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{10+}; e + Fe^{11+}; e + Fe^{12+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{13+}; e + Fe^{14+}; e + Fe^{15+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{16+}; e + Fe^{17+}; e + Fe^{18+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{19+}; e + Fe^{20+}; e + Fe^{21+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{22+}; e + Fe^{23}; e + Fe^{24+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{25+}; e + Fe^{26+};
THEORETICAL ENERGY RANGE: Undef
Woods, D. T.; Shull, J. M.; Sarazin, C. L.
Recombination coefficients for iron ions.
Astrophys. J., Part I **249**, 399 (1981) United States

REF. NO. = 11672
(E05)IONIZATION: e + Fe^{18+}; e + Fe^{17+}; e + Fe^{16+}
(E05)IONIZATION: e + Fe^{15+}; e + Fe^{14+};
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{18+}; e + Fe^{17+}; e + Fe^{16+}
(E06)RECOMBINATION (ELECTRON-ION): e + Fe^{15+}; e + Fe^{14+};
EXPERIMENTAL ENERGY RANGE: 480-680 eV
Isler, R. C.; Crume, E. C.; Arnurius, D. E.
Ionization and recombination coefficients for Fe XV-Fe XIX.
Phys. Rev. A **26**, 2105 (1982) United States

The *Atomic Data for Fusion* ("Redbook") Series

Volume 1 *Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules*, C.F. Barnett, ORNL-6086 (1990). (Includes ALADDIN files).

Volume 3 *Particle Interactions with Surfaces*, E.W. Thomas, ORNL-6088 (1985).

Volume 4 *Spectroscopic Data for Iron*, W.L. Wiese (NIST), ORNL-6089 (1985).

Volume 5 *Collisions of Carbon and Oxygen Ions with Electrons, H, H_2, and He*, R.A. Phaneuf, R.K. Janev, and M.S. Pindzola, ORNL-6090 (1987). (Includes ALADDIN files).

Volume 6.1-3 *Spectroscopic Data for Titanium, Chromium, and Nickel*, W.L. Wiese and A. Musgrove (NIST), ORNL-6551/V1-3 (1989).

Other Recent Data Assessments and Recommendations

Assessment of Ion-Atom Collision Data for Magnetic Fusion Plasma Edge Modelling, R.A. Phaneuf, Atomic and Plasma-Material Interaction Data for Fusion (Supplement to Nuclear Fusion), **2**, 75 (1992).

Status and Critical Assessment of the Database for Collisions of Be^{q+} and B^{q+} ions with H, H_2, and He, R.A. Phaneuf, R.K. Janev, H. Tawara, M. Kimura, P.S. Krstic, G. Peach, and M.A. Mazing, Atomic and Plasma-Material Interaction Data for Fusion (Supplement to Nuclear Fusion), **3**, 105 (1992).

Critical Assessment of Atomic Collision Cross-Section Data for Fusion Plasma Applications, R.A. Phaneuf, Physica Scripta (1993).

Recommended Cross Sections for State-Selective Electron Capture in Collisions of C^{6+} and O^{8+} Ions with Atomic Hydrogen, R.K. Janev, R.A. Phaneuf, H. Tawara, and T. Shirai, Atomic Data and Nuclear Data Tables (1993).

Current Projects

- Establish CFADC *Atomic Data Workstation.*
- Resume work towards Volume 2 of the "Redbook" Series.
- Assess existing data and produce theoretical cross sections for H recyling and He ash removal in ITER.
- Convert archival bibliographic tape files to contemporary format.
- Through consultant's contract with Dr. A.Ya. Faenov, produce compilations of data in ALADDIN format concerning processes of current interest.

The CFADC *Atomic Data Workstation*

Following the recent trend to provide information "on-line" and over a large national or international computer network, the ORNL CFADC has proposed to establish an *Atomic Data Workstation.*

This workstation would allow the dissemination of atomic data to the fusion community in a new, much more efficient way, and would allow totally new services to be provided without substantial work load increases for the CFADC staff.

A Hewlitt-Packard Model 755 has been purchased and will be delivered by October 1, 1993. The first step will be to implement a modern database management tool, such as INGRES, through which to operate the bibliographic and numerical databases.

INTERNET access will be allowed so that users can interactively use the ALADDIN and bibliographic databases.

Volume 2 of the "Redbook" Series

Electron-Impact of Ions, Atoms, and Molecules

Data pertaining to electron-impact continues to be a major area of focus for the requests that the CFADC receives. Therefore, we have attempted to restart the efforts to produce Volume 2 of the Redbook series concerning these reactions.

Due to human resource limitations, this project is necessarily a collaborative effort. Jean Gallagher (NIST) and John Broad (JILA) will participate as co-editors with us, and the labor will be divided. For example, the CFADC will concentrate primarily on the gathering of bibliographic data for all electron-impact processes and numerical data for ionization. A partial list of targeted reactions is given in the example.

In order to focus efforts and maintain some stream of production, we will work towards dividing the total list of reactions into groups and attempt to publish periodically results for these groups.

The CFADC *Atomic Data Workstation* is anticipated to be a key tool in the production of this volume of recommended data, by providing a central resource for maintenance of the bibliographic data, linking through the database management system of the gathered numerical data, communication of these data amongst the editors, and as the vehicle to effect final production. That is, plotting, wordprocessing, line fitting, and rate coefficient facilities resident on the workstation will allow the data to be directly published from a single machine.

I. IONIZATION

1. $e + H, D, T > H^+, D^+, T^+ + 2e$ $E_e = E_{th} - 20$ keV
2. $e + H(2s), D(2s), T(2s) > H^+, D^+, T^+ + 2e$ $E_{th} - 20$ keV
3. $e + H(n), D(n), T(n) > H^+, D^+, T^+ + 2e$ $E_e = E_{th} - 10$ keV
4. $e + H_2 > H_2^+ + 2e$ $E_e = E_{th} - 200$ keV
5. $e + He > He^+ + 2e$ $E_e = E_{th} - 20$ keV
6. $e + He^+ > He^{2+} + 2e$ $E_e = E_{th} - 20$ keV
7. $e + He(2^3S) > He^+ + 2e$ $E_e = E_{th} - 20$ keV
8. $e + He(2^1S) > He^+ + 2e$ $E_e = E_{th} - 20$ keV
9. $e + He > He^{2+} + 3e$ $E_{th} - 20$ keV
10. $e + He^+(2s) > He^{2+} + 2e$ $E_{th} - 20$ keV
11. $e + O_2 > O_2^+ + 2e$ $E_{th} - 20$ keV
12. $e + O > O^+ + 2e$ $E_{th} - 20$ keV
13. $e + C > C^+ + 2e$
    $e + C^{n+} > C^{(n+1)+}$
    $e + C > C^{2+}, C^{3+}, \ldots$
14. $e + N_2 > N_2^+ + 2e$
    $e + N_2^{n+} > N_2^{(n+1)+}$
    $e + N_2 > N_2^{2+}, N_2^{3+}, \ldots$
15. $e + Fe > Fe^+ + 2e$
    $e + Fe^{n+} > Fe^{(n+1)+}$
    $e + Fe > Fe^{2+}, Fe^{3+}, \ldots$
16. $e + Ne >$ ions $T_e = 1$ eV - 10 keV
17. $e + Ar >$ ions $T_e = 1$ eV - 10 keV
18. $e + Kr >$ ions $T_e = 1$ eV - 10 keV
19. $e + CH_4 >$ ions $T_e = 1$ eV - 10 keV
20. $e + H_2O >$ ions $T_e = 1$ eV - 10 keV

Ionization of Ba, Tl, Rb, Cs, Mg, Be, B, Ne, Ar, Kr, G, Mo, Ta, W, C_mH_n

II. DISSOCIATION

21. $e + H_2 > H + H + e$ $T_e = 1$ eV - 5 keV
22. $e + H_2 > H^+ + H + 2e$ $T_e = 1$ eV - 5 keV
    $e + H_2 > H^+ + H^- + e$
23. $e + H_2(v) > e + H_2(v') > H^+ + H^- + e$; 1 - 100 eV
24. $e + H_2^+ > H^+ + H^+ + e$ T_e = thresh - 1 keV
25. $e + H_2^+(v) > H^+ + H^-$ T_e = thresh - 1 keV
26. $e + H_2^+ > 2H$ T_e = thresh - 1 keV
27. $e + H_3^+ > H_2^+ + H + e$ T_e = thresh - 1 keV
28. $e + H_3^+ > 2H^+ + H + e$ T_e = thresh - 1 keV
27. $e + H_3^+ > H_2^+ + H + e$ T_e = thresh - 1 keV
29. $e + H_3^+ > 3H$ T_e = thresh - 1 keV
30. $e + H_3^+ > 3H^+ + 3e$ T_e = thresh - 1 keV
31. $e + H_3^+ > H_2^+ + H^-$ T_e = thresh - 1 keV
32. $e + H_3^+ > H_2^{+*} + H^-$
33. $e + H_3^+ > H^+ + 2H$
34. $e + O_2 > O^+ + O + 2e$
35. $e + O_2 > 2O + e$
36. $e + O_2 > 2O^+ + 3e$
37. $e + H_2O >$ neutral products
38. $e + H_2O^+ >$ products
39. $e + CH_4 >$ products
40. $e + CH_4^+ >$ products
41. $e + CH_3^+ >$ products
42. $e + CH_2^+ >$ products

43. e + CH^+ > products

ELECTRONIC EXCITATION

44. e + H(1s) > H(2p)

45. e + H(1s) > H(2s)

46. e + H(1s) > H(3s)

47. e + H(1s) > H(3p)

48. e + H(1s) > H(4s)

49. e + H(2s) > H(n)

50. e + H_2 > H + H(2p)

e + H_2 > + H(n=3)

e + H_2 > + H(n=4)

51. e + D_2 > e + D + D(2s,2p,n=3,n=4)

52. e + H_2 > e + H_2(v = 1,2,3)

53. e + H_2 > e + H_2(1230A, B, C, D) ?

Werner bands

54. e + H_2 > e + H_2(Lyman bands)

55. e + H_2^+ > H_2(v = 0)

56. e + H_2^+ > H_2(3 PI u , v*)

57. e + H_2^+ > H_2(v**)

58. e + H_3^+ > H_3(v**)

59. e + He(1^1S) > He(4^1S, 3^1P, 4^1D, 4^3S, 3^3S)

60. e + He(1^1S) > He(2^1P, 2^1S, 2^3S, 2^3P)

61. e + He(2^3S) > He(2^3P, 3^1P, 3^3P)

62. e + He^+(1s) > He^+(2s, 2p, 3s, 3p, etc.) ?

63. e + He^+(1s) > He^+(2p, 3s, 3p, 4s, etc.) ?

64. e + O_2 > O_2^*

65. e + O($2p^34s$) > O^*

66. e + C($2p^2$) > C^*

67. e + Fe, Cr, Ni, Be, B, Mo, Ta, W, Ga, Ne, Ar, Kr > A^*

68. e + Ti > Ti^*

DISSOCIATIVE EXCITATION

69. e + H_2(v) > H^*

70. e + H_2^+(v) > H^*

71. e + H_3^+(v) > H^*

72. e + O_2(v) > O^*

73. e + O_2^+(v) > O^*

RADIATIVE RECOMBINATION

74. e + H^+ > H^*

75. e + He^+ > He^*

76. e + He^{2+} > He^+

ELECTRON ATTACHMENT

77. e + H > H^-

78. e + O > O^-

79. e + O_2 > O_2^-

80. e + C > C^-

Elastic Heavy-Particle Cross Sections

Through requests from plasma modellers, the A+M Data Unit of the IAEA has identified an urgent need for elastic and diffusion cross sections for edge-plasma modelling.

These low energy (1-500 eV) heavy particle $(H,D,T,He,H_2)^{q+}$ collisions are important in the edge and divertor regions, under conditions of high recycling in next step reactors (ITER).

The data is of great importance for addressing the isssues of particle transport in helium ash exhaust and hydrogen recyling.

In collaboration with J.H. Macek and S.Y. Ovchinnikov (University iof Tennessee and ORNL) we have begun calculating a number of these cross sections since general, comprehensive tablulations do not exist.

The CFADC Archival Bibliographic Data

Before the advent of the CFADC on-line, PC-based database system, bibliographic records were stored on tape from a mainframe computer. Entries since 1978 (totalling about 25,000) are available on the on-line system, but those dating from about 1950 to 1977 (about 45,000) may be searched only through the hardcopy documents that were periodically published.

Due to the rapidly changing hardware associated with the ORNL data processing services, the archival tapes will soon be no longer readable or able to be backed up or copied.

We have begun the process to convert these records to contemporary format so that they too may be placed on-line. Recent requests for low energy, heavy-particle elastic cross sections, for example, highlight the usefulness of these records.

After transfering the records to contemporary media, we have obtained the generous help of Jean Gallagher, Pheobe Fagan, and Gerry Dalton at NIST in beginning to convert the old, coded references into a form decipherable by current database programs.

Compiled Data for Processes of Current Interest:

A.Ya. Faenov and A.I. Magunov

Compilation of Dielectronic Recombination Rate Coefficients for H-like Ions

Compilation of Dielectronic Recombination Rate Coefficients for Electron Impact Excitation of He-like Ions

Compilation of Cross Sections and Rate Coefficients for Electron Impact Excitation of Be-like Ions

Compilation of Cross Sections and Rate Coefficients for Electron Impact Excitation of Li-like Ions

Compilation of Cross Sections and Rate Coefficients for Electron Impact Excitation of Be^{2+} and C^{5+} Ions

Compilation of Characteristics of Autoionization States of Li Atom and He-like Ions

TEXT.JUL July 13, 1993

Electron Impact Ionization of Multicharged Ions at ORNL: 1985-1992*

D. C. Gregory and M. E. Bannister
Oak Ridge National Laboratory

ABSTRACT

Absolute cross sections are presented in graphs and tables for single ionization of forty-one ions, multiple ionization of four ions, and for dissociation and ionization of two molecular ions by electron impact. This memo is the third in a series of manuscripts summarizing previously published as well as unpublished ionization cross section measurements at ORNL; contents of the two previous memos are also referenced in this work. All work tabulated in this memo involved ion beams generated in the ORNL-ECR ion source and utilized the ORNL electron-ion crossed beams apparatus. Target ions range from atomic number Z=8 (Oxygen) to Z=92 (Uranium) in charge states from +1 to +16.

I. Introduction

Our understanding of the atomic processes which are important in the ionization of atomic ions has progressed greatly in the last decade, primarily due to numerous collaborations between theoreticians and experimentalists involving ions of widely varying atomic number and charge. Advances in ion sources, data collection and analysis techniques, and energy resolution on the experimental side have inspired more sophisticated theoretical models and calculations. Similarly, theoretical insights and advanced computational techniques have led to predictions which guided experimentalists toward more meaningful work.

As a result of the understanding gained from this symbiotic relationship, the cross section for ionization of any given ion by electron impact could probably be calculated within 20% today, given relatively modest resources and attention. This was certainly not true fifteen years ago, when direct ionization was considered by most modelers and other cross section users to be the only important process for almost all ions. It is now understood that various indirect processes contribute to, and indeed often dominate, total ionization.

One of the purposes behind the seemingly patternless collection of measurements summarized here is a search for "interesting" cross sections, those that reveal unexpected or seemingly unexplainable features. It is these surprises which lead to advances in our understanding of the ionization process. Another theme behind the measurements involves the interests of the fusion energy community. This research project receives primary support from DOE's Office of Fusion Energy, and it has emphasized specific data needs of the fusion program as an important part of the quest for general understanding discussed above. The targets presented here are

* **Excerpt from ORNL Technical Memo, in preparation**

Element		Initial Charge State															
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
3	Li																
4	Be																
5	B		2	1													
6	C		2	12	1												
7	N		2	12	1	1											
8	O		2	1	12	1*											
9	F		2														
10	Ne			2													
11	Na																
12	Mg																
13	Al		2														
14	Si	*	*	2	*	*	*	*									
15	P																
16	S				*												
17	Cl		2			*											
18	Ar		2	2	1	2	*	*	*								
	$Ar^{\dagger}$				2												
19	K																
20	Ca																
21	Sc																
22	Ti		2	2		*						*					
23	V																
24	Cr						*	*	*		*			*			
25	Mn																
26	Fe		2			*	*			*		*		*		*	
27	Co																
28	Ni			2		*	*	*	*				*		*		
29	Cu		2	2													
30	Zn																
31	Ga																
32	Ge																

Element		Initial Charge State															
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
33	As																
34	Se																
35	Br																
36	Kr		2	2	*			*	*	*							
	Kr†				2												
40	Zr			2													
51	Sb			2													
54	Xe		2	2	2	2	2*		*								
	Xe†				2		*		*								
	Xe‡						*										
72	Hf			2													
73	Ta			2													
92	U										*			*			*
	U†										*			*			

[1] Reference 1. ORNL/TM 7020 Crandall et al.

[2] Reference 2. ORNL/TM 9501 Gregory et al.

* This report. ORNL/TM Gregory & Bannister

† Double ionization.

‡ Triple ionization.

"Cross Sections Evaluation and Handling at Orsay"

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Work in progress in the unit of Atomic Physics of Fusion Plasmas (PAPF) of the Laboratory of Gases and Plasma Physics (LPGP) at Orsay is partly related with the evaluation of ion - atom collision cross sections of interest to fusion, total for ionization and total and partial (n,l resolved) for charge transfer. In collaboration with the group of theory of the LPGP and with external collaborations we have calculated "ab initio" an extensive amount of cross sections. This work lead to sets of evaluated data which, as is the case with the non-evaluated ones, have to be conveniently stored and ordered in order to be handy for everyday use, but also for a wide distribution with plasma modelling applications in mind.

As it was often observed, the form of data storage is crucial and may greatly contribute to their application. In the light of discussions held in previous DCN meetings and of well known implementations (e.g. the "red books" [1], the review of the first IAEA A+M Data Unit CRP on atomic collision data [2] etc) we are developing a curve storage system through corresponding sets of parameters based on curve fitting. This database is similar to CHART (Charge Transfer Between Atoms and Molecules) [3] implemented in Nagoya and, as is the case for the bulk of data collected at Oak Ridge by CFADC (Controlled Fusion Atomic Data Center) can be directly put in ALADDIN format because of the ASCII data files used [4]. It could then easily made available through the A+M Data Unit of the AIEA in PC diskette form.

We are here briefly presenting the available data and the principles of the software implementation necessary for their storage and use.

Available data

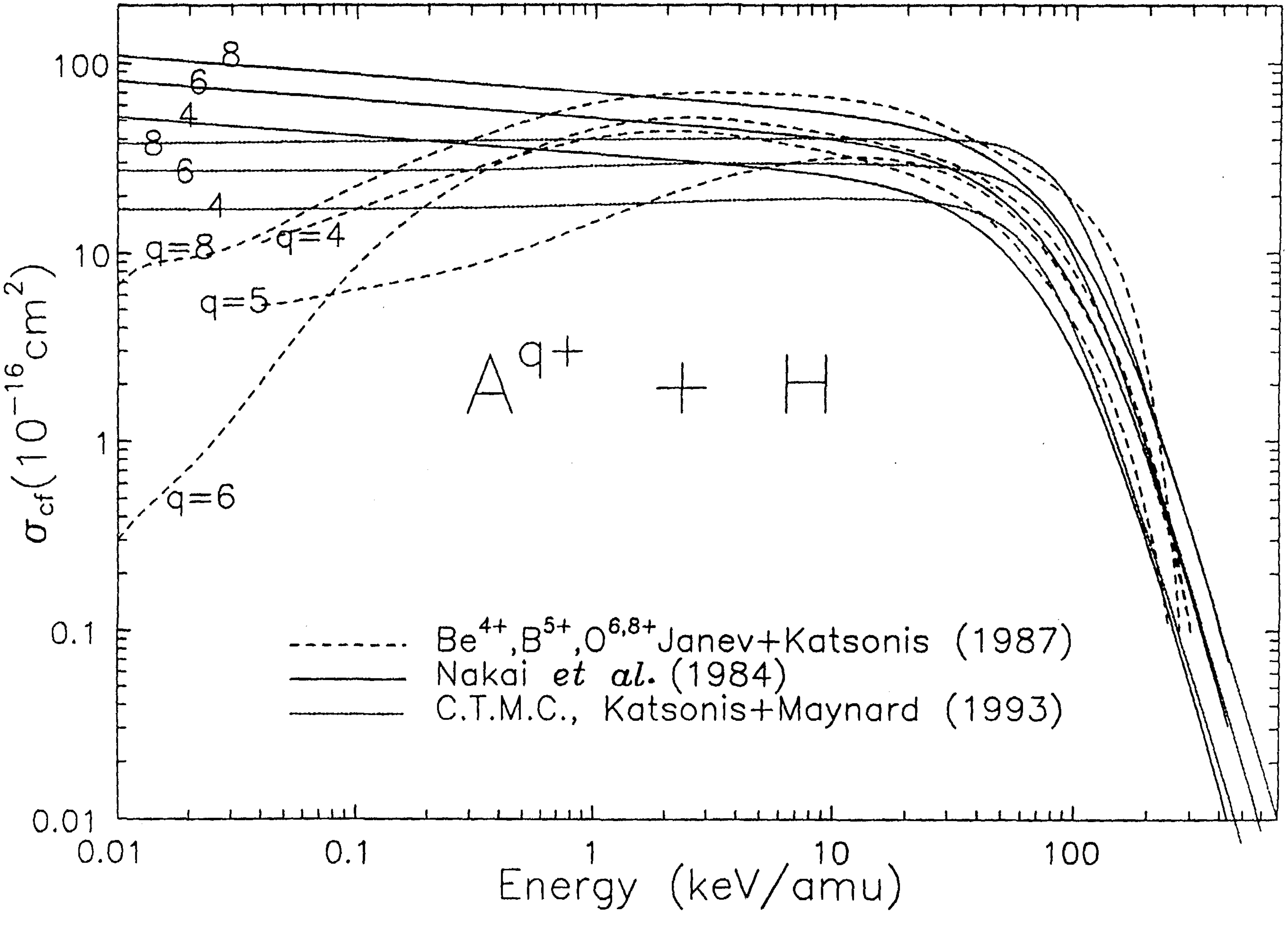
As the process of parametrization is under way, we rather present here a list of the totality of the data calculated and/or evaluated, even if they are not all yet in parametric form:

A^{q+} + H collisions
Energy range: 10 ev/amu to 5 Mev/amu
One e ionization cross sections.
One e charge transfer,
total cross sections all $Z < 75$, all q;
partial n-resolved cross sections, $q=3$ to 6.

A^{q+} + He collisions, totally stripped ions, $Z = 1$ to 28
Energy range: 1 kev/amu to 1 Mev/amu
Simple and double ionization cross sections.
Simple and double total charge transfer.

He^{+} + A^{q+} collisions, totally stripped ions, $Z = 1$ to 18
Energy range: 1 kev/amu to 5 Mev/amu
Ionization and total charge transfer cross sections.

Moreover, some dielectronic recombination and electron impact ionization data have been put in parametric form.



100
10
1
0.1
0.01
0.01
0.1
1
10
100
Energy (keV/amu)
$\sigma_{cf}(10^{-16}cm^2)$
8
6
4
8
6
4
q=8
q=4
q=5
q=6
A^{q+} + H
$Be^{4+}, B^{5+}, O^{6,8+}$ Janev+Katsonis (1987)
Nakai *et al.* (1984)
C.T.M.C., Katsonis+Maynard (1993)

Figure 1

The available sets are not meant to cancel the gaps among the available detailed evaluations or to replace existing values, but to constitute rather complete homogeneous collections for use in various applications. As an example we are giving in Fig. 1 a set of total charge transfer cross sections for A^{q+} + H collisions for totally stripped ions with q = 4, 6 and 8 in a wide energy range. Previously available parametrized evaluated data from [2] and theoretical data from [5] are also given for comparison. It is to be noted that the parametrizations shown in the Fig. 1 are based to "ad hoc" empirical formulas, except for [2] where a minimax polynomial of degree ten was used to fit the available data.

Choice of parametric forms and handling of data

It has been previously realized that the use of least squares fitted polynomials may lead to substantial deviations from values expected between data points and outside them; the problem is increasing for higher degree polynomials. Therefore, in the common case of lack of convenient empirical formulas, Chebyshev polynomials were often used instead of the standard ones. Such an implementation is given and documented in [1]. Rational functions of Padé type are superior to polynomials in some cases (whenever poles are found in the curve to be parametrized) and therefore are strongly recommended [6]. Rational polynomial fitting is readily available within common workstation softwares as Mathematica. We are commonly using a standalone curve fitting programme based in algorithms given in [6], in a C language implementation described in [7]. This programme called RPFT is able to perform fitting of Chebyshev polynomials or rational functions, to arbitrary sets of data points. Extrapolation and optional keyboard input for calculating test results is also possible. The (x,y) data pairs are given as input in ASCII type files. In order to be able to judge on the simplicity of use of RPFT, its standard help screen is given in Fig.2.

Figure 2 *RPFT help screen*

```
USAGE: rpft LL=a UL=b NN=n ND=m [-DIG=n -XLN -YLN] file

   LL=a   a is the lower limit of theregion for fit
   UL=b   b is the upper limit of the region for fit

   ND=m | m>0: rational function, denominator degree m,
   NN=n |      numerator degree n.  1<=m<=10  1<=n<=10
        | m=0: Polynomial degree n.  1<=n<=20

 -DIG=n   (optional) n = number of significant digits
               for coefficients on output. Default=7.
   -XLN   (optional) Transform X values to ln(X)
   -YLN   (optional) Transform Y values to ln(Y)

   file   File with input X Y data points, 1 per line

All command line parameters except DIG, XLN and YLN are
required. They may be in any order, upper or lower case
```

References

[1] C.F. Barnett et al., Oak Ridge National Laboratory, "Atomic Data for Fusion" series, "Red Book", e.g. ORNL-6086/v1 (1990); R.A. Phaneuf et al., Oak Ridge National Laboratory, "Atomic Data for Fusion" ORNL -6090/v5 (1987).

[2] R.K. Janev and K. Katsonis, Nucl. Fusion **27**, 1493 (1987).

[3] T. Kato et al., "Atomic Database in NIFS", in Proceedings of the IAEA Technical Committee Meeting on "Atomic and Molecular Data for Fusion Reactor Technology", Cadarache, Oct. 1992, p. 60.

[4] D.R. Schultz et al., "Compilation of Atomic Data for Fusion by the ORNL Controlled Fusion Atomic Data Center", as in Ref.[3] p. 52.

[5] Nakai et al., Annual Report of the Radiation Center of Osaka Prefecture **25**, 19 (1984).

[6] W.H. Press et al., "Numerical Recipes", second edition, Cambridge University Press, Cambridge 1992.

[7] L. Smith, "Curve Fitting with Extrapolation" The C users Journal, June 1993.

Progress Report on the A+M Data Activities at Nuclear Data Center, Japan Atomic Energy Research Institute (JAERI) July 1992 - September 1993

Toshizo Shirai

Compilation and evaluation work is continued for making the 4th edition of Evaluated Atomic and Molecular Data Library (JEAMDL-4) for fusion under collaboration with the JAERI Research Committee on Atomic and Molecular Data and with NIST and ORNL in the US-Japan Fusion Cooperation Program.

1. Recent Activities and Work in Progress

Analytical least squares fits has been made to the cross sections recommended in ORNL redbook vol. I for total and partial electron capture in collisions of H, H_2, He and Li atoms and ions with atoms and molecules [1]. Similar work is now in progress on excitation and spectral line emission cross sections and will be published within a year. In parallel, we continue to compile recent experimental cross sections for these collision processes in order to compare with redbook data and also to examine the validity of the analytical expressions employed for extrapolation.

Cross sections for single-, double- and triple-electron capture have been measured for the carbon ions passing through the CO_2, CH_4, C_2H_6 and C_3H_8 gas targets at energies between 0.5 and 5 keV/amu [2] under a research contract with Kyoto University. The cross sections hardly depend on incident energy, but depend on the charge of the incident particles and the ionization potential of the molecules. Multiple-electron capture processes are predominant in these molecules studied here.

Critical evaluation of spectroscopic data of particular interest to the fusion community was completed for highly ionized krypton ions [6] and is now undertaken for the Ga ions. A series of monographs are already published for the Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Mo ions. These monographs will be put into a book with addition of more recent data of the Ti, Fe, Ni and Mo ions.

A workshop was held on particle-material interactions such as plasma-facing materials in ITER, radiation damage in carbon materials, trapping, emission and permeation of hydrogen in metals, and heavy ion-solid surface interactions [7].

2. Recent Publications

Cross Section Data

1. JAERI-M 93-117: "Analytic cross sections for collisions of H, H_2, He and Li atoms and Ions with Atoms and Molecules. I," R. Ito, T. Tabata, T. Shirai and R.A. Phaneuf.
2. JAERI-M 93-202: "Charge-changing collision cross sections of low-energy carbon ions with carbon containing molecules," N. Hamamoto, T. Tanaka, A. Itoh, N. Imanishi, M. Saito, Y. Haruyama and T. Shirai.
3. Atom. Data Nucl. Data Tables 55, (1993): "Recommended cross sections for state-selective electron capture in collisions of C^{6+} and O^{8+} ions with atomic hydrogen," R.K. Janev, R.A. Phaneuf, H. Tawara and T. Shirai.

Spectroscopic Data

4. J. Phys. Chem. Ref. Data 22, No.5 (1993): "Spectral data and Grotrian diagrams for highly ionized chromium, Cr V - Cr XXIV," T. Shirai, T. Nakagaki, J. Sugar and W.L. Wiese.
5. J. Phys. Chem. Ref. Data, in press: "Spectral data and Grotrian diagrams for highly ionized manganese, Mn VII - Mn XXV," T. Shirai, T. Nakagaki, K. Okazaki, J. Sugar and W.L. Wiese.
6. J. Phys. Chem. Ref. Data, in submission: "Spectral data and Grotrian diagrams for highly ionized krypton, Kr V - Kr XXXVI," T. Shirai, K. Okazaki and J. Sugar.

Particle-material Interaction Data

7. JAERI-M 92-134: "Report of the 1991 workshop of particle-material interactions for fusion research," edited by the Research Committee of A+M data.

COMPUTER DATA BASE FOR FUSION REACTOR MATERIALS

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Directions of our Activity

- Improvement of ALADDIN software.
- Collection and evaluation of data on thermomechanical properties of materials.

Original ALADDIN version peculiarity

1. Flexible system of data representation, so its possible to support a wide range of data types
2. ASCII (text) data files format
3. Supporting online data documentation with associated dictionary files.
4. Command based programm, designed on FORTRAN 77

New database programm...

1. is menu-driven, easy to use, provides context sencitive help;

2. produces screen graphics and metafile for hardcopy;

3. in addition to sequentual searches through database file, builds a database index and makes search trough index, increasing search speed;

4. provides simple visual database navigation and records selection according to given Hierarchical labels;

5. Several input database files may be opened simultameously and linked logically to act as one big database;

6. Program designed on C and compiled by Microsoft C 6.0

Hierarchical labels set

I Label	II Label	III Label	IV Label
GRAPHITE	ISOTROPIC	MPG-8,H451,POCO,MPG-6	
	ANISOTROPIC	B-2, etc.	
	PYROLITIC	PG,APG,UPV-1,UPV-1T,HORG etc.	
	DOPED	PG-Ti,PG-TiK etc.	
CFC (Carbon Fiber Composite)	CHOPPED F. BASED	1-D, 2-D, 3-D, n-D	TRADE NAME
	CONTINUOS F. BASED	1-D, 2-D, 3-D, n-D	TRADE NAME
	DOPED	1-D, 2-D, 3-D, n-D	
BERYLLIUM	POWDER MET.	S65-B	
	CAST	TRADE NAME	
	SPRAED	TRADE NAME	
CARBIDES	SiC	RSiC,SiSiC,SSiC,SbSiC,SiCFC	TRADE NAME
	TiC	TRADE NAME	
LIQUID metals	GALLIUM BASED	Ga, Ga-In-Sn etc.	
	LITHIUM BASED	Li, Pb-Li etc.	
STEELS	AUSTENITIC	TRADE NAME	
	MARTENSITIC	TRADE NAME	
	FERRITIC	TRADE NAME	
Ni&ALLOYS	Ni	-	
	AGE-HARDENING		TRADE NAME
	NON-AGE-HARDENING	-	
Cu&ALLOYS	Cu	OFHC,ELECTROLITIC	TRADE NAME
	SOLUTION STRENGTHENED	TRADE NAME	
	DISPERSION STRENGTHENED	TRADE NAME	
	PRECIPITATION HARDENED	TRADE NAME	
W&ALLOYS	POWDER met.	W, W-ALLOY	TRADE NAME
	CAST	W, W-ALLOY	TRADE NAME
	SPRAYED	W, W-ALLOY	TRADE NAME
Ta&ALLOYS	Ta	TRADE NAME	
	Ta ALLOYS	TRADE NAME	
Mo&ALLOYS	POWDER met.	Mo,Mo ALLOY	TRADE NAME
	CAST	Mo,Mo ALLOY	TRADE NAME
V&ALLOYS			
Nb&ALLOYS			
LOW ACTIV ALLOYS	AUSTENITIC		
	FERRITIC		

Boolen labels set

N°	Boolen label	Description
1.	PROPERTY	Property is printed in entry*)
2.	AUTHOR	First (or one) author of source (reference)
3.	SOURCE	Data Reference
4.	MANFUL	Material manufacturer
5.	MATERIALS	Description of the materials including: - introduction - basic information; - method of production; - chemical composition; - thermomechanical treatment; - lattice parameters; - grain size; - microstructure characteristics; - semiproducts description (geometry, dimensions etc.) - etc.
6.	SAMPLE-DESC	Description of the studied samples: - sample geometry; - sample orientation in semiproduct - sample orientation to load/measurement parameters; - sample thermomechanical treatment if it is different of materials; - sample fracture mode; - sample identification ; - etc.
7.	TEST-COND	Description of the test conditions: - laboratory; method of testing; - environment; strain control; - pre-test exposure; - irradiation parameters * Reactor/facility; * Flux; * Energy spectrum; * Dose/fluence; * Temperature;

Data

At the same time with software modification, the material data collection work was started. And now we have the following information:

- Pyrolitic graphites: PG(Phizer), APG(Phizer), PG(Goodrich), APG(Goodrich UPV-1, UPV-1T, HOPG;
- Graphites: MPG-8, POCO, H-451, RCT, OAM-91, USB-15, RF CFC
- Stainless steel: 3161, RF steels
- Tungsten: pure W, W + Re alloys
- Be and Be alloys: pure Be, S-65-B, S-200-E, RF Be, Be-Al alloys

Current Activities

- Collection and evaluation of materials data in accordance with ITER request. (Be, V, Cu-alloys, Ti and Ti-alloys)
- December 1993: first redaction of Be properties data base should be sent to ITER.

Thermomechanical Properties list:

- Physical Properties
  - T_m, T_B
  - Thermal conductivity
  - Specific heat
  - Density
  - Emmisivity
  - Evaporation rate
- Mechanical Properties
  - Ealstic modulus
  - Ultimate strength
  - Yield strength
  - Elongation
  - Fatigue
- Influence of n-irradiation on material properties
  - Physical (swelling, thermal conductivity, etc.)
  - Mechanical

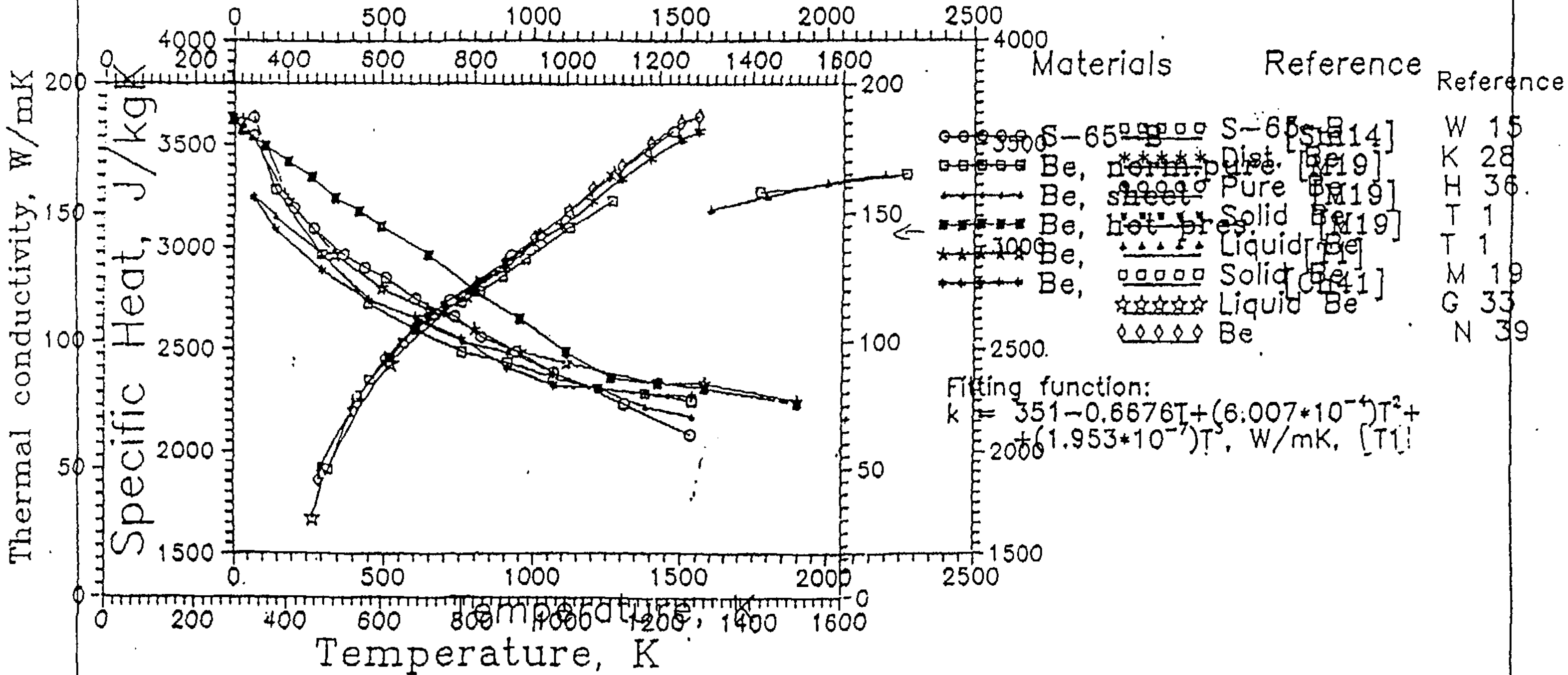
COMMON INFORMATION OF BERYLLIUM PROPERTIES

Atomic number	- 4
Atomic weight	- 9.01
Melting temperature	- 1556K [E18, D22], 1557K [P23, M19, S24], 1558K [W25] 1562K [B26]
Boiling temperature	- 2757K [L16], 3243K [M19], 3142K [K120], 2676K [W25], 2757K [E18], 2768K [A27], 2744K [N29], 2723±50K [P23]
Heat of fusion	- 1300 J/g [L16], 1083 J/g [M19] 1633±38 J/g [K28]
Heat of evaporation	- 36600 J/g [L16], 24700 J/g [M19] 37000 J/g [P31]
Crystalline lattice	- hexagonal-close-packed a = 0.22855nm, c = 0.35840nm [E1]

BERYLLIUM
Specific Heat

BERYLLIUM

Thermal conductivity vs. temperature



INTERNATIONAL ATOMIC ENERGY AGENCY

Atomic and Molecular Data Unit

Report of Activities: July, 1992 to September, 1993

Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (12th Meeting of the A+M Data Centres and ALADDIN Network)

Prepared by: J. Botero
September 21, 1993

AREAS OF INTEREST

- Atomic and Molecular Collisions
- Atomic and Molecular Structure and Spectra
- Plasma-Surface Interactions
- Material Properties

As Applied to:

- Current: Thermonuclear Fusion
- Planed Extensions:
  - Life Sciences: Biophysical Modelling of Radiation Induced Damage of Subcellular Structures; Monte Carlo Calculations of Track Structure Analysis of Radiation Induced Biological Effects.
  - Environmental Sciences: A+M Data Needs for Modelling Ozone Layer Photo-Chemistry Dynamics; Data Base for A+M Processes of Greenhouse Gases.

STAFF AND EQUIPMENT

- Staff
  - 3 Physicists
  - 1 Secretary and Support
- Equipment
  - IBM RS6000/340
    - 64 Mbytes of RAM

    * 1 (2) Gbytes of Hard Disc
    * Operating System: UNIX
  - 3 IBM PC 386
    * 8 Mbytes RAM
    * 40-80 Mbytes Hard Disc
    * Operating System: MS/DOS, MS/Windows
  - Access to:
    * Vax 4000 (VMS)
    * IBM Main Frame (TSO)
- Communications
  - EARN/BITNET: rnd@iaeal, rng@iaeal
  - INTERNET
    * Anonymous ftp account: user "anonymous" or "ftp"
    * AMDIS on-line service: user "aladdin" password "aladdin"
    * IP Address: ripcrs01.iaea.or.at

PROJECTS

- Data Base Development
- Data Evaluation and Recommendation
- Coordinated Research Projects

1. Data Base Development

    - **A**tomic and **M**olecular **D**ata **I**nformation **S**ystem (**AMDIS**): On-line service for:

        - ALADDIN interface and data base (currently works with ALADDIN V.1.0, implementation of new interface, and possibly Data Base Management System are under study).
        - Spectroscopic Data (NIST)*: ALADDIN format is not appropriate for spectroscopic data base. It will use the interface developed by NIST (D. Kelleher).
        - IAEA Bibliographic Data Base*: Need to be down-loaded from the IBM main frame. Searching for DBMS (as above).
        - A+M and PSI Computer Code Library*

    - ALADDIN.C (PC version) : Nearly completed. In collaboration with G. Yushko. It will have improved search capabilities, tree structure of hierarchical labels, graphics (including PostScript) capabilities.

    - New ALADDIN formated data

        - Sputtering (IAEA and IPP)
        - Hydrogen Data Base (IAEA)

    - Implementation of Spectroscopic Data Base (NIST)

    - Bibliographic Data Base: 32500 entries, dating from 1950 to present. It has to be down-loaded from the IBM main frame.

        - Mantain the IAEA Bibliographic Data Base
        - Publish the International Bulletin on Atomic and Molecular Data for Fusion (new Format), published semiannually.

2. Data Evaluation and Recommendation

- "Cross Sections for Collision Processes of Hydrogen Atoms with Electrons, Protons, and Multiply Charged Ions", R. K. Janev and J. J. Smith
  - Electron Impact Processes: Excitaion, Ionization.
  - Proton Impact Processes: Excitation, Ionization, Electron Capture.
  - Collision Processes with He^{2+}: Excitation, Ionization, Electron Capture.
  - Collision Processes with Highly Charged Ions: Excitation, Ionization, Electron Capture.
- Sputtering Data Base: An Evaluated Data Base for Sputtering of Light Ions. (Thomas, Janev, Botero, Smith and Qiu) Sputtering yield for normal incidence of light ions (H^+, D^+, and He^{2+}i of Be, B, C, Al, Ti, Fe, Ni, Cu, Mo, W, and Au.
- Lithium Data Base: In progress. (Aumayer, Janev, Smith)
- Helium Data Base: In progress. (Janev, Botero)
- Particle Exchange Reactions: In progress. (Botero, Janev, Smith)
- Be and B Data Base: In progress. (Botero, Janev)
- Material Properties Data Base: In progress. (Langley, Barabash)
- Plasma-Surface Interaction Induced Erosion Data Base: In progress. (Langley)

3. Coordinated Research Projects

- Medium and High Z Impurities in Fusion Plasmas.
- Plasma-Surface Interaction Induced Erosion of Fusion Reactor Materials.
- A+M Data for Fusion Edge Plasmas.
- Reference Data for Thermo-mechanical Properties of Fusion Reactor Plasma Facing Materials*.
- Tritium Retention and Release of Fusion Reactor Plasma Facing Materials*.
- Radiative Cooling of the Plasma Edge*.

Progress Report on Atomic and Molecular Data at QUB

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This is a short report to describe the activities of the Atomic and Molecular Data Unit at Queen's University of Belfast. The work carried out on data analysis during the past year is described below.

1. In spite of funding problems efforts have been made to keep the electron ionization database up to date and its information available to anyone asking for data. Information from the database has been forwarded to a number of scientists around the globe.

2. A paper on "Recommended Electron Excitation rate for Iron Ions above 100 eV has been prepared for publication. This paper provides experimental and theoretical data for the electron impact excitation of FeI to FeXXVI and its assessment and corrects an earlier paper.

3. We wished to investigate the usefulness of the CIAMDA index and of the Bulletin. Could the information in the Bulletin not be found by searching in INSPEC? This has led to research on a comparison of CIAMDA 80 with results obtained from a search with INSPEC and CHEMABS. It is coming to a conclusion, and preliminary results are included in the following tables. An attempt is being made to explain why the two systems do not match.

   It is clear from the tables that there is a real need for the Numerical Data index found in the Bulletin. It is surprising that CHEMABS and INSPEC did not perform better and that their recall of papers for these data items were as low as 23% and 24% respectively.

TABLE 1

Example of Data Entries in the retrospective Computer Index in Atomic and Molecular Data for Fusion (CIAMDA) published by the IAEA

Process	Energy	Th/Ex	Ref
$H + N^{4+}$			
ionisation	1 - 100 keV	T	11748
ionisation	38 - 200 keV	T	5560
ionisation	0.10 - 10 MeV	T	4900
ionisation	0.10 - 10 MeV		5560
excitation		E	5560
excitation		T	5560
charge transfer	0.10 - 1 keV	T	10336
Charge transfer	0.90 - 6.3 KeV	E	10675
charge transfer	1 - 100 keV	T	11748
charge transfer	38 - 160 keV	E	5560
charge transfer	38 - 130 keV	T	5560
charge transfer	0.10 - 10 MeV		5360
charge transfer	0.010 - 1.6 MeV	E	10598

TABLE 2

Example of Data Entries in the current Awareness Bulletin of Atomic and Molecular Data for Fusion published by the IAEA

reaction	Process	Energy range	Th/Ex	Ref
e + Fe^{8+}	ionisation	1 - 100 keV	Th	210
e + Fe^{16+}	excitation		Th	132
e + Fe^{16+}	ionisation	1 - 100 keV	Th	210
e + Fe^{16+}	recombination		Th	132
e + Fe^{21+}	excitation	1.22 keV	Th	131
e + Fe^{24+}	recombination	10 - 500 M°K	Th	150
e + Ni	ionisation		Ex	139
e + Ni^{3+}	ionisation	36.6 - 991 eV	Ex	205
e + Ni^{23+}	excitation		Th	131
e + Cu	elastic scattering	3.8 - 100 eV	Th	182
e + Cu	elastic scattering	6 - 100 eV	Th	183
e + Cu	excitation	3.8 - 100 eV	Th	182
e + Cu	excitation	6 - 100 eV	Th	183
e + Cu	ionisation		Ex	139
e + Cu	angular scattering	6 - 100 eV	Th	183
e + Cu^{2+}	ionisation	0.03 - 1.48 keV	Ex	205

TABLE 3

COMPARISON OF CIAMDA 80 AND CHEMABS

Description of search (CIAMDA Terminology)	No of CIAMDA refs published 1967-80	No of refs retrieved on CHEMABS 1967-80	No of CIAMDA Refs retrieved on CHEMABS	% of CIAMDA refs retrieved on CHEMABS
$Li^+ + H_2$ ionisation	3	4	1	33.3
$Ar^+ + H_2$ charge transfer	19	18	11	57.9
Kr + H elastic scattering	2	16	2	100.0
$e^- + C^{4+}$ ionisation	9	11	1	11.1
$CO + H^+$ excitation	11	1	0	0
$N^{5+} + H_2$ charge transfer	3	4	3	100.0
$G_2^+ + D_2$ interchange react	6	9	0	0
$e^- + Zn$ ionisation	17	53	7	41.2
$Ne + He^{++}$ excitation	2	1	0	0
$H + Si^{++}$ charge transfer	2	3	2	100.0
$e^- + Cs^+$ recombination	11	2	1	9.1
$Fe^{++} + H$ charge transfer	1	2	1	100.0
$O^+ + H$ charge transfer	8	11	3	37.5
$e^- + Hg$ ionisation	69	81	31	44.9
Ni + H ionisation	1	7	0	0
$Sn + H^+$ ionisation	9	0	0	0
$H^+ + H_2$ ionisation	20	5	1	5.0
$e^- + Kr^{++}$ excitation	3	3	1	33.3
$e^- + Na$ elastic scattering	28	110	17	60.7
$Li^+ + He$ elastic scattering	17	30	7	41.2
$H^+ + H_2$ total scattering	1	1	0	0
$O^+ + O$ interchange react	1	0	0	0
$H + H^+$ charge transfer	148	2	0	0
$e^- + S^{6+}$ recombination	1	0	0	0
$O^{++} + He$ charge transfer	3	7	2	66.6
$e^- + Ar^{++}$ excitation	1	4	0	0
$e^- + K^{++}$ excitation	2	1	0	0
$H_2 + C^*$ interchange react	2	13	0	0
$H_2 + H$ ionisation	20	70	6	30.0
He + Cs charge transfer	2	11	0	0
TOTAL:	424	483	98	23.1

TABLE 4

COMPARISON OF CIAMDA 80 AND INSPEC

Description of search (CIAMDA terminology)		No of CIAMDA refs published 1971-1979	No of refs retrieved using INSPEC (1971-1979)	No of CIAMDA refs retrieved on INSPEC search	% of CIAMDA refs retrieved on INSPEC
$Li^+ + H_2$	ionisation	3	1	0	0
$Ar^+ + H_2$	charge transfer	13	10	6	46.2
$e^- + B^+$	total scattering	1	0	0	0
$Kr + H$	elastic scattering	1	7	0	0
$e^- + C^{++}$	ionisation	7	5	0	0
$H_2 + He^+$	excitation	11	10	1	9.1
$CO + H^+$	excitation	8	4	2	25.0
$N^{5+} + H_2$	charge transfer	3	2	2	66.7
$H_2^+ + D_2$	interchange react	3	4	0	0
$e^- + Zn$	ionisation	11	34	3	27.3
$Ne + He^{++}$	excitation	1	1	0	0
$H + Si^{++}$	charge transfer	2	0	0	0
$e^- + Cs^+$	recombination	6	1	1	16.7
$Fe^{++} + H$	charge transfer	1	0	0	0
$O^+ + H$	charge transfer	4	7	1	25.0
$e^- + Hg$	ionisation	41	84	28	68.3
$Ni + H$	ionisation	1	11	1	100.0
$Sn + H^+$	ionisation	9	0	0	0
$H^+ + H_2$	ionisation	15	24	0	0
$e^- + Kr^{++}$	excitation	3	1	0	0
$e^- + Na$	elastic scattering	28	24	10	35.7
$Li^+ + He$	elastic scattering	10	3	1	10.0
$H^+ + H_2$	total scattering	1	12	0	0
$H^+ + Mg$	excitation	2	0	0	0
$O^+ + O$	interchange react	1	17	0	0
$H + H^+$	charge transfer	100	52	2	2.0
$e^- + S^{6+}$	recombination	1	0	0	0
$O^{++} + He$	charge transfer	3	1	0	0
$e^- - Cs$	excitation	32	55	19	59.4
$Kr + He^*$	ionisation	10	71	4	40.0
$HD^* + H_2$	deexcitation	2	2	0	0
TOTAL:		334	443	81	24.3

Appendix 4

Priorities in A+M Compilation, Evaluation and Generation for ITER

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Outline

1. ITER EDA Status
2. ITER Divertor Concept Selection
3. Particle and Power Control Issues
4. A+M Data for Disruption Erosion Modeling
5. ITER Diagnostics

1. ITER EDA Status

- Joint Central ITER Teams Assembling
- Concept Formulation
- Working Tasks Formulation

Basic Conceptual Changes (with Resp. to ITER CDA)
(Current Ideas)

- Increased Thermal Power ($1GW_{th} \rightarrow 3GW_{th}$)
  (somewhat increased size)
- No Non-Inductive Current Drive
- No NBI Heating
- L-mode Operation
- Dense Cold Gas (or radiative?) Divertor
- Shifts in Priorities for PFC Materials
  (C-based, SS → Be, V, W/Mo)

2. Divertor Concepts Currently Discussed

- **High Density Cold Gas Divertor**

  * Plasma and gas parameters:

  $T_e \sim 0.2 - 100eV$

  $T_e \sim 10^{12} - 10^{17}\ cm^{-3}$

  $n_{H_2} \sim 10^{12} - 10^{17}\ cm^{-3}$

  $n_{Ho} \sim 10^{12} - 10^{16}\ cm^{-2}$

  * Main Power Extraction (Dissipation) Mechanisms:
  Charge Exchange,
  Dissociative cooling,
  Momentum transfer

  * Cold H_2 introduced in divertor region/channel at high rate

- **Radiative Divertor**

  * Te ~ 1 - 100 eV, $n_e \sim 10^{12} - 10^{15}\ cm^{-3}$
  $n_{Ho} \sim n_{H_2} \sim 10^{12} - 10^{15}\ cm^{-3}$ (still high recycling)

  * Appropriate, strongly radiating impurities (Kr, ...) deliberately introduced in divertor channel/chamber at necessary rates

  * Plasma energy extraction mechanisms:
  electron impact excitation, ionization

- **Innovative Concepts (?)**

3. A+M Data Related to Power Exhaust Issue

(A+M Processes in the Plasma Edge and Divertor Regions)

The issue: $\frac{1}{5}$ of fusion power is of thermal nature (α-particle heating) and has to be exhausted from reactor

- 40% is assumed to be radiated out in the main plasma region (bremsstrahlung, etc).

- 60% goes into the edge/divertor region

  ~ 350 MW for ITER (if $P_f \simeq 3\ GW_{th}$)

- Main relience on impurity radiative cooling
- Additional cooling/power dissipation defines divertor concept
  - * high density divertor
    - power dissipation through CX and momentum transfer processes (cooling of ion plasma component through high recycling and then plasma thermalization)
  - * radiative divertor
    - plasma power exhaust through enhanced impurity radiation (seeded/injected impurities in controlled manner) (cooling through energy extraction from electron plasma component)

A) <u>High Density Divertor: A+M Processes</u>

$$T_e \sim 0.2 - 100\ eV\ ,\ n_{H^o}|_{\max} \sim 10^{16}\ cm^{-3};\ n_{H_2}|_{\max} \sim 10^{17}\ cm^{-3}$$

$$n_e|_{\max} \sim 10^{17}\ cm^{-3} \qquad n_{He} \sim 10^{14}\text{-}10^{15}\ cm^{-3}$$

* All A+M Processes for Complete Collisional Radiative Models for He, H_2 and H

- For H CR-model database completed
- For He CR-model database completed for processes involving ground state;
  - * improvement needed for processes involving excited states, particularly for heavy-particle collisions;
- For H_2 CR-model: significant gaps exist in processes invovling electronically and vibrationally excited states;
- Elastic/momentum transfer processes for ion-neutral and neutral-neutral collisions (neutrals: H, H_2, He)

<u>new aspects</u> due to high densities and low T_e:

- three-body processes
- particle exchange reactions (reactive collisions)
- resonant radiation capture (radiation transfer problem, plasma opacity

- excitation transfer processes

$$\text{e.g. } H^* + H^0 \rightarrow H^0 + H^*$$

$$H^* + H_2^0 \rightarrow H^0 + H_2^*$$

$$\rightarrow 2H^0$$

$$\rightarrow H^0 + H^*$$

- line profiles

* Processes of e^-, H^+, H^0, He^0 (He^+, He^{2+}) and H_2^0 (H_2^+) with impurities

- Impurities: Be, B, C, Ti, V, Fe, Ni, Cr, Mo, W
- Charge states: q=0-3(5)
- Processes with e^-: excitation, ionization, recombination

  He^{2+}, He^+, H^+: cx with excited neutral H^0, H_2^0, He^0:

  cx, px with low-q ions

* Radiative processes (transition probabilities) of low-q metallic ions (and spectra)

B) Radiative Divertor (?)

* All processes involved in a CR model for a selected A^{q+} impurity: processes with e-, H^+, He^0, H_2^0; A^q: q=0-Z. Candidates for A^{q+}: Kr (Si, Xe, ... ?)

* All processes involved in a "normal", high recycling divertor

4. A+M Data Related to Particle Exhaust/Control

A) Helium Exhaust

- Complete CR-model for He
- Elastic/momentum transfer processes of He^0 with ions, and He^{2+}, He+ with neutrals
- In high density divertor: particle interchange/reactive collisions of He^0, He^+, He^{2+}; three-body collisions
- He (He^+, He^{2+}) - surface processes (reflection, release)

(Data base far from adequate)

B) Impurity Control

- All A+M collision processes involved in impurity transport
- Impurity generation particle-surface int. processes (sputtering, self-sputtering, reflection, other impurity release processes)

(Data base for low-q heavy ions rather poor)

Note on particle-surface processes (for high density divertor)

Sheath potential: $V \simeq 2T_i + 3.5\ q$

$$T_i \sim T_e \quad q=1\text{-}3 \quad ; \quad T_e \gtrsim 1\text{eV}$$

Quantum ion-surface processes important such as: resonant neutralization, Auger processes

5. A+M Data for Disruption Erosion Modeling

Current approach: To avoid plasma disruptions in ITER Completely
No clear way how to achieve this goal!

- Disruption erosion is associated with formation of an evaporated cloud in front of the surface
- Question about shielding effect of this ablated plasma (barrier to further deposition of plasma energy to the wall)

  Vapor cloud parameters: $T_e \sim$ 1-5eV; $n \sim 10^{16}\text{-}10^{17}\ \text{cm}^{-3}$

  Composition: mix of hydrogen plasma and impurity plasma
- Major issues:
  - Energy transfer from hot hydrogen plasma to cold impurity plasma
  - Impurity plasma radiation

A+M data required: CR-model for impurity in question (all processes with e^-, H^+, including three-body processes, and radiation capture (cloud opacity)

6. A+M Data Needs for Plasma Diagnostics

6.1. X-ray core plasma spectroscopy

- Expected core plasma temp. for ITER:

  $T_{e,i}$ ~ 30-40 keV

- Medium Z (wall) impurities fully ionized
- Need for injection of moderately high-Z impurities for VUV or X-ray diagnostics

- PPPL Proposal: Kr injection (in controlled amounts)
  at T_e 30-40 keV He-like ions of Kr predominate in the centre
- A+M Data Required: 1) All daa for determining of ionization stage distribution
  2) Very accurate data for n ≥ 3 dielectronic satelites (including spectroscopic information and collitional-radiative information for satellite formation and decay processes)

6.2. Edge Plasma Diagnostics

Required knowledge of:

- plasma density and temperature profiles
- impurity radial profiles
- impurity and neutral particle (in) fluxes

A+M Data: Similar to those required for divertor plasma (incl. neutral gas) modeling (Needed)

Major Diagnostics:

- H_α-diagnostics: needs accurate knowledge of all processes involving H, H_2, H_2^+ leading to population and destruction of n=2 and n=3 H-levels

* In a high density divertor:
  - excitation transfer (radiation trapping)
  - molecular processes

- Impurity radiation spectroscopy (e.g. Be^{q+}, C^{q+}): Needs accurate knowledge of all processes related to production of selected diagnostic lines

6.3. Active Neutral Beam Based Diagnostics

a) charge exchange recombination spectroscopy: H-beam and He-beam (beam energy: 80-200 keV)

$H^0, He^0 + A^{Z+} \rightarrow H^+, He^+ + A^{(Z-1)+}$ (nl)

A+M Data for Beam Attenuation kinetics: CR model for Beam atoms (intermediate to high energy range)

b) Beam-Emission Spectroscopy: H, He-beams (beam energy: 80-200 keV)

Basis: Radiation from beam excited atoms (n=3-4) (beam energy: 80-200 keV)

- Processes involved in beam penetration calculations
- Detailed cross section knowledge of $n \leq 4$ kinetics

c) He beam alpha particle diagnostics: He^{+*} emission, He^0 particle analysis (Beam energy: 200-300 keV)

- A+M Data for He-beam penetration
- $He_b^0 + He^{2+}$ SSEC | "plume ions" problem
- $He_b^0 + He^{2+}_{(\alpha)} \rightarrow He^{2+}_b + He^0_{(\alpha)}$

Appendix 5

Proposed Points to Consider in Session 3: ALADDIN Implementation and Developments; Possibilities for Technical Improvements: Comments from all Data Centres.

- Frequency of the DCN Meetings: 2 years?
- Technical Aspects
  - Numerical Data.
    - ALADDIN format for exchange
    - ALADDIN interface versus commercial: Having an exchange format, DC's may easily use different interfaces (DBMS).
    - Refinement and Enhancement of ALADDIN Labeling schemes.
    - On-line Service. How useful? Possible users.
    - Sharing of Technical Information Among Data Centers.
    - News Letter for Recommended/Evaluated Data.

- Bibliographic Data
  - International Bulletin on Atomic and Molecular Data for Fusion.
    - Frequency
    - Format
    - Input from DC's
  - Inclusion of Numerical Data in the Bulletin.

- Exchange
  - Improve communication among data centres.
  - Exchange of information: Evaluated data, row data, bibliographic data.
  - Exchange information on DBMS software developments and applications among DC's.

- Applications of A+M Data beyond Fusion.

- Collaboration Among DC's.