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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (11th Meeting of A+M Data Centres and ALADDIN Network)

15-16 June 1992, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared by R.K. Janev

February 1993, Vienna

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

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (11th Meeting of A+M Data Centres and ALADDIN Network)", held on June 15-16, 1992, in Vienna is briefly described. The meeting conclusions on the priorities in A+M data compilation, evaluation and generation, and a plan of actions related to the implementation of these priorities are also provided.

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1. INTRODUCTION

On June 15-16, 1992, the IAEA organized the regular Advisory Group Meeting on "Technical Aspects of Atomicc and Molecular Data Proccessing and Exchange" (11th Meeting of Atomic and Molecular (A+M) Data Centres and ALADDIN Network) with the objectives to review the progress in the A+M data related activities in the data centres, the methods and procedures applied in the data processing and exchange, the developments in the ALADDIN system, and to co-ordinate the working plans for the next period. The meeting was attended by 15 participants from 14 data centres **(see Appendix 1).** Only the Belfast Queen's University A+M data centre was not represented at the Meeting. The NIST (Gaithersburg) Reference Data Programme and the JILA (Boulder) data centre activities were for the first time represented at this series of Advisory Group Meetings.

2. MEETING PROCEEDINGS

The Meeting was opened by the Head of IAEA A+M Data Unit and, after adopting the Agenda **(see Appendix 2)**, its work proceeded in four sessions:

(1) Current activities of the A+M data centres,
(2) Status of ALADDIN, data processing and exchange,
(3) Priorities in A+M data compilation and evaluation,
(4) Meeting conclusions and reccommendations.

In Session 1, progress reports on the activities of individual data centres during the period September 1991 - June 1992 were presented. These reports, which are reproduced in **Appendix 3**, describe the highlights of the work of data centres on A+M data compilation, evaluation and generation, the data centre publications during the reporting period, the status of ongoing programmes and the plans for immediate future work. Some of the reports address also technical aspects of their work, such as manpower situation, computer equipment, etc. 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 establishment spectroscopic data bases in their centres. The recent data compilation and evaluation work at NIST includes energy level data bases for S, Cu, Ga, Kr, wavelength data bases for Mg, Fe, Al, S, Cr, Co, V, Cu, transition probability data bases of the heavy elements (such as Mo). The work in progress at this data centre includes data compilation and evaluation for the energy levels of Cl, Cr, Zn, wavelengths for Na, Si, Mn, Kr, Ga, and transition probabilities for the C-, N-, and O-like ions. The near future plans include work on the M- and N-shell elements (energy levels and wavelengths), He-, Li- and B-like isoelectronic ions (transition probablities), and publication of a spectroscopic data volume in the ORNL "Red book" series on H, D, T, He, C, N and O.

Dr. Faenov described the ongoing spectroscopic data compilation, evaluation and generation work at VNIIFTRI (and the collaborating institutions), and the structure of their spectroscopic data base SPEKTR. About 320,000 spectroscopic records are contained in this data base using the FOXPRO2 software. The VNIIFTRI data centre currently extends its activity also in the area of A+M collisional data, mainly for elecctron impacct processes (excitation, ionization, dielectronic recombination). The ongoing work includes electron-impact excitation data for the H-like ions, Be^{2+}, C^{5+} (transitions up to the 5l states), dielectronic recombination in H-like ions Be^{3+}, C^{5+}, Al^{12+}, Ca^{19+} on $n^{1,3}L$ states, with n=1-9 and L=S...G, and O^{q+} and Fe^{q+} isonuclear sequences.

Spectroscopic data compilation activity is also being pursued at the JAERI NDC-A+M Data Unit, mainly in collaboration with the NIST data centre, and a progress report on it was presented by **Dr. T. Shirai**. Completion of the spectroscopic data bases for ionized Cr and Mn was reported, as well as the similar work in progress for KrV - KrXXXVI. Dr. Shirai also reported on the JAERI NDC-A+M Data Unit activities in the area of A+M collisional data, the highlight of which include an analytic fit representation of all the Barnett's recommended data on H, H^+, H_2^+, He^+ and He^{2+} electron capture collisions with atoms, molecules and ions of fusion interest (contained in the recently published ORNL "Red book", vol. 1), and the similar fits for the C^{6+}, O^{8+}-H recommended state-selective cross sections.

The presentation of the ongoing work on A+M collisional data bases in the A+M Data Centre Network continued with the presentation of **Dr. D.R. Schultz** (ORNL, CFADC), who reported on the continued bibliographic data compilation activity of CFADC, recent cross section data evaluation efforts of this centre in collaboration with IAEA, NIFS (Nagoya) and JAERI for electron capture and other heavy particle collision processes involving Be^{q+}, B^{q+}, C^{6+}, O^{8+} ions, and on the initiated project for establishing a data base for the elastic and momentum transfer processes in ion-neutral and neutral-neutral processes relevant for the neutral particle transport in the plasma edge. Dr. Schultz also described the status of the CFADC efforts on establishing a universally accessible Atomic Data Workstation at ORNL CFADC for on-line use of the bibliographic and ALADDIN formatted numerical A+M data bases. **Dr. H. Tawara** (NIFS, Nagoya) reported on the recent A+M data compilation and evaluation activities, which include: electron-impact excitation data for ground-state and metastable He atoms, data for processes relevant for the polarization plasma spectroscopy, and high-energy ion-hydrogen atom stripping reacctions. Generation of electron-ion excitation cross sections and ion energy level calculations, performed jointly with coworkers from the Moscow Institute of Spectroscopy, have also been reported by this data centre. **Dr. E. Menapace** (ENEA NDC-A+M Data Unit, Bologna) reported on the theoreticcal model developments at ENEA for calculation of the ro-vibrational spectra of polyatomic molecules (such as hydrocarbons), photoionization of complex atoms and ions, and particle reflection from sufaces at low impact energies. The first results obtained from these models were shown, demonstrating their advantages and potentials. Of particular interest for generation of particle-surfacce interaction data for fusion is the molecular-dynamics code for particle reflection, which reflection, which can access the energy region below 10 eV, where the standard particle-surface collision simulation codes (such as TRIM and MARLOWE) encounter conceptual difficulties for their application. **Dr. K. Katsonis** (GAPHYOR, Orsay) presented the bibliographic activity of this centre during the reporting period, providing statistics on the number of entries in their bibliographicc data base (as of June 15, 1992, total number of entries was about 15,600), and its structural features. Dr. Katsonis also described the work in progress on cross section calculations for heavy particle collision processes by using a classical trajectory Monte Carlo code, as well as some published and new results.

The data activity and its results of the A+M data centre at the Kurchatov Institute, Moscow, was presented by **Dr. V.A. Abramov**. In the reporting period, this activity has included: preparation of bibliographic data files from Russian publications as input to the IAEA A+M data bibliographic Bulletin, collection and generation (including experimental methods) of cross section data for low-Z (Li, Be, B, C) and high-Z (Ga, Cs, Mo) elements, A+M data bases for modelling the Li- and Cs-beam penetration in fusion plasmas, and calculations of radiative cooling rates for C-seeded plasmas (with inclusion of charge exchange of impurities on the residual hydrogen atoms). The data generation activities at the Kurchatov Institute in the area of particle-surface interaction processes (sputtering, radiation-enhanced sublimation, synergistic effects in the simultaneous two-ion implantation) were also described in Dr. Abramov's presentation.

Dr. V. Piksaikin (Obninsk NDC-A+M Group) described the A+M data activities in the Obninsk NDC, including a data base on ionization differential cross sections for proton ccollisions with He and Ar, and oscillator strengths and transition probability calculations for Ca^+, Cd^+ and Zr^+ ions using the ATOM code (of Vainshtein and Shevelko). An analytic fit representation for the ionization differential cross sections has been devised, allowing for two (or three, in some cases) fitting parameters. These data are ccurrently being ALADDIN formatted. **Dr. J. Yao** (Chinese NDC-A+M Data Group, Beijing) reported on the data compilation and ALADDIN data formatting work at CNDC, involving electron-impact excitation and ionization collisions of atoms and ions in the energy range up to 100 keV, and heavy-particle electron capture and ionization collisions of H, H_2, He, Li, Fe atoms with their ions. Dr. Yao also described the results obtained from the PANDA-U code on light ion (H, D, T, He-3, He-4) reflecction coefficients from solids (Be, B, C, Al, Si, Ti, Fe, Ni, Cu, Mo, W and Au). These calculations, performed by Dr. Luo Zhengming, incorporate the effects of surface potential barrier. The CNDC A+M Group compiles data on hydrogen trapping/detrapping on surfaces, as well as particle desorption data for certain elements and materials. The work in progress in the electron capture data compilation was also described. The activities of the Chinese Research Association for A+M Data (CRAAMD) in the reporting period were presented by **Dr. Yubo Qiu** (IAPCM, Beijing). The highlight of these activities are: preparation and publication of the first volume of the Chinese Bulletin on A+M Data, compilation, evaluation, parametric representation and ALADDIN formatting of a large body of electron-impact collisional data (published in several CRAAMD Reports) on excitation and ionization of atoms and ions, dielectronic recombination, as well as data on photoionization and spectroscopic properties of atomic ions (energy levels, wavelengths, oscillator strengths). A general overview of the CRAAMD A+M data base, its structure and functional organization, was also given in the presentation of Dr. Qiu.

The Atomic Collision Cross Sections Data Centre at JILA (Boulder) was for the first time represented at the A+M Data

Centre Network meetings by its Director, **Dr. J. Broad**. Dr. Broad presented the main objectives of the Centre, its structure, manpower and computer equipment, its bibliographic and numerical data activities in the areas of A+M and Optical physics, and the major current and planned projects of the Centre in these areas. The content of many of the JILA A+M and Optical (spectroscopic) data bases is relevant to fusion (e.g. the planned compilation and assessment of electron-impact excitation of atomic ions, and the gas lasers data base), so that the contribution of this data centre to the objectives of the A+M Data Centre Network could be significant. This contribution could particularly be important in facilitating the data exchange between the existing large data generation programmes (such as OPACITY and IRON) and A+M Data Centre Network and in providing technical advice in establishing the ORNL on-line accessible workstation data base. **Dr. J.W. Gallagher** (NIST, Standard Reference Data Programme, Gaithersburg) described the reference data bases at NIST in various areas (from Analytic Chemistry to Thermophysical Properties of Fluids). The most relevant for the present Advisory Group was the content of the NIST standard reference data bases in the fields of Molecular Structure and Spectroscopy (vibrational and electronic energy levels of fusion edge plasma molecules), chemical kinetics (reaction rates for certain gas-phase reactions occuring in the plasma edge), and the Material Properties data bases (structural and thermophysical properties, performance properties including mechanical corrosion, and phase equilibria). While the NIST atomic and ionic spectroscopy programmes have already been incorporated in the A+M Data Centre Network activity for fusion, similar working relationship of the Network with the NIST programmes in the areas of molecular spectroscopy data and material properties would be mutually beneficial.

At the end of this session **Dr. R.K. Janev** (IAEA, A+M Data Unit) presented the activities of the IAEA A+M Data Unit in the reporting period. Apart from reviewing the standard Unit's activities related to the maintenance of recommended A+M numerical data bases, their updating, ALADDIN formatting and extension, the work in progress on the finalization of the data bases for H-, He- and Li-beam penetration into plasmas was also described. Information was given on the status of Be- and B-data base projects, the results produced so far within three research A+M and PSI data programmes co-ordinated by the IAEA, and the Unit's activity extension into the area of material properties data for fusion. The IAEA Data Unit's efforts on improvement of ALADDIN interface shell were also briefly described.

Prof. F.J. Smith of the Queen's University of Belfast A+M Data Centre has not been able to attend the Meeting. However, a brief report on the activity and recent developments in this data centre has been obtained from Prof. Smith after the Meeting, and this report is also reproduced at the end of **Appendix 3**.

During the subsequent two sessions, the Advisory Group participants had in-depth discussions on the status, implementation and recent developments of the ALADDIN system, and regarding the priorities in the data compilation and evaluation work for the next period. The summaries of these discussions are given in the next two sections of the present Report. The conclusions and recommendations of the Advisory Group have been formulated and adopted during the last session of the Meeting and are summarized in Section 5 of this Report.

3. SUMMARY OF THE DISCUSSIONS CONCERNING IMPLEMENTATION AND DEVELOPMENT OF THE ALADDIN SYSTEM

(Prepared by D.R. Schultz, ORNL and J. Botero, IAEA)

Comments of the representatives from the thirteen international data centres present at this meeting indicated that the ALADDIN data format and system are continuing to mature as the internationally accepted medium for atomic and molecular data exchange and processing for controlled fusion plasma research. It was reported that the ALADDIN software has been ported on an ever increasing variety of computers ranging from IBM PCs to workstations and mainframes. However, the need for a number of extensions and additional utilities was pointed out. Among these extensions and utilities, two were discussed as first priority.

In order to facilitate data processing, compilation, evaluation and recommendation of data, a more user-friendly interface to the software is required. It was reminded that in the previous data centres meeting preliminary work on such an interface, developed by V. Osorio and J.J. Smith (IAEA), was presented. The consensus of the participants at the present meeting was that now that J. Botero had been hired by the IAEA A+M Data Unit, the work should be continued to complete this, or a similar graphical interfacce. Another option available to individual data centres is to supplement the ALADDIN software with commercially available data base software as a shell. **Dr. A. Faenov** (VNIIFTRI) demonstrated such a possibility using the data base program FOXPRO. **Dr. E. Menapace** also stated that ENEA had written a code which serves as an interface between ALADDIN and their local format.

The main users of A+M data are the plasma modellers. Therefore, the second important extension pointed out at the meeting was the interface to the plasma modelling programs. These interface programs, whenever available, should be shared among data centres. The IAEA A+M Data Unit agreed upon making informal inquires to the main plasma modellers as to whether or not such programs have been or should be developed.

Another important development of the ALADDIN system will be the inclusion of spectroscopic data and the establishment of a standard format for its entry. Last year a preliminary standard was proposed by **W. Wiese** (NIST) and was approved by the Advisory Group. A few details still remain to be worked out, but Wiese indicated that he felt that they could be resolved quickly once another difficulty was overcome. This difficulty centers about the transformation of the NIST spectroscopic data into the proposed ALADDIN format, from the ORACLE format in which it is currently stored. J. Botero (IAEA) and D. Schultz (ORNL) offered their assistance in making the conversion.

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.

D. Schultz also described preliminary work directed towards the establishment of a work station at ORNL which will allow universal access to the A+M bibliographic data base currently maintained there. He also asked for input from the other data centers concerning the implementation of ALADDIN on that platform, in collaboration with the IAEA A+M Data Unit.

Thus, with the advent in the near future of utilities to facilitate the interface of ALADDIN both with humans and plasma modelling codes, and its wide spread use to disseminate data, the system is reaching a solid standing as the accepted medium of A+M data exchange.

4. PRIORITIES IN A+M DATA COMPILATION AND EVALUATION

The discussion on priorities in A+M data compilation and evaluation work at the A+M data centres has reflected the fact that the ITER R+D plans, as proposed by the ITER Physics Group during the last year of ITER CDA, contain a degree of uncertainty related to the possible modifications of some technical aspects of the design concept during the ITER EDA phase, which may affect the content of the atomic physics involved. However, the Advisory Group took the position that the impurity control and particle and power exhaust aspects will continue to be very important design issues during the ITER EDA, and that they have certain atomic physics content which is invariant to the design modifications. On the other hand, the ongoing and planned experiments on the operating large tokamaks have already formulated a wide range of urgently required A+M data. On this basis, and keeping in mind the present status of the available evaluated data bases, as well as the manpower and data generating potentials of the A+M data centres, the Advisory Group adopted the following priorities in the A+M data compilation, evaluation and generation work for the next period: (The data centres and other institutions from which a major contribution is expected in satisfying the priority needs are also indicated).

A. Spectroscopic Data

(1) Transition probabilities for the He-, Li-, Be-, B-like isoelectronic ions (NIST, JAERI, VNIIFTRI),
(2) Energy levels, wavelengths, transition probabilities for high-Z impurities (Ga, V, Mo W) and for Kr (NIST, JAERI, VNIIFTRI, Kurchatov Institute),
(3) Updating and compilation of spectroscopic data bases for Be^{q+} and B^{q+} ions (including publication in the ORNL "Red book" series) (NIST, ORNL).

B. Collisional Data for Plasma Edge Studies

(Includes: neutral particle transport modelling and diagnostics, H-recycling, He-exhaust).

(1) 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^+ (ORNL, ENEA, IAEA).
(2) Ro-vibrational excitation of H_2 and H_2^+ by electron and proton impact in the energy range from threshold to ~ 500 eV (JAERI, ENEA).
(3) 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) (McKoy, NIFS).

(4) 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 (NIFS, Kurchatov Inst., IAEA, JAERI, JET, FOM-Amsterdam).

(5) 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) (IAEA, Lebedev Inst., ANL, Belfast Univ., GAPHYOR, ORNL, others).

(6) Further development of the data bases for hydrocarbons (all processes with electrons and protons) (NIFS), H_2O and CO (NIFS), and Be-, B- oxides and hydrides (including their ions) (NIST-Gallagher).

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

C. <u>Radiative Plasma Cooling</u>

C.1. <u>Plasma core region</u>

(1) Electron impact processes (excitation, ionization, radiative and dielectronic recombination) of medium- and high-Z impurities (Ti, Ni, Cr, Fe, Mo, W, Ga, V) (Kurchatov Inst., JILA, CRAAMD, CNDC, others).

(2) Charge exchange collisions of A^{q+} (A as above) with H, H^+ and He^{2+} (GAPHYOR, IAEA).

Note: Pertinent energy range for C.1 is from a few keV to 30 keV.

C.2. <u>Plasma edge region</u>

(1) Electron impact processes involving low-, medium- and high-Z impurities in low charge states ($q \le 5$). The most important low-Z impurities are Be and B. (For C and O the data base is in good shape) (Contributors: same as in B(5) and C.1(1)).

(2) Collisions of A^{q+} ($q \le 5$) with H, He, H_2, including

state-selective electron capture (IAEA, GAPHYOR, ORNL, NIFS, JAERI, Kurchatov Inst.).

(3) 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) (LANL, NIFS, Kurchatov Inst., GAPHYOR, ORNL).

Note 1: Pertinent energy range for C.2 is from 1 eV (or threshold) to 500 eV.

Note 2: If the charge exchange/momentum transfer scheme of divertor plasma cooling is accepted for ITER, the required A+M information is that described in B(1)-B(7).

Note 3: The optimum data base required for calculation of the radiative cooling power of a given chemical species coincides with that of the corresponding collisional-radiative model (including also charge transfer on H).

5. MEETING CONCLUSIONS AND RECOMMENDATIONS

The presentations and discussions at the Advisory Group meeting regarding the A+M and PSI 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:

A. 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 seems to be adequate to follow both the fusion needs for such data and the rate of data generation by the atomic physics community. 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 data compilation efforts are currently still being done mainly in the fusion laboratories, i.e. outside the A+M Data Centre Network. The Agency only partly co-ordinates this data compilation activity (through a Co-ordinated Research Programme and a number of Research Contracts), although the results of this activity in various institutions are being regularly collected and processed by the IAEA A+M Data Unit. It is highly desirable that the members of the A+M Data Centre Network expand more vigorously their effort in the PSI data compilation area, and that some of the most active fusion-laboratory-based groups (such as that in IPP Garching) which collect and evaluate PSI data be included in the A+M (and PSI) Data Centre Network. A similar statement can be made also regarding the material properties data for fusion.

The Advisory Group commends the progress in A+M and PSI data compilation field made by the two Chinese data centres (CRAAMD and CNDC-A+M Group) and wellcomes the co-operation with the JILA A+M data centre, and the development of a broader working relationship with the NIST reference data programmes.

2) The Advisory Group is of the opinion that the present level of the data evaluation effort, particularly in the areas of A+M collisional and PSI 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 data 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.

B. Data Processing and Exchange (ALADDIN)

1) The implementation of ALADDIN in the data management, processing and exchange practices of A+M data centres can now be considered as well established, as far as the collisional and PSI data are concerned. The conversion of NIST numerical spectroscopic data files from ORACLE into ALADDIN format still depends on developing an appropriate computer code to automate the conversion. The IAEA and ORNL data centres could provide the necessary advisory and technical assistance to NIST to accomplish this task. The ALADDIN structure has recently been extended (IAEA, PPPL and Efremov Institute) to incorporate data on material properties. The Efremov Institute in St. Petersburg is now maintaining a large material properties data base in ALADDIN, which is also available at the IAEA. This ALADDIN data base is supplemented also with a graphical interface.

2) The development of a graphical interface shell for ALADDIN, initiated by the IAEA, is to be continued and

finalized as soon as possible. The IAEA and Efremov Institute versions of this interface shell have to be optimized and fused into one. This, 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 1993.

3) The data exchange between the members of A+M Data Centre Network follows well established procedures and is rather intense. This exchange includes both evaluated and non-evaluated numerical data, transported between the centres by various means (including electronic mail). The establishment of a user-accessible ALADDIN data base workstation at the ORNL data centre should considerably enhance the data exchange and dissemination process. The bibliographic reference data exchange is currently confined to the IAEA and ORNL, NIST, GAPHYOR and Kurchatov Institute data centres. The publication of the bibliographic Bulletin on A+M data for fusion should resume its regular rate in 1993.

4) There is an increasing number of requests from the fusion A+M and PSI data users for preparation of data files not only for the quantities directly related to the A+M and PSI processes, but also for composite quantities, such as collisional-radiative rates, radiative cooling rates, etc. In order to meet such needs, as well to enable the IAEA A+M Data Unit with a capability for significant and independent contributions to the completion of certain A+M or PSI data bases, it is necessary to further enhance the technical base of the Unit, both in terms of computer equipment and additional technical manpower.

C. Priorities in Data Compilation, Evaluation and Generation

1) The long-term priorities in A+M and PSI data compilation, evaluation and generation, as established by the IFRC Subcommittee on A+M Data for Fusion at its September 1990 meeting, remain still unchanged (see IAEA Report INDC(NDS)-244/M9). Some modifications, or changes in emphasis, may be expected from the analyses at the planned Technical Committee Meeting (TCM) on "A+M Data for Fusion Reactor Technology" to be held in October 1992 in Cadarache, France.
2) The short-term priorities in the A+M and PSI data activities, particularly in relation with the reactor plasma edge studies and the radiative plasma cooling, are those listed in Section 4 of this Report. It is also expected that the TCM in Cadarache will provide a broader list of urgently required data for the operating and next-generation fusion devices. This new data requirements should complement the list in Section 4.

Appendix 1

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (11th Meeting of A+M Data Centres and ALADDIN Network)"

15 - 16 June 1992, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

Dr. Yao Jinzhang	Chinese Nuclear Data Center, Institute of Atomic Energy, P.O. Box 275(41), Beijing, **CHINA**
Dr. Yubo Qiu	Institute of Applied Physics and Computational Mathematics, No. 6 Huayuan Road, Hai-Dian District, P.O. Box 8009, Beijing 100088, **CHINA**
Dr. K. Katsonis	GAPHYOR, Laboratoire de Physique des Plasmas, Université de Paris XI (Paris-Sud), 15, Rue G. Clemenceau, F-91405 Orsay Cedex, **FRANCE**
Dr. E. Menapace	ENEA-C.R.E. "E. Clementel", Viale Ercolan 8, I-40138 Bologna, **ITALY**
Dr. T. Shirai	Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Naka-gun, Ibaraki-ken 319-11, **JAPAN**
Dr. H. Tawara	National Institute for Fusion Science, Nagoya 464, **JAPAN**
Dr. V.A. Abramov	Institut Atomnoi Energii I.V. Kurchatova, Ploshchad I.V. Kurchatova, Moscow D-182, 123182, **RUSSIAN FEDERATION**
Dr. A. Faenov	All Union Research Institute for Physical Technical and Radiotechnical Measurements, VNIIFTRI, 141570 Mendeleevo, Moscow Region, **RUSSIAN FEDERATION**
Dr. V. Piksaikin	Centr po jad. dannym, Fiziko-Energetichesky Institut, Ploschad Bondarenko, 249 020 Obninsk, Kaluga Region, **RUSSIAN FEDERATION**

Dr. J.T. Broad Joint Institute for Laboratory and Astrophysics (JILA), University of Colorado, Colorado 80309, **U.S.A.**

Dr. J.W.Gallagher National Institute for Standards and Technology (NIST), US Department of Commerce, Gaithersburg, MD 20899, **U.S.A.**

Dr. D.R. Schultz Oak Ridge National Laboratory, MS-6372, Bldg. 6003, P.O. Box 2008, Oak Ridge, Tennessee 37831-6372, **U.S.A.**

Dr. W.L. Wiese National Institute for Standards and Technology, US Department of Commerce, Atomic and Plasma Radiation Division, Gaithersburg, MD 20899, **U.S.A.**

IAEA

R.K. Janev IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, **AUSTRIA**

J. Botero IAEA Atomic and Molecular Data Unit, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, **AUSTRIA**

Appendix 2

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (11th Meeting of A+M Data Centres and ALADDIN Network)"

15 - 16 June 1992, IAEA Headquarters, Vienna, Austria

MEETING AGENDA

MONDAY, June 15

09:30 - 09:45	- Opening - Adoption of Agenda	(Room: A-07-42)
Session 1:	**Current Activities of the A+M Data Centres**	
Chairman:	**Abramov**	
09:45 - 11:00	Reports from Data Centres: Wiese (NIST), Faenov (VNIIFTRI), Shirai (JAERI)	
11:00 - 11:15	**Coffee break**	
11:15 - 12:30	Reports from Data Centres: Schultz (ORNL), Tawara (NIFS), Menapace (ENEA)	
12:30 - 14:00	**Lunch**	
Session 1:	**Cont'd**	
Chairman:	**Wiese**	
14:00 - 15:50	Reports from Data Centres: Delcroix/Katsonis (GAPHYOR), Abramov (Kurchatov Institute), Piksaikin (Obninsk), Yao Jinzhang (IAE, Beijing)	
15:50 - 16:05	**Coffee break**	
16:05 - 18:00	Reports from Data Centres: Gallagher (NIST), Broad (JILA), Qiu Yubo (CRAAMD), Janev (IAEA)	

TUESDAY, June 16

Session 2:	**Status of ALADDIN, Data Processing and Exchange**
Chairman:	**Menapace**
09:30 - 10:45	ALLADIN implementation and developments: Comments from Data Centres (all participants)
10:45 - 11:00	**Coffee break**
11:00 - 12:00	Possibilities for technical improvements of data processing and exchange procedures
12:00 - 12:30	Demonstration of new softwares (Faenov)
12:30 - 14:00	**Lunch**
Session 3:	**Priorities in A+M data Compilation and Evaluation**
Chairman:	**Janev**
14:00 - 15:30	- Priorities in A+M data compilation and evaluation related to ITER EDA needs - Co-ordination of data activities within the Data Centre Network and with ITER EDA - Plan of DCN activities for near future
15:30 - 15:45	**Coffee break**
Session 4:	**Meeting Conclusions and Recommendations**
Chairman:	**Janev**
15:45 - 17:00	Formulation and adoption of meeting conclusions and recommendations

17:00 - **Adjourn of the Meeting**

Appendix 3

Reports from the A+M Data Centres for the period September 1991 - June 1992

Data Centers on Atomic Spectroscopy at NIST

Progress Report for 1991/92

W.L. Wiese

	Director	Workforce
1. Atomic Energy Levels and Wavelengths	W.C. Martin	2 Professionals
2. Atomic Transition Probabilities	W.L. Wiese	1 1/2 Professionals
3. Spectral Line Shapes and Shifts	W.L. Wiese	Occasional Guest

NIST data compilations:

	Energy Levels	Wavelengths	Transition Probabilities
Recent Work Areas: (compilations last 2 years)	S, Cu, Ga, Kr	Mg, Fe, Al, S, Cr, Co, V, Cu	Selected heavy elements, such as Mo
Work in Progress:	Cl, Cr, Zn	Na, Si, Mn, Kr, Ga	C Sequence N Sequence O Sequence
Near Future Plans:	Volume on H, D, T, He, C, N, and O for ORNL ("Red Book" series)		
	M-shell elements (Na-Ar) N-shell elements (Cu-Mo)	N-shell elements	Selected heavier elements (metals) B Sequence Li Sequence He-Sequence

Database development:

1. Bibliographic databases (ORACLE software):

   Atomic Energy Levels since 1985,

   Atomic Transition Probabilities since 1980,

   Line Shape and Shift Parameters since 1920.

2. Numerical databases:

   General Spectroscopic database → E, λ, A

   Data entered:

Energy Levels (λ's)	→	Na, Mg, Al, Si, P, S, Cu, Kr, Mo
		Fe-group elements
		Rare earths
Transit. Probabilities	→	Fe-group elements

Recent Publications

W.C. Martin, R. Zalubas, and A. Musgrove,
Energy Levels of Sulfur, S I through S XVI,
J. Phys. Chem. Ref. Data 19, 821-880 (1990).

J. Sugar and A. Musgrove,
Energy Levels of Copper, Cu I through Cu XXIX,
J. Phys. Chem. Ref. Data 19, 527-616 (1990).

T. Shirai, Y. Funatake, K. Mori, J. Sugar, W.L. Wiese, and Y. Nakai,
Spectral Data and Grotrian Diagrams for Highly Ionized Iron, Fe VIII-XXVI,
J. Phys. Chem Ref. Data 19, 127-275 (1990).

J.R. Fuhr and W.L. Wiese,
Atomic Transition Probabilities, CRC Handbook of Chemistry and Physics, 71st Edition
(CRC Press, Boca Raton, Fl. 1990).

T. Shirai, T. Nakagaki, J. Sugar and W.L. Wiese,
Spectral Data and Grotrian Diagrams for Highly Ionized Vanadium, V VI through V XXIII,
J. Phys. Chem. Ref. Data 91, 273-390 (1992).

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 (September 1991 - June 1992) 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: wave-lengths, energy levels, transitions probabilities); creating 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. Inverse populations investigations in multicharged ions plasma and creation of recombination lasers on the ion transitions in laser-produced plasmas.

IV. Investigation of emission of laser-produced plasma, expended under external actions (interactions of two laser-produced plasma jets, interaction of laser-produced plasma with different obstacles, gas and magnetic field).

V. Creation of different x-ray spectroscopic equipment.

I. a) Now we have agreement between LLNL and MISDC about improving of atomic physic database which is created in our Center during 6 years. LLNL placed at MISDC IBM PS/2 computer with enough big hard disk. During this year we did conversion to PC computer formats all data which we had an old EC computer . We change our software for PC database. Now we are using FoxPro 2 as a basic software and writing some applied software our Database contains now wavelengths, energy levels, transition probabilities, ionization potentials and excitation crossections. MISDC placed at LLNL our Database with software for testing and work. Now our Database is working with 320,000 records. The time for complicated search is not more than one minute.

b) We continue collecting, evaluating data on electron impact excitation, ionization and dielectronic recombination etc. Conversion all of these data to ALADDIN format and send them to IAEA. (See Appendix

c) We continue working to improve the accuracy of measurements wavelengths in traditional hot dense plasma experiments. We suggest new experimental scheme for laser-produced plasma experiments. Using Iohan's scheme spectrograph and measuring spectral lines with spatial resolution were allowed us to register spectra in wavelengths region 12 ÷ 17 Å with spectral resolution $\frac{\Delta\lambda}{\lambda} \sim 3 \div 5.10^3$. The wavelengths of He-like ions of F VIII were measured with the accuracy $5 \div 8.10^{-5}$.

d) We began to study the possibility of using exploding wire, x-pinch plasmas for precise measurements of wavelengths. Such plasma sources are very interesting because they have small sizes ($10 \div 100\ \mu$), hot temperature (up to $1 \div 3$ keV) and high electron density (up to $10^{23} \div 10^{24}$). In such experiments ions with spectroscopic symbols up to 70 were registered. Using the Iohan's scheme with spherical mica crystals were allowed us to register He-like spectral lines with transitions up to $n = 12 \rightarrow n' = 1$ and have spectral resolution $\frac{\Delta\lambda}{\lambda} \sim 3 \div 5.10^3$. We hope that it is allowed us to do very precise measurements of wavelengths in the nearest future.

II. a) Intensities and Line Shapes for exploding wire and X-pinch plasmas are very interesting due to unique parameters of these plasmas. Our Center together with Dr. S.A. Pikuz from Lebedev Physical Institute began to carry out experiments to investigate Line Shapes and intensities from different part of X-pinch. Now we did experiments with Al wires. Later we hope that for Ti wires we will have plasma with electron density $10^{23} \div 10^{25}$ cm^{-3}.

b) We continue our joint experiments with GSI (Germany), ITEP (Moscow) for spectroscopy investigations of plasma produced by high energy heavy ion beam. It were two group of experiments. We measured visible spectra in spectral range 2000 ÷ 6000 Å and soft x-ray spectra with the help of multichannels pinholes.

It has been demonstrated that the spectroscopic techniques can be applied successfully for the diagnozing of plasma with parameters $N_e = 1,4.10^{17}$ cm^{-3} and $T_e = 0,8$ eV which were determined from the intensity ratio of the 4f-3d and 4s-3p lines of Mg II and from electron impact broadening of the 4f-3d line. It was shown that the X-ray emission coming from the surface of the target is its characteristic radiation caused by excitation processes in ion atom collisions. It was investigated plasma density and temperature parameters in the case of the two colliding plasmas, created heavy-ion Kr^+ ions heating Mg-foil with mass thickness 100 mg/cm^2 and slab target spaced by 5 mm. It was shown that the temperature and density were essentially increased in colliding region.

Appendix

VNIIFTRI activity on the storing of electron-ions collision data.

Following data have being compiled and submitted in ALADDIN format to the Atomic and Molecular data Unit of IAEA:

cross sections and rate coefficients for the electron impact excitation of H-like ions Be^{2+} and C^{5+} from the ground state to nl=4l,5l states, calculated in the Coulomb-Born approximation by the ATOM program code. Taken from "Electron impact Excitation Cross Sections and Rate Coefficients for 1s-4l,5l transitions in BeIV and CVI Ions" , I.L. Beigman, Lebedev Physical Institute (unpublished).

rate coefficients for the dielectronic recombination in H-like ions Be^{3+}, C^{5+}, Al^{12+}, Ca^{19+} on the $n^{1,3}L$ states with n=1...9 and L=S...G, calculated in configuration interaction method with account of 205 autoionization states and 77 states below ionization threshold. Taken from "Rate Coefficients for Dielectronic Recombination in H-like Ions BeIV, CVI, AlXIII, CaXX", O.I. Zatsarinny (unpublished).

rate coefficients for the dielectronic recombination in Fe^{q+} and O^{q+} ions. Taken from "Rate Coefficients for Dielectronic Recombination", I.L.Beigman et.al, Preprint of Lebedev Physical Institute n. 7, (1981) in Russian.

The evaluation function codes and data identification labels dictionary file have been also submitted.

Progress Report on the A+M Data Activities at Nuclear Data Center (NDC), Japan Atomic Energy Research Institute (JAERI) October 1991 - May 1992

Toshizo Shirai

A four-year program from April 1992 was started for making the fourth edition of Evaluated Atomic and Molecular Data Library (JEAMDL-4) for fusion. This program is pursued by the JAERI/NDC in collaboration with the JAERI Research Committee on Atomic and Molecular Data and with researchers in NIST and ORNL under the U.S.-Japan Fusion Cooperation Program.

1. Recent Activities and Work in Progress

A work on analytic fits has been continued for (1) the total electron capture cross-sections by H, H^+, H_2^+, He^+ and He^{2+} colliding with atoms, molecules and ions and (2) the state-selective electron capture cross sections for H^+ colliding with atoms and molecules. Analytic expressions are given in functional forms to make it possible to extrapolate the Barnett's recommended data. The fifty-nine ALADDIN formatted expressions have been sent to the IAEA/NDS/A+M Unit. They reproduce well the recommended data within the uncertainty of them. In order to estimate the accuracy of the extrapolation, however, experimental measurements and/or sophisticated calculations are required, especially at low collision energies.

Similar analytic fits have been made for recommended cross sections for state-selective electron capture in collisions of C^{6+} and O^{8+} ions with atomic hydrogen.

Evaluation of spectroscopic data was completed for highly ionized chromium and manganese ions in joint work with NIST. A similar work is now in progress for Kr V-Kr XXXVI. A survey and collection has been made of bibliographic data on Ga ions. Data accumulation is not so large.

Differential cross sections for the 1s-2s,2p excitations of ions from He^+ to C^{5+} by electron impact were calculated in a close-coupling approximation with 1s, 2s, and 2p states.

2. Recent Publications

Cross Section Data

1. Phys. Rev. A 45, 6902 (1992): "Differential cross section for the excitation of hydrogenlike ions from He^+ to C^{5+} by low energy electron impact," Y. Zou and T. Shirai.
2. JAERI-M (1992) to be submitted: "Analytic expressions for the collision cross-sections 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.

Spectroscopic Data

3. J. Phys. Chem. Ref. Data 21, 23 (1992): "Spectral data and Grotrian diagrams for highly ionized cobalt, Co VIII - Co XXVII," T. Shirai, A. Mengoni, Y. Nakai, J. Sugar, W.L. Wiese, K. Mori, and H. Sakai.
4. J. Phys. Chem. Ref. Data, 21, 273 (1992): "Spectral data and Grotrian diagrams for highly ionized vanadium, V VI - V XXIII," 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 chromium, Cr V - Cr XXIV," T. Shirai, T. Nakagaki, J. Sugar, and W.L. Wiese.
6. J. Phys. Chem. Ref. Data, submitted: "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.

3. Activity Plans for 1992 to 1993

3.1 Analytic fits for collision cross-sections

The work on analytic fits for recommended cross sections will be extended to other processes of state-selective electron capture, and excitation and spectral emission of H, H_2, He, and Li atoms and ions in collisions with atoms and molecules.

3.2 Spectral data of highly ionized atoms for fusion

A series of monographs are already published of spectra of highly ionized atoms from Ti to Cu, Kr, and Mo. We have a plan to collect these monographs under one cover. Data will be superseded by more recent data published to December 1991.

CONTROLLED FUSION ATOMIC DATA CENTER

Progress Report for 1991/92

D.R. Schultz

ORNL STAFF:

R. A. Phaneuf (Director) [20%]
M. I. Kirkpatrick (Information Assistant) [100%]
D. R. Schultz [20%]
C. C. Havener [5%]
F. W. Meyer [5%]

CONSULTANTS UNDER CONTRACT:

H. B. Gilbody
E. W. McDaniel
M. S. Pindzola
E. W. Thomas
T. J. Morgan
(A. Ya Faenov)

OTHER PARTICIPANTS:

I. Alvarez
C. Cisneros
R. K. Janev
H. Tawara
T. Shirai

MISSION

* To identify, compile, evaluate, and recommend atomic collision data needed in fusion research.

CONTINUING ACTIVITIES

* Maintenance of an on-line bibliographic data base (by ORNL staff, consultants)
* Compilations of recommended atomic collision data for fusion applications (Redbooks, topical reports)
* Development and implementation of universal data base and exchange system and computer data bases (ALADDIN)
* Deduction of scaling laws and parametrizations of atomic data to facilitate applications in fusion.
* Identification of data needs and data base assessments for fusion applications.
* Coordinate activities and collaborate with International Atomic and Molecular Data Center Network.
* Answer individual requests for atomic data for fusion applications (1-2 per week)

ORNL CFADC bibliographic database

1978 - present

on-line "local area network" using dBaseIII
approximately 24,200 entries
on the order of 1500 entries/year added

circa 1950 - 1978

hardcopy files, published bibliographies
archive tapes exist
estimated to be about 25,000 entries
plans to explore feasibility of converting tapes
  to dBaseIII compatible file

Redbook Compilations:

Collisions of H, H_2, He and Li Atoms and Ions with Atoms and Molecules, C. F. Barnett, ORNL-6086 (1990). [+ ALADDIN Database]

Spectrocopic Data for Titanium, Chromium and Nickel, W. L. Wiese and A. Musgrove (NIST), ORNL-6551 (1989).

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). [+ ALADDIN Database]

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

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

Other Database Assessments

Recommended Cross sections for State-Selective Electron Capture in Collisions of C^{6+} and O^{8+} Ions with H, H_2 and He, R. K. Janev, R. A. Phaneuf and H. Tawara, *Atomic Data Nucl. Data Tables* (submitted).

Assessment of Ion-Atom Collision Data for Magnetic Fusion Plasma Edge Modelling, R. A. Phaneuf, (Atomic and Molecular Data Supplement, *Nuclear Fusion* (to be published, 1992).

Status and Critical Assessment of the Data Base 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 Molecular Data Supplement, *Nuclear Fusion* (to be published, 1992).

Atomic and Molecular Data Requirements for Fusion Plasma Edge Studies, H. Tawara and R. A. Phaneuf, *Comm. At. Mol. Phys.* 21, 177 (1988).

CURRENT PROJECTS AND PLANS

* Collaboration with IAEA, NIFS, and JAERI data centers on recommended data base for state-selective electron capture in collisions of C^{6+} and O^{8+} with H.

* Collaboration with JAERI Data Center on parametrization of "Redbook" Volume 1 data.

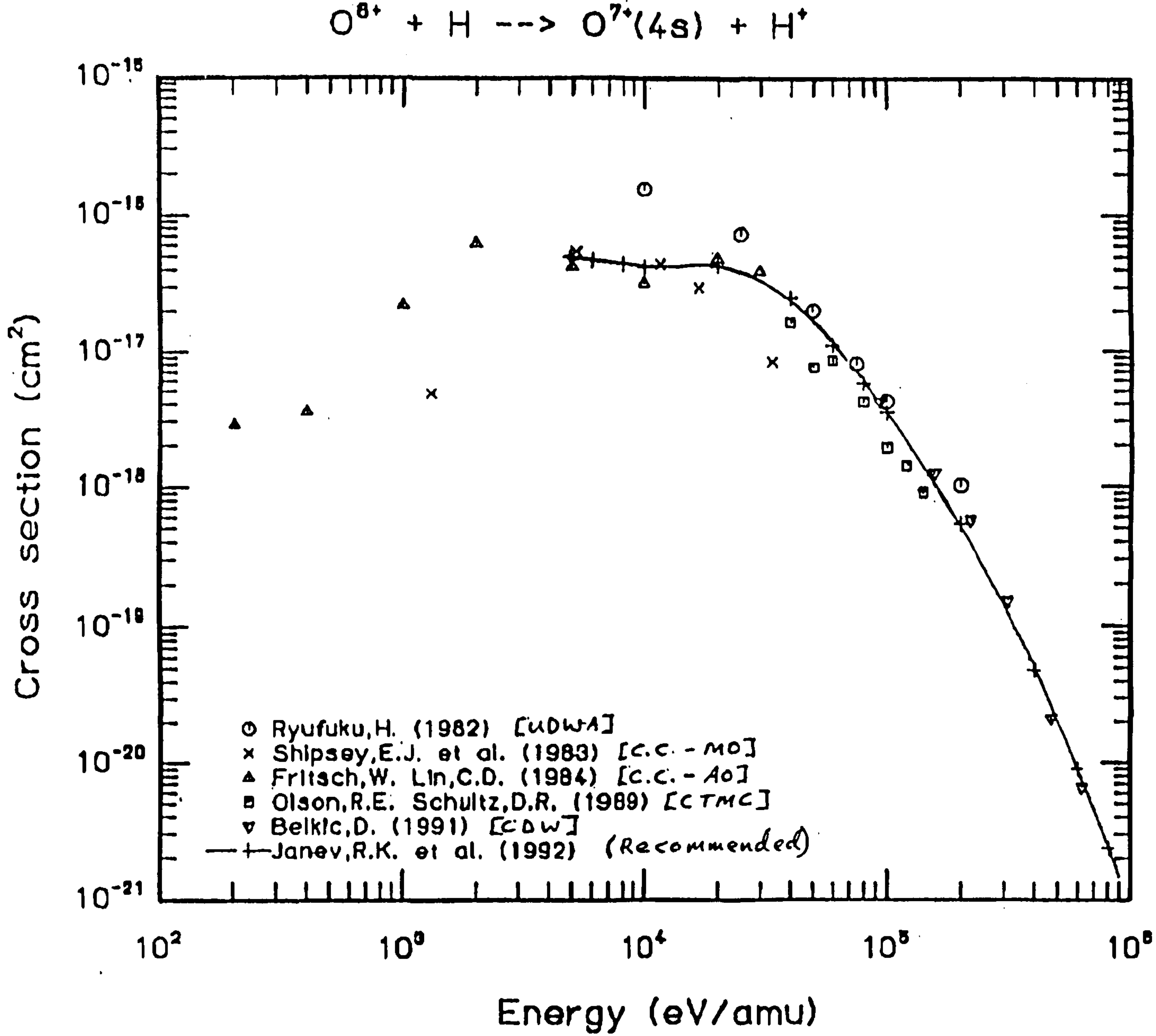
* Data base assessment for collisions of Be^{q+} and B^{q+} ions with H, H_2, and He at edge-plasma relevant energies for ITER.

● Data base assessment for elastic scattering of multicharged impurity ions from H, H_2, and He at edge-plasma relevant energies (+ theoretical calculations) for ITER.

* Data base assessment for H recycling and He - ash removal in ITER.

● Establish universally accessible Atomic Data Workstation containing on-line bibliographic and ALADDIN numerical data bases.

* Coordinate data input and analysis for CAMOS Questionnaire on Future Opportunities in Atomic, Molecular and Optical Sciences.


O8+ + H --> O7+(4s) + H+
Cross section (cm2)
10-15
10-16
10-17
10-18
10-19
10-20
10-21
Energy (eV/amu)
102
103
104
105
106
Ryufuku,H. (1982) [UDWA]
Shipsey,E.J. et al. (1983) [C.C. - MO]
Fritsch,W. Lin,C.D. (1984) [C.C. - AO]
Olson,R.E. Schultz,D.R. (1989) [CTMC]
Belkic,D. (1991) [CDW]
Janev,R.K. et al. (1992) (Recommended)

State-Selective Electron Capture Cross Sections

$C^{6+} + H(1S) \rightarrow C^{5+}(3l) + H^{+}$

Energy [eV/amu]	Velocity [cm/s]	σ(3s) [cm²]	σ(3p) [cm²]	σ(3d) [cm²]	σ(n=3) [cm²]
1.40E+03	5.20E+07	5.14E-19	1.65E-18	1.14E-18	3.31E-18
2.00E+03	6.21E+07	2.56E-18	6.68E-18	3.64E-18	1.29E-17
4.00E+03	8.78E+07	1.83E-17	3.66E-17	1.79E-17	7.28E-17
6.00E+03	1.08E+08	3.05E-17	7.21E-17	3.76E-17	1.40E-16
8.00E+03	1.24E+08	3.48E-17	9.85E-17	5.85E-17	1.91E-16
1.00E+04	1.39E+08	3.57E-17	1.08E-16	7.74E-17	2.21E-16
2.00E+04	1.96E+08	3.13E-17	1.06E-16	1.46E-16	2.83E-16
4.00E+04	2.78E+08	1.66E-17	6.22E-17	1.54E-16	2.33E-16
6.00E+04	3.40E+08	9.11E-18	3.92E-17	1.14E-16	1.63E-16
8.00E+04	3.93E+08	5.82E-18	2.58E-17	7.60E-17	1.08E-16
1.00E+05	4.39E+08	4.10E-18	1.64E-17	4.83E-17	6.90E-17
2.00E+05	6.21E+08	8.25E-19	2.84E-18	8.10E-18	1.18E-17
4.00E+05	8.78E+08	9.84E-20	2.61E-19	7.66E-19	1.13E-18
6.00E+05	1.08E+09	1.61E-20	4.88E-20	1.48E-19	2.14E-19
8.00E+05	1.24E+09	4.09E-21	1.12E-20	2.80E-20	4.34E-20
1.00E+06	1.39E+09	1.25E-21	3.64E-21	6.50E-21	1.14E-20

Accuracy:

E ≤ 4 keV/u	Indeterminate
4 < E(keV/u) ≤ 1000	30-40%

Comments:

(1) In the energy region below 4 keV/u, there is only σ(3l) data at E ~ 1.2 keV/u from the 33-MO coupled channel calculations of Green et al. [10]. The cross sections are about a factor of fifteen smaller than the corresponding values of σ(3l) at E ~ 4 keV/u. In the energy range 4-20 keV/u the recommended cross sections are based on the results of Green et al. and their accuracy is probably better than 30%.

(2) In the energy range between 40 and 100 keV/u, the recommended cross sections are based on the CTMC results of Olson and Schultz [17] which have an intrinsic uncertainty of 30-40%. At E = 100 keV/u the CTMC value agrees with the CDWA value of Belkic et al. [19] within the same accuracy. At energies above 200 keV/u, the recommended cross section follows the CDWA data.

(3) For the σ(3p) and σ(3d) cross sections, there is good agreement between all the available data, including the UDWA results of Ryufuku [18] for E > 75 keV/u, and the accuracy of these cross sections is estimated to be about 30%.

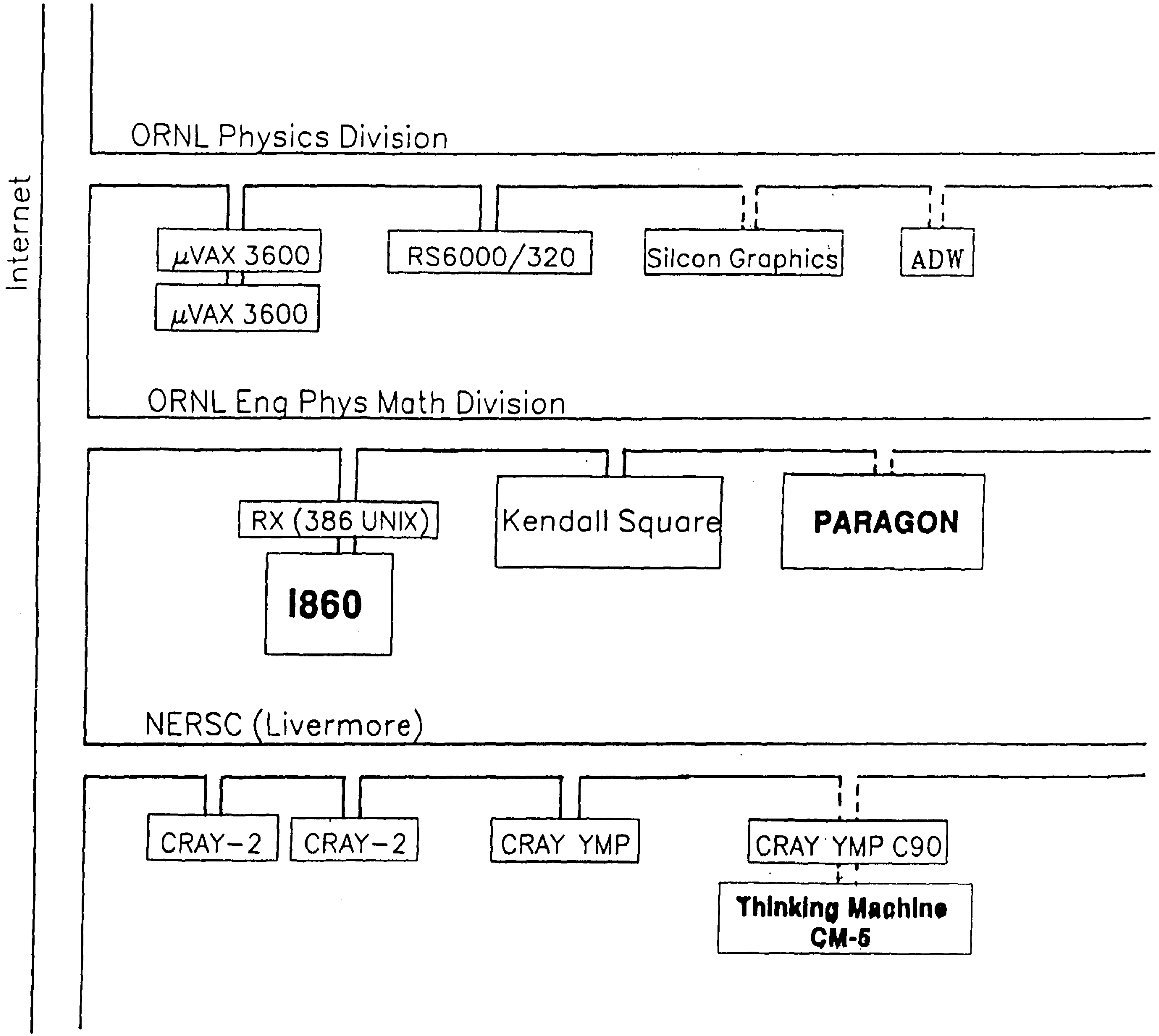
Atomic Data Workstation

The establishment of a workstation through which the Data Center may disseminate atomic data relevant to fusion energy research in accordance with its mission has been proposed by the Data Center and approved by the Office of Fusion Energy.

The workstation will be a multi-user machine which will be accessible via telnet to the fusion energy community and will provide a human interface to the Data Center resources.

Specifically, the atomic data stored in the ALADDIN format and the Data Center's bibliographic database will be available through the workstation.

The anticipated baseline capabilities may be illustrated by an example of a typical interactive session.


Internet
ORNL Physics Division
μVAX 3600
μVAX 3600
RS6000/320
Silcon Graphics
ADW
ORNL Eng Phys Math Division
RX (386 UNIX)
I860
Kendall Square
PARAGON
NERSC (Livermore)
CRAY-2
CRAY-2
CRAY YMP
CRAY YMP C90
Thinking Machine
CM-5

Interactive session on the atomic data workstation

- *user TELNETs to Atomic Data Workstation*

```
> telnet 128.219.20.xxx
```

- *user logs in*

```
username: cfadc
cfadc's password:
```

- *menu appears*

```
                Welcome to the ORNL
        Controlled Fusion Atomic Data Center
             Atomic Data Workstation

Select an item:
     [1] run ALADDIN
     [2] search CFADC bibliography
     [3] ftp ALADDIN or bibliography data file
     [4] message to CFADC
     [5] exit
```

• *user selects [2] and bibliography menu is accessed*

```
CFADC BIBLIOGRAPHIC DATABASE

SELECT ITEM
     [1] Category+Reactants search
     [2] other searches
     [3] exit bibliography
```

• *user selects Category+Reactants search*

```
PLEASE ENTER A REACTION CATEGORY: E06

PLEASE ENTER THE REACTION OF INTEREST: e + Fe^1^7^+

WRITE TO SCREEN OR TO FILE (S or F): S
```

• *after using the ALADDIN program, the user transfers the output to his computer*

```
FTP files to remote site

THE FILES YOU HAVE CREATED THIS SESSION ARE:
     bib.out
     aladdin.out

FTP> connect 128.111.60.01
connected, enter username: smithra
password
FTP> put bib.out, aladdin.out
FTP> quit
```

• *the user logs off and the workstation compiles statistics on what resources were used*

Scrape-off layer elastic/diffusion database

Through requests from plasma modellers, the Atomic and Molecular Data Unit of the IAEA has identified an urgent need for elastic and diffusion (momentum transfer) cross sections for fusion plasma scrape-off layer modelling.

The collision systems of interest involve all heavy particle species found in the edge plasma, i.e. A^{q+} + H, He, where, in particular, A=(H, He, Li, Be, B, C, O and Fe) in the energy range of 1 to 1000 eV.

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

IAEA Consultants' Meeting on an Atomic Data Base for Hydrogen Recycling and Helium Removal from Fusion Reactors, June 11-12, 1992, Vienna, Austria

Plan for producing elastic/diffusion database

1. Search CFADC bibliographies for pertinent data for (i) the elastic total cross section, (ii) the diffusion cross section and (iii) the elastic differential cross section from which the diffusion cross section is derived

2. Compile/evaluate available data

3. Participate in calculations to fill in the gaps in the existing data

4. Produce recommended data and scalings

Preliminary evaluated status of existing data

Elastic Collisions of 1 to 1000 eV A^{q+} + H, He

Ion Species	Elastic Total Cross Section	Elastic Diff. Cross Section	Diffusion Cross Section
Hydrogen	B	F	F
Helium	B	F	F
Lithium	N	N	N
Beryllium	N	N	N
Boron	F	N	N
Carbon	F	F	N
Oxygen	F	F	N
Iron	N	N	N

A to F: decreasing amount of data available

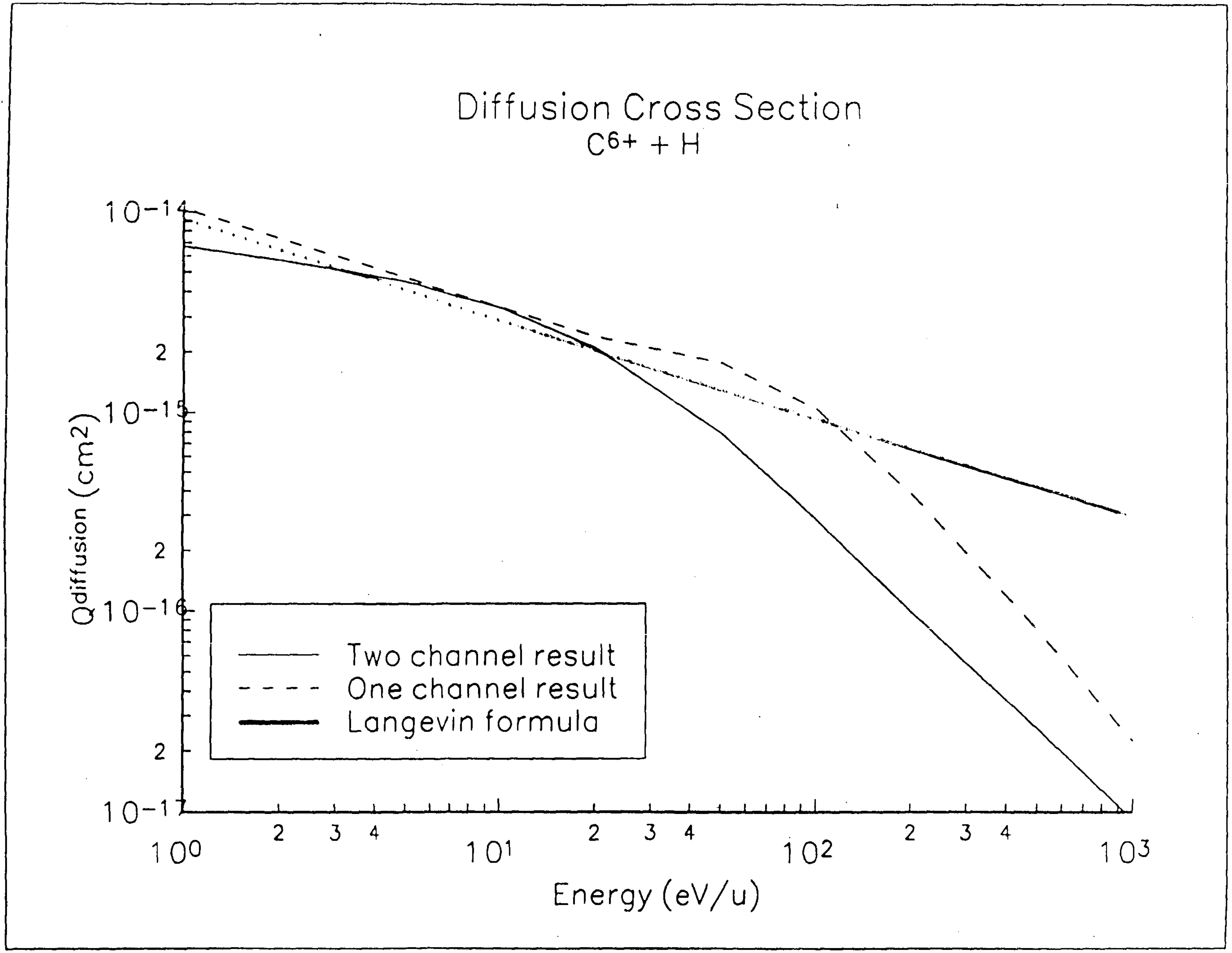
N: no data available

- The conclusion reached after the preliminary search for existing data is that the vast majority of the required cross sections will have to be calculated.

- For the one electron systems (e.g. C^{6+} + H) and for the resonant cases (H^{+} + H, He^{+} + He) reasonable, simple quantum mechanical models should be sufficient and relatively easy to implement.

- Due to the complex nature of the quantum mechanical calculations (many-states, many-channels) that would be required to treat the remaining low energy ion-atom collisions, some simplified models will be required to handle the large number of collision pairs and impact energies.

- To serve as a benchmark of the simplified models (e.g. classical scattering method) we have performed a quantum mechanical calculation including the most important interactions for C^{6+} + H collisions.


Diffusion Cross Section
C6+ + H
10−14
2
10−15
2
10−16
2
10−17
Qdiffusion (cm2)
100
2
3
4
101
2
3
4
102
2
3
4
103
Energy (eV/u)
Two channel result
One channel result
Langevin formula

Progress Report 1991/1992

National Institute for Fusion Science

1992.6.17-19 Hiro Tawara

Activities in 1991/1992

1) Data compilation of electron capture cross sections for the following collisions :

a) C^{5+} + H -> C^{5+}(nl)

b) O^{8+} + H -> O^{7+}(nl)

Data evaluation and recommendation over the collision energy 10^4-10^6 eV/amu and for nl=(3-8)l for C^{5+} and nl=(4-9)l for O^{7+} ions with accuracies better than 50 % have already been made under collaboration of IAEA, Oak Ridge and NIFS last summer and submitted to Atomic Data and Nuclear Data Tables. Also under collaboration of JAERI, we are trying to fit the recommended data to analytical formula proposed by IAEA. In further activities, we include other related data to these processes over the collision energy 10^2-10^6 eV/amu over nl=(1-9)l and n=10-15 for C^{5+} and nl=(1-12)l and n=13-20 for O^{+} ions to show general trends, though the accuracies might not be good in the outside of the recommended parameters above.

2) Compilation of excitation cross sections of He atoms $1s^2\ ^1S$ - 1snl and 1s2s ^1S, ^3S -> 1snl and 1s2p ^3P -> 1snl has been finished and reported in NIFS-DATA-15.

3) Polarization phenomena of photons from plasmas, which might be used for their diagnostics, and related basic processes have been reviewed and reported in NIFS-DATA-16.

4) Data compilation and estimation for electron stripping cross sections for impurity C^{i+} (i=0-5) and O^{i+} (i=0-7) ions in collisions with atomic hydrogen :

These processes become important when the neutral beam injection (NBI) energy increases up to a few 100 keV to 1 MeV in large tokamaks. The electron stripping of these impurities result in the increase of effective nuclear charge of plasma Z_{eff} near the edge region where impurities are plenty. The results have been reported in NIFS-DATA-17.

5) Calculations of excitation cross sections and energy levels for various ions have been performed under collaboration of Dr. U. Safronova.

Internal Reports

1) T.Kato, Y.Itikawa and K.Sakimoto, NIFS-DATA-15 (March, 1992)
   Compilation of excitation cross sections for He atoms by electron impact
2) T.Fujimoto, F.Koike, K.Sakimoto, R.Okasaka, K.Kawasaki, K.Takiyama, T.Oda and T.Kato, NIFS-DATA-16 (April, 1992)
   Atomic processes relevant to polarization plasma spectroscopy
3) H.Tawara, NIFS-DATA-17 (April, 1992)
   Electron stripping cross sections for light impurity ions in colliding with atomic hydrogens relevant to fusion research

Related publications

1) P.Hvelplund, S.K.Bjornelund, H.Knudsen and H.Tawara, Phys. Scripta 45 (1992) 231
   Electron capture in collisions between medium velocity multiply charged ions and H and H_2
2) T.Kato and U.I.Safronova, Opt. Spectrosc. 70 (1991) 291
   $1s^22s^2$-$1s^22s2p$-$1s^22p^2$ excitation cross sections for O V, Si XI, Fe XIII, MO XXXIX
3) T.Nakano, H.Toyoda and H.Sugai, Japanese J. Appl. Phys. 30 (1991) 2908
   Electron impact dissociation of methane into CH_3 and CH_2 radicals
   I. relative cross sections
4) T.Nakano, H.Toyoda and H.Sugai, Japanese J. Appl. Phys. 30 (1991) 2912
   Electron impact dissociation of methane into CH_3 and CH_2 radicals
   II. absolute cross sections

ALADDIN activities

Some ionization cross sections and rate coefficients from ALADDIN have been put into Macintosh.

COMPUTATIONAL ACTIVITIES ON A+M DATA AT ENEA. Italy

by E.Menapace

1) Department for advanced technology development. Computing Division.

Nuclear Data and Codes Laboratory

i) Molecular vibrational-rotational structures and electron-molecule collision processes.

(A.Mengoni)

The extension of the algebraic approaches to the calculation of rotational and vibrational spectra of polyatomic molecules is in progress. Starting from the Vibron Model based on the U (4) algebra for the single molecular bond (Ref.1), the extension of coupled U (4) algebras has been completed for triatomic molecules in the linear and non-linear configuration cases.

For 4-atom molecules, the coupling or three U (4) is manageable and good results have been recently obtained for planar configurations.

For molecules containing more atoms, a model based on the U (2) algebra has been recently proposed. The advantage of using such a model is that the numerical calculations required, reduce to the diagonalization of a single Hamiltonian in a space where the angular momentum does not come into play. This allows, in principle, the treatment of the vibrational structure for molecules with a large number of atoms. For example, the vibrational spectrum of such molecules as UF_6, SF_6, WF_6, and C_6H_6 have been recently calculated.

The calculation of infrared intensities within the framework of this model requires the calculation of matrix elements of operators such as

$$T = \exp (-\lambda n_{\pi}).$$

In the case of U (2) algebra this calculation is particularly simple. In the Figures 1 and 2, examples of this type of calculations are given. The matrix elements of the operator T are given as a function of v_1, for two typical v values. In the figures, the comparisons are made between the complete numerical calculations, involving a diagonalization of a U (2) Hamiltonian, and three different types of analytical expression (Ref. 2). The agreement between the complete numerical calculations and the analytical expressions is rather good.

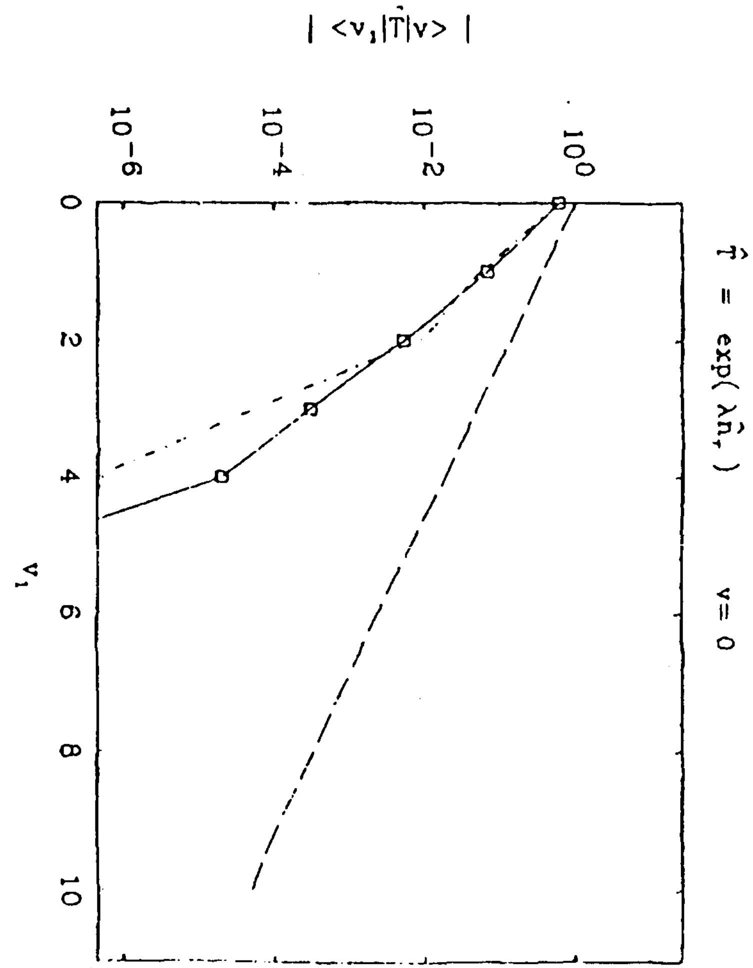
The possibility of calculation for the scattering cross sections in the e^--molecule collision process within this model takes advantage of the results given above. At the present time, this kind of application is under investigation.

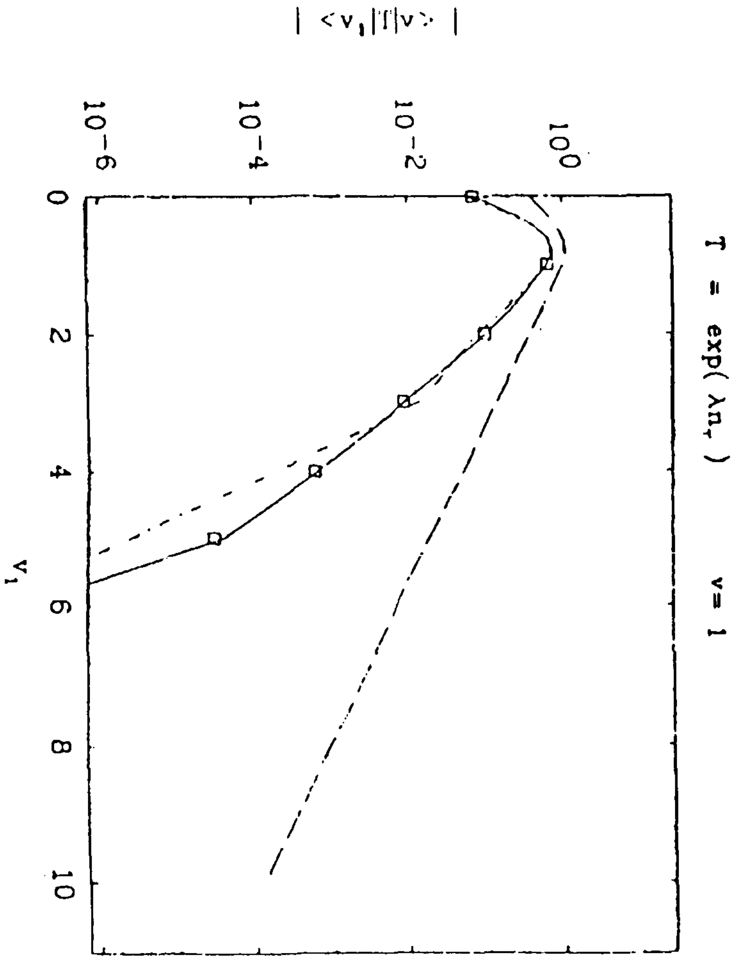
Referencies.

1) F.Iachello: "Algebraic method for molecular rotation-vibration spectra". Chem. phys Lett. 78 (1981), pag.581.

Number of vibrons $N = 20$
$\lambda = -0.05$

□ Numerical
— Analytical (Ref. 2)
-·- Power expansion of $\hat{T}$ (2nd order)
- - - $e^{\lambda' |v_1 - v|}$, $\lambda' = N\lambda$





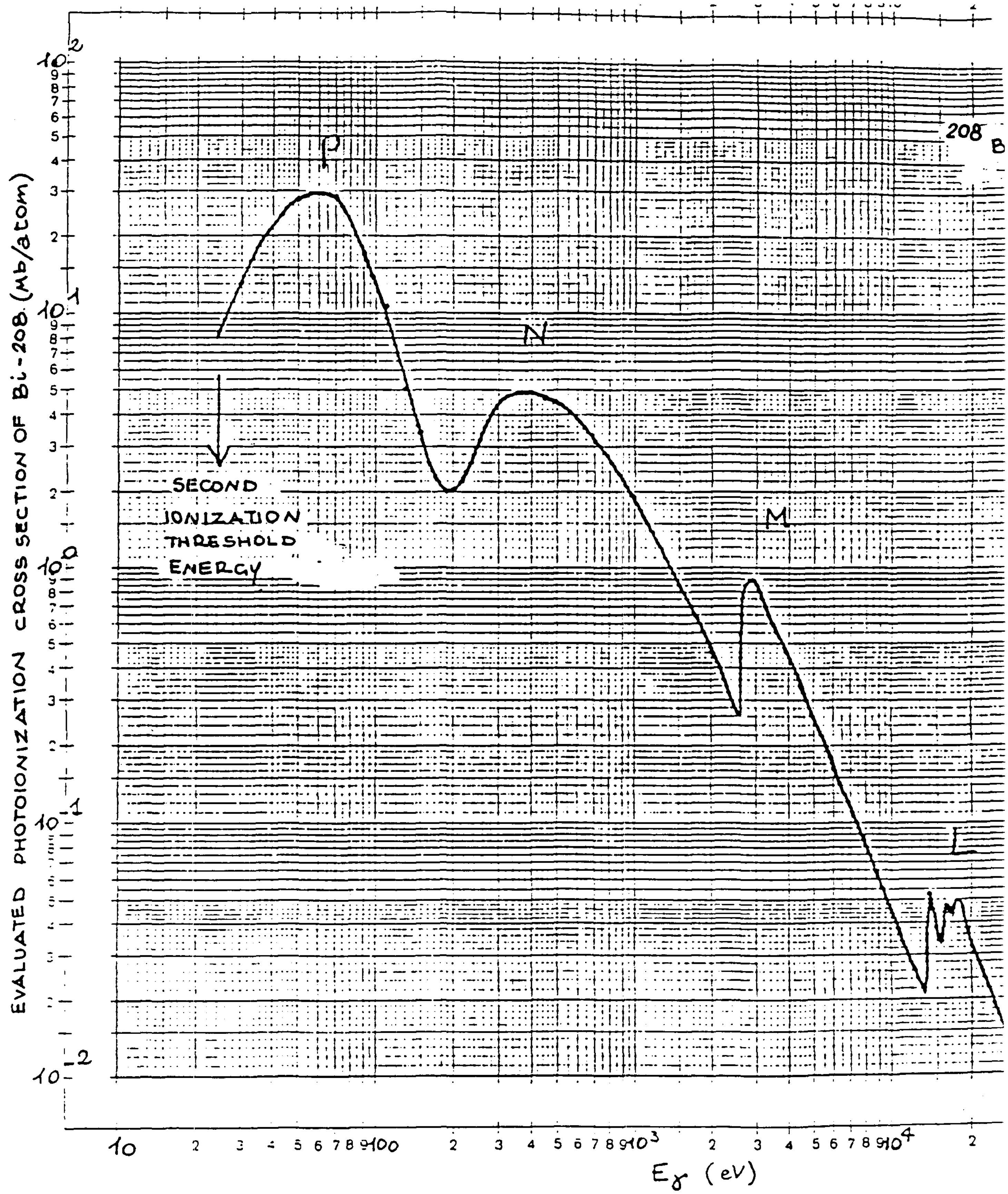
2) F.Iachello, A.Leviatan and A.Mengoni: "Algebraic approach to molecular rotation-vibration spectra III. Infrared intensities". J. Chem. Phys. 95 (1991), pag.1449.

ii) Evaluation of photoionization cross section of ^{208}Bi (G.Maino).

In order to investigate the feasibility of a unconventional FEL device for the Bi $^{+}\rightarrow$ Bi^{++} ionization process required in the heavy-ion driven inertial fusion (ENEA reports RT/INN/90/35 and 90/46) the photoionization cross section of ^{208} Bi has been evaluated in the energy range between 10 and 10^4 e V. The results shown in fig.1 are based on both standard theoretical calculations and avaible information from experiments and systematics.

For that concerns both experimental data sources and theoretical investigations with the corresponding systematics a critical analysis of the recent literature on the matter has been performed with main reference to the following references:

1) J.H.Hubbell, Atomic Data 3 (1971) 241;
2) J.H.Scofield, "Theoretical photoionization cross sections from 1 to 1500 keV", Lawrence Livermore Lab. report UCRL 51326 (1973);
3) I.M.Band, Yu.I.Kharitonov and M.B.Trzhaskovskaya, Atomic Data and Nuclear Data Tables 23 (1979) 443;


EVALUATED PHOTOIONIZATION CROSS SECTION OF Bi-208 (Mb/atom)
208 B
P
N
M
L
SECOND
IONIZATION
THRESHOLD
ENERGY
Eγ (eV)

4) B.L.Henke, P.Lee, T.J.Tanaka R.L.Shimabukuro and B.K.Fujikawa, Atomic Data and Nuclear Data Tables 27 (1982) 1;

5) E.B.Saloman and J.H.Hubbell, "X ray attenuation coefficients (total cross sections): comparison of the experimental data base with the recommended values of henke and the theoretical values of Scofield for energies between 0.1 and 100 keV", National Bureau of Standards report NBSIR 86 3431 (1986);

6) E.B.Saloman, J.H.Hubbell and J.H.Scofield, Atomic Data and Nuclear Data Tables 38 (1988) 1;

7) E.B.Saloman, J.H.Hubbell and Berger, SPIE 911 (1988) 100;

8) D.K.Trubey, M.J.Berger and J.H.Hubbell, "Photon cross sections for ENDF/B VI", in Proceed. of ANS Topical Meeting, Santa Fe, 9/13 April 1989.

2) ENEA-INN Project for Innovative Metallic Materials

i) Elastic and inelastic energy loss rates of slow protons on Fe surface. (submitted for pubblication)

(A.Ventura, V.Rosato)

It has been recently attempted the simulation of the behavior of slow protons ($1eV<E_{in}<50eV$) interacting with a [100] Fe surface at T=300 K, by means of Molecular Dynamics.

A suitable N-body potential [1,2] has been used to reproduce the thermal behavior of the metallic host. Metal-proton interaction has been derived, in the Embedded Atom Method [3] scheme, by evaluating the electronic density experienced by the proton at each point of its trajectory. This information has been further used to evaluate the inelastic energy losses through the introduction of a friction term $F=\beta v$ acting on the projectile alone. The friction coefficient β has been taken proportional to the first-order transport cross section for electrons with momentum close to the local Fermi value.

The obtained results are reported in the following Table, where E_{in}=incident energy, R_N=particle number reflection coefficient, E_{out}=average energy of reflected protons, R_E=energy reflection coefficient, E_{el}=average elastic energy loss, E_{inel}=average inelastic energy loss.

E_{in} (eV)	R_n	E_{out}(eV)	R_E	E_{el}(eV)	E_{inel}(eV)
1.0	0.30	0.8445	0.253	~0	0.2252
5.0	0.64	3.678	0.471	0.671	0.651
10.0	0.68	6.986	0.475	1.543	1.471
50.0	0.65	33.724	0.438	9.676	6.600

[1] V.Rosato et al., Phil.Mag.A59 (1989) 321
[2] F.Cleri, V.Rosato, in preparation
[3] M.S.Daw, M.I.Baskes, Phys.Rev.B29 (1984) 6443

GAPHYOR Atomic and Molecular Data Centre

Activities during year 1992

J.L.Delcroix,D.Humbert, K.Katsonis, 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, C.M.Ferreira, L.Hrachova, K.Katsonis, C.Lalo, P.Lightfoot, J.Masanet, P.Ranson, A.Ricard, M.Yousfi

**Centre de Données GAPHYOR, Université de Paris-Sud, Bat. 212
91405 ORSAY CEDEX, FRANCE - FAX. 69417844**

**presented at the 11th Atomic and Molecular
Data Centre Network Meeting
IAEA, Vienna, 15-16 June 1992
Rapport GA-9/257**

1. SOME STATISTICS.

As of the 15th of June 1992, the total number of entries in the files was about 250,000 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-June-92)

	SECTION 1	SECTION 2	SECTION 3	SECTION 4	SECTION 5	TOTALS
	Structure	Photon. Coll.	Electron. Coll.	Atom.,Mol.Coll	Macro.Pro.	
1 ELEMENT	44896	7394	13518	7626	4546	**77980**
2 ELEMENTS	53341	5771	4879	35851	7447	**107289**
3 ELEMENTS	24860	2590	910	20962	2805	**52127**
4 ELEMENTS	5215	523	110	6021	826	**12695**
TOTAUX	**128312**	**16278**	**19417**	**70460**	**15624**	**250091**

Table 2: Number of entries by process in each section (15th-June-92)
(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	71816	AN	1858	SN	1132	SN	1139	PV	1148
CP	271	SN	495	SC	469	SP	103	FT	1685
DP	3426	SC	315	EL	1752	SC	643	VR	154
NP	881	EL	208	EX	5118	EL	804	ZT	133
PE	2725	FF	84	ER	574	EN	2002	CO	135
VR	32166	EX	1722	DX	189	EX	2638	DN	656
TR	12813	ER	412	XX	464	ER	1195	VI	753
IN	1057	DX	104	DO	46	DX	8011	CT	818
DT	229	XX	65	IN	5035	XX	2317	TD	312
DS	1777	DO	89	RC	213	DO	295	PE	270
XX	79	IN	6416	RR	174	TE	2159	EN	2661
EA	1041	DT	536	RE	115	IN	7500	DM	58
		DS	3517	RO	68	TI	29	RN	935
		NL	149	RD	560	DT	984	FE	359
		PR	300	RS	605	10	4198	CE	160
				AT	1655	0-	264	ME	625
				DT	59	1-	7	DE	177
				DS	893	IM	352	PI	490
				BS	223	RI	464	AT	452
				PR	100	XD	659	DT	70
						CX	3720	PC	67
						C1	1302	FI	31
						CA	285	MI	887
						S1	636	DI	185
						SR	135	DA	41
						IR	14965	RC	162
						IH	967	LA	928
						IA	88	MD	96
						ID	681	ST	1121
						AS	4371		
						AH	205		
						DS	2949		
						DH	146		
						KE	701		
						PR	3548		
Σ	128281	Σ	15821	Σ	19444	Σ	70462	Σ	15569

[1] J.L. DELCROIX Gas-phase chemical database (Elsevier 1988)]
[2] GAPHYOR HANDBOOK 1992-1

2 CHANGES IN CLASSIFICATION SCHEME

No change has been introduced since the last meeting. We are presently studying changes in the classification scheme for gas(plasma)-surface interactions.

3 DIRECT ENTRY AND UPDATING SITUATION

The situation has not changed very much since the last meeting. However it is now improving progressively for Eastern European Journals with the entrance into our Science Experts Group of two new colleagues : A.Faenov from Moscow and L.Hrachova from Prag.

4.GAPHYOR HANDBOOK 92-1

The major achievement during this year has been the publication of GAPHYOR HANDBOOK 92. This book is designed to help anybody who is interested in a new field of research, or looks for recent developments in a given field. It can also be used as a help to on-line retrieval. It is then a selection taken from the whole GAPHYOR Database of the data which are best suited for those purposes. The selection criteria depend on quality, but also on the actuality of data. More precisely the selection is made as follows:

1-Assigning a value index to every GAPHYOR record. This index is the sum of nine partial indexes V1 to V9 as shown in Table 1. These partial indexes depend on the quality of data (IN1 à IN6), the publication year (AN), the journal (JO), and the process described in the record (PR) in every section (SE). The notations used are explained in Explanation of tables of the Handbook.

2-Record selection
-we first set up a catalog of multiplets included in the Database. We call a multiplet the set of records having the same values of elements, reactants and process. For every multiplet we choose the record with the largest value index. We note the multiplicity MULT i.e. the number of records included in this mutiplet. This number is shown in the last column of the Handbook tables, instead of the geographical informations of the GAPHYOR tables.
-to decrease the total volume of the Handbook we eliminate all the records of little interest with a value index smaller than a minimum value. In the first volume(see below) the minimum value has been set respectively to 25, 27, 8, for sections 3, 4, 5.

3-Division in two volumes. The first volume (shown at the meeting) includes the data from sections:

3 Electron collisions
4 Collisions between atoms and molecules (including chemical reactions)
5 Macroscopic properties of gases

The second volume will cover the two other sections:

1 Properties of isolated atoms and molecules
2 Photon collisions

Finally, the Table 4 shows **some statistics** relating the Handbook to the whole Database. The average multiplicity is only about 1.6. But this low value is the result of a large number of cases with MULT=1 (unusual processes) and of a small number of case with MULT>10 (well known processes). One notes also that the Handbook covers about 70% of the subjects (multiplets) included in the base while the other 30% are considered of little interest.

Table 3:

Rules for calculating the value index

IN 1		IN 2		IN 3		IN 4		IN 5		IN 6		AN		JO		SE 3		SE 4		SE 5	
	V1		V2		V3		V4		V5		V6		V7		V8	PR	V9	PR	V9	PR	V9
W	10	I	3	=	10	A	3	:	10	E	5	91	10	JCP	10	SN	5	SN	5	PV	2
S	10	8	2			L	2	F	5	R	5	90	9	PR/A	10	EL	5	EL	5	DN	2
K	10	Q	1			J	1	G	5			89	8	JPC	9	EX	5	EX	5	VI	2
P	10					H	1	Y	2			88	7	CHPL	9	DX	5	DX	5	CT	2
U	10							Z	2			87	6	JP/B	8	XX	5	XX	5	TD	2
C	10											86	5	JRD	8	IN	5	TE	5	EN	2
V	10											85	4	ADND	7	RR	5	IN	5	DM	2
<	10											84	3	JACS	7	RE	5	TI	5	ME	2
												83	2	JMSC	6	RO	5	DT	5	PI	2
												82	1	IJMS	6	RD	5	10	5	AT	2
														JDPn	5	RS	5	0-	5	DT	2
														JMSP	5	AT	5	1-	5	PC	2
														CHPH	4	DT	5	IM	5	MI	2
														MOL	4	DS	5	RI	5	DI	2
														THCA	3	BS	5	XD	5	DA	2
														JFII	3	SC	5	CX	5	MD	2
														ZP/D	2			C1	5	ST	2
														JMSR	2			CA	5	FT	1
														PSC	1			S1	5	FE	1
														IJCK	1			SR	5	CE	1
														EACC	1			IR	5	DE	1
																		IH	5	FI	1
																		IA	5		
																		ID	5		
																		AS	5		
																		AH	5		
																		DS	5		
																		DH	5		
																		KE	5		
																		SP	2		
																		SC	2		
																		EN	2		

Table 4:

Comparative statistics of HANDBOOK 92-1 and of the whole Database (03-1-92)

	Section 3	Section 4	Section 5	Σ
Records in Base	21000	80000	18000	119000
Multiplets in Base	9427	56727	10163	76317
Multiplicity in Base	2,2	1,4	1,8	1,6
Multiplets in Handbook	6803	40406	6991	54200
Eliminated multiplets	2624	16321	3172	22117
% élimination	28%	29%	31%	29%

5. NUMERICAL DATA ON MULTIPLY CHARGED ION COLLISIONS.

Work on evaluation of cross section values relevant to fusion is part of the scientific project "Atomic Physics of Fusion Plasmas", recently established in the Laboratoire de Physique des Gaz et des Plasmas by Dr. K. Katsonis in collaboration with Dr. G. Maynard; Miss F. El Balghiti (PhD student) is also participating in this project, which is scheduled to be upgraded to form an European Network. Prof. R. Janev of the IAEA has collaborated in the present scientific project to obtain the presented results.

Since September 1991 the evaluation of ionisation and charge transfer cross sections for collisions of ions with H and He atoms lead to the following results:

1 - Collisions of multiply charged ions with He atoms:

- Classical Trajectory Monte Carlo (CTMC) calculations of collision cross sections for medium Z impurity ions (Ti^{q+}, Cr^{q+}, Fe^{q+} and Ni^{q+}, q = 4, 6, 8, 10) colliding with He lead to cross sections for the following process:

i) One-electron total and partial (n - level selective) electron capture and electron loss and

ii) Double capture, transfer ionisation and two electron loss.

- Previous CTMC calculations for totally stripped low Z impurity ions (Be^{4+}, C^{6+}, O^{8+} and Ne^{10+}) colliding with He have been finalised; the same kind of cross sections as in the medium Z case have been calculated.

A detailed evaluation on the basis of all the currently available theoretical and experimental data has been performed and charge state scaled cross sections for one- and two-electron loss have been derived in analytic form, valid in a wide energy range (R.K. Janev, G. Maynard and K. Katsonis, Nucl. Fusion, in press.).

2 - Low Z multiply charged ions collisions with H.

In this domain, an extensive programme of calculations and evaluations of C^{q+} and Be^{q+} ionisation and charge transfer cross sections for collisions with H has been accomplished and the obtained results are under preparation for publication. This work was motivated because, although extensive evaluations have been lately available (e. g. D. Belcic, R. Gayet and A. Salin, At. Dat. Nucl. Data Tab. **51**, 59, 1992), the status of these data is yet unsatisfactory and an extension of the studied collision energy region down to 10 eV/amu is needed.

Activity report at the Russian Scientific Centre "Kurchatov Institute" 1991/1992

V.A.Abramov
Institute of Nuclear Fusion,123182,Moscow,
The Russian Federation

The present activities on the field of collection,dissimination and evaluation of (A+M) data for fusion which are performed in the Institute of Nuclear Fusion (former the Plasma Physics Department of the I.V.Kurchatov Institute of Atomic Energy) are connected both the present tokamak research and the ITER design study.As previously,the collection of (A+M) data published in the Soviet literature have been done.The corresponding collection is submitted to the publication in the "International Bulletin on Atomic and Molecular Data for Fusion".

Because of the present interest to the problem of the luquid-metal limiter in the T-3M tokamak , the ionization rates for Ga neutral atom and ions by an electron impact have been compiled and reported.The atomic data relevant to the problem of the penetration of Cs-beam in the T-10 tokamak are analyzed.The new model to describe the interaction of Li-beam with fusion plasmas is developed (V.S.Lisitsa et al.).This semianalytical model allows to consider the atomic beam-plasma interaction by a refined manner. Because of the large interest to low -Z material coatings inside fusion devices the ionization,excitation and charge exchange data for different Be,B and C ions in colliding with electron and neutral hydrogen atoms have been compiled and evaluated (G.I.Krotova).The analysis of the data base for the rates of different atomic and molecular processes determing the recycling value in the T-10 tokamak was made by A.Yu.Pigarov et al.This result is included in the paper presented at the 10-th International Conference on Plasma Surface Interactions in Controlled Fusion Devices.

The calculations of radiative cooling rates for C-seeded plasmas with taking into account the charge exchange of impurity ions in colliding with neutral hydrogen atoms have been performed by V.A. Abramov et al. The data base for charge exchange cross-sections published by R.Janev,R.Phaneuf and M.Pindzola has been used.These results are included in the paper by V.A.Abramov et al. presented at the 19-th EPS Conference on Controlled Fusion Research and Plasma Physics.

The group headed by Dr.V.A.Belyaev performs the experimental investigation of the molecular hydrogen ions dissociation due to self-collisions at the low energies.The measurements of the ionization cross-sections of Ga^{+q} (q=1-3) by an electron impact will be performed in this year.Energy range is E_{thr} -100 eV.In principle,there is possibility to measure the charge exchange cross-sections for the collision Ga 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 processes of radiation erosion (sputtering,radiation-induced sublimation)are considered in details.The process of chemical sputtering for carbon-graphite materials doped with boron(USB-15,carbide boron,graphites doped with boron in volume) are studied in model experiments on the interaction of a solid surface with hydrogen isotope ion beams and plasma beams.The phenomenon of enrichment of the surface layer by boron in USB-15 is found.This phenomenon is explained by the reverse boron deposition at the target. The deposition of hydrogen atom implanted in graphite materials (beam energy is 10 keV,fluence is 10^{19} cm^{-2} ,T is 100-1200 C) is measured by the recoil nucleon method.

The synergistic effects at the simulteneous implantation of H^+ and He^+ ions,$H^+$and O^+ ions are studied in detail.The main synergistic phenomenon is the large enhancement of hydrogen concentration in the surface layers.It is shown that ions H^+ and O^+ create traps for hydrogen atoms.The total amount of traps increases when the ion mass increases.

On-going and future activities:

1) Data compilation related impurities such as carbon-hydrogen molecules which affect on the recycling coefficient
2) Data compilation of ionization and excitation cross-sections of different boron ions by an electron impact (and also rates) including the data presented at the IAEA meeting on data for Be and B ,June 11-13,1991,Vienna)
3) Evaluation of excitation cross-sections (rates) for different nickel ions by an electron impact (in collaboration with Lebedev Institute)
4) Calculation of the radiative cooling rates for B-seeded plasmas

Activities in the atomic and molecular data at Nuclear Data Centre of Physics and Power Engineering Institute

Obninsk, Russia

Progress report 1991-1992

prepared by V.Piksaikin

In frame of the program on the A+M data for nuclear excited plasmas a compilation and evaluation work has been completed of the ionization differetial cross sections (IDCS) for collisions of proton with helium and argon atoms /1/. The calculation of the transition probabilities and oscillator strenghts has been carried out for CaII, CdII and ZnII ions for a wide variety of radiation transitions/2/.

Collision data. Evaluation of the experimental data on the differential cross section for ejection of electrons from helium and argon atoms by proton impact (IDCS) /1/.

On the bases of critical analysis of the compiled experimental data the IDCS systematic errors were estimated as 25% for all electron and proton energies. The experimental values corresponding to Auger lines for argon (near 200 eV electron energy) were not included in evaluation. Several experimental data for electron energies lower 10 eV were eliminated from evaluation. Another processes ,e.g. nuclear interaction for several MeV proton energies, were not considered.

The criteria by which the IDCS fitting expression was chosen were as follows:

- the equation should be simple and have a small number of parameters;
- the physics of process should be accounted for;
- the linear least squares method (LSM) should be used with clear

estimation of final errors;

- the equation should not take into account a fine structure of cross sections (Auger lines).

In different models of calculation the IDCS is proportional to electron energy in power from -2 to -3. Besides the monotonic dependence in the IDCS there is a binary collision peak corresponding to maximum energy transfer to electron by projectile E = 4*T, where T = E *(M/m), M and m are masses of proton and electron . The fitting equation was chosen as

$$dS/dE=\exp(a)*(E+I)**b \tag{1}$$

where dS/dE - the IDCS, E - the electron energy, I - the ionization energy of atom, a,b - adjustable parameters.

In calculations the analytical expression (1) was linearized in respect to the parameters and variable ln(E+I) and then the LSM procedure was used for fitting. The IDCS was represented by one or two straight-line segments over intervals corresponding to two energy ranges of ejected electrons: from 0 to approximatly 4*T and other part of spectrum. In calculation procedure the ln(dS/dE) values for the fixed values of ln(E+I) were used. The evaluation was made in three steps:

- the experimental data of each author were approximated by one or two linear segments. As a results of this step the evaluated parameters and their variance-covariance matrix were obtained;

- on the second step the obtained results were used in calculation of the adjustable parameters for each proton energy;

- on the third step a continuous dependence of the IDCS for proton energy range 0.1-5.0 MeV was determined from the evaluated parameters for discrete values of proton energy.

Some of the evaluation results are presented in figs.1-3.

Analyses of the obtained results shows that the fitted dependences give the IDCS for He and Ar atoms within the accuracy of experimental data. The evaluated data will be put in the ALADDIN format data base.

Present method being a few modified can be used for evaluation of similar cross sections for different targets and projectiles.

Spectroscopic data. Calculation of atomic transition probabilities for CaII, CdII and ZnII ions /2/.

The calculation has been carried out using the central field approximation. Radial function was obtained on the basis of the "ATOM" code developed by Vanshtein and Shevelko. The optically allowed transitions (only for $\lambda < 10^5$ Å) were considered. The calculated values of the absorbtion osclllator strengths and transition probabilities for CaII, CdII and ZnII ions are given in Tables 1-3 (see Appendix). Spectroscopic characteristics presented in Tables 2 and 3 are the following: E_j, E_i - the energies of the lower and upper states measured from the ground state of ion; λ_{ij} - the wavelength; g_i, g_j - the statistical weights; f_{ji} - the absorbtion oscillator strength and A_{ij} - the transition probability. Table 1 along with above characteristic contains also the oscillator strengths values from the NBS compilation /7/ by Wiese et.al., deviation Δ between the present results and Wiese et.al. data /7/ and literal class of accuracy: C - for uncertainties within 25% and D - for uncertainties within 50%.

In the vast majority of transitions the obtained results for CaII ion are within the uncertainties of Wiese et.al. data. In case of CdII and ZnII ions there was no data of other authors for comparison.

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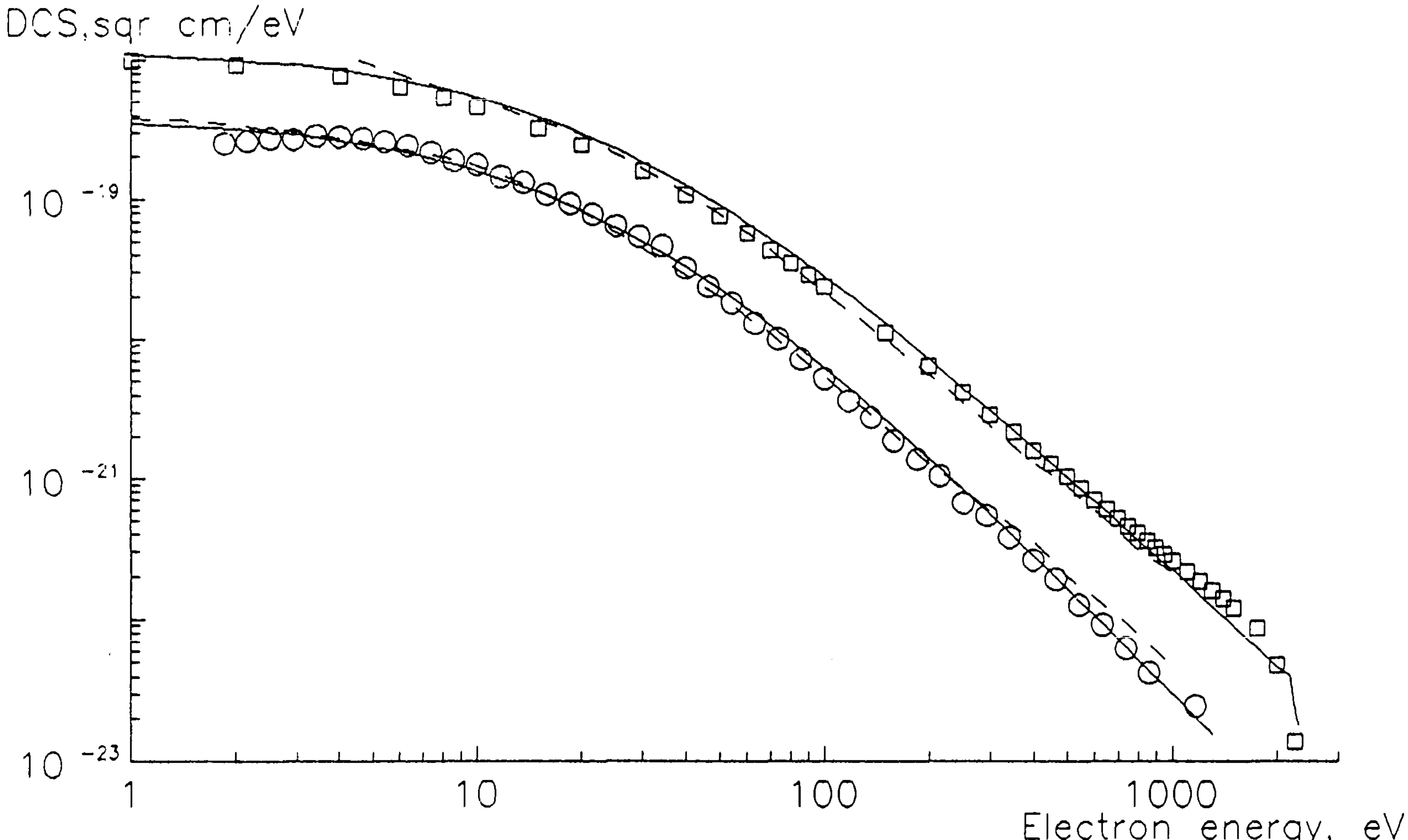

Fig.1. Ionization Differential Cross Sections of He by Protons. Upper lines and points for 1.0 MeV protons, lower – for 5.0 MeV. Solid lines – present evaluation, dashed lines – theoretical values from paper /6/, points – experimental data /3/.

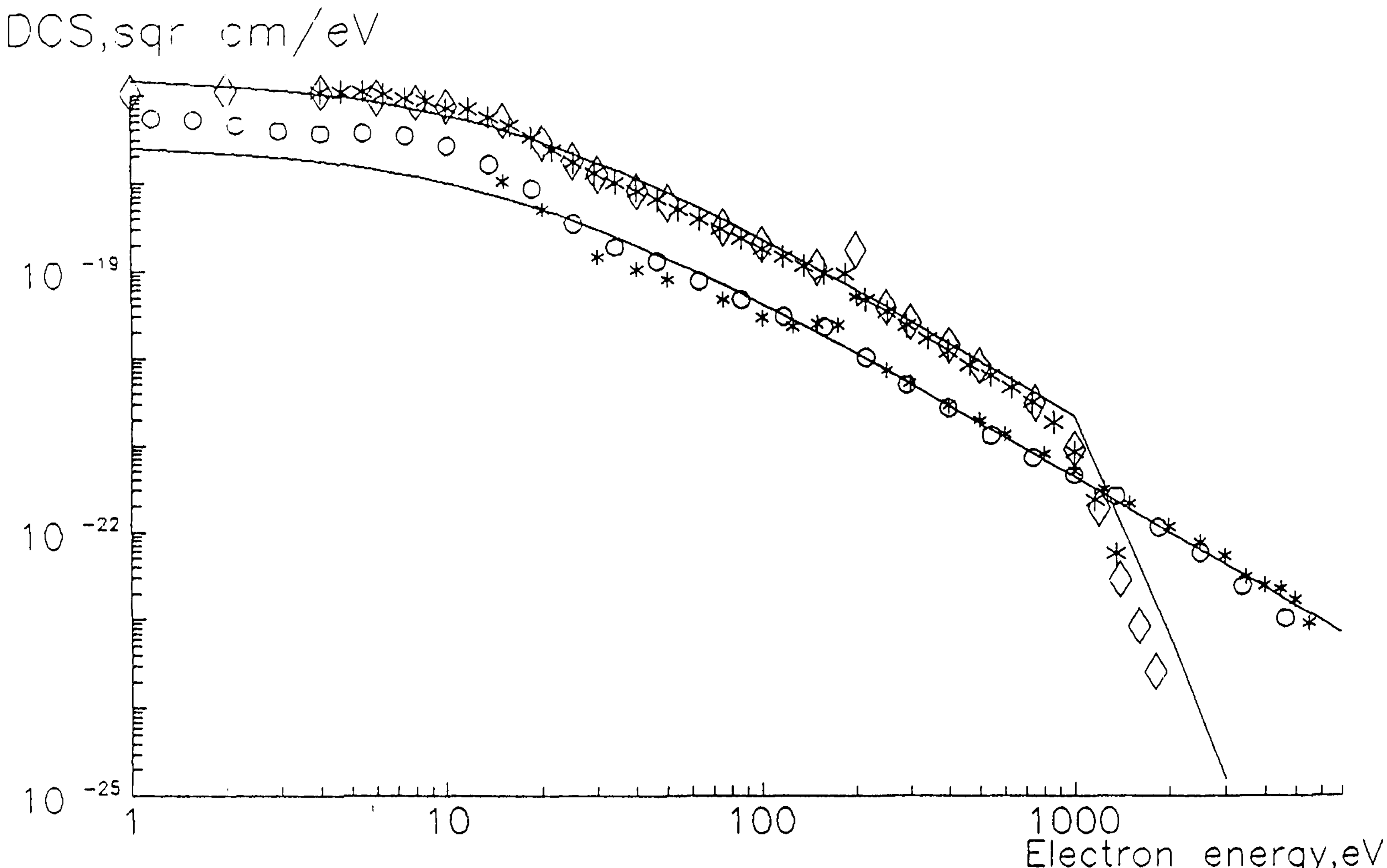

Fig.2. Ionization Differential Cross Sections of Ar by Protons.
Upper line and points for 0.5 MeV protons, lower – for 4.2 MeV.
Solid lines – present evaluation, points – experimental data /4/.

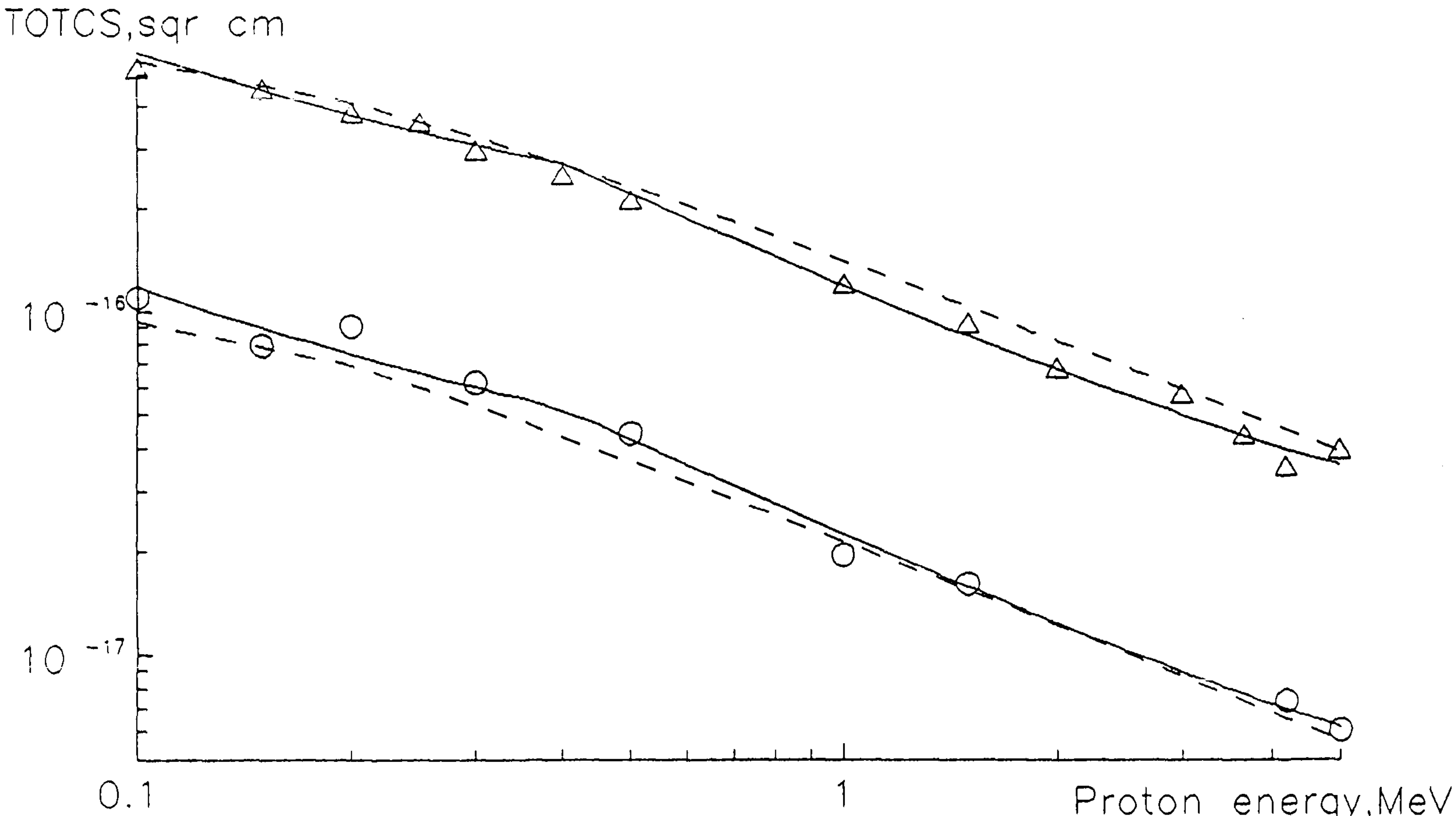

Fig.3. Total Ionization Cross Sections.
Solid lines and points – present evaluation (see text),
Dashed lines – evaluation by Rudd e.a. /5/.
Upper lines and points for Ar, lower – for He.

ACTIVITIES RELATED TO THE RESEARCH OF A & M DATA FOR NUCLEAR FUSION AT CNDC

Jinzhang YAO
Chinese Nuclear Data Center
Institute of Atomic Energy , Beijing, China

A. Database for Ion - Atomic Collision Processes

A primary atomic and molecular database for controlled thermonuclear fusion was formed on Micro-VAX-II and IBM-PC computers at Atomic and Molecular Data Group , CNDC. An ALADDIN format for storage and exchange of atomic and molecular data was adopted. At present, retriavable A+M data at CNDC contain:

1) Collision ionizations of atoms and ions (Z=1-92) with electron in range of incident energy 10 eV - 100 KeV;
2) Collision excited cross sections and rate coefficients of C,O,He atoms and ions with H,H2 and He;
3) Collision ionization,excitation,electron capture, electron emission and asocciation of H,H2,He,Li and Fe atoms, ions and molecules with H,H2,He and Li atoms and their ions.

B.Plasma Surface Interaction

Luo Zhengming et al. have developed a new program PANDA -U version 2. It is a modified version 1 of PANDA-U to consider the influence of potential barrier on the surface. Reflection coefficient data of H, D, T, He-3 and He-4 projectiles from a surface of solids including Be, B, C, Al Si, Ti, Fe, Ni, Cu, Mo, W and Au elemental targets have been calculated. Yao Jinzhang and Fang Shaohong have analysed the reflection data for oblique incidence.

Li Yexiang compiled the trapping data of Hydrogen and its isotopic. The desorption data of some elements including Stainless stell, Iron and Nickel have been collected and evaluated by Zhang Di.

C.Charge Exchange Collision

Wang Nanming has compiled charge exchange collision data of Hydrogen atom and molecule with multicharge ions including C(q+), O(q+), Li(q+), Fe(q+), Al(q+), Mo(q+) and Au(q+) $q \leqslant Z$

He Fuging et al. will measure K-electron ionization cross sections of metallic atoms by electron impact. The experimental equipment was installed.

Database of CRAAMD

Qiu Yubo, Jia Baolin

Institute of Applied Physics and
Computational Mathematics
(P.O.Box 8009, Beijing 100088 China)

Abstract

Database of CRAAMD was founded informally at The Institute of Applied Physics and Computational Mathematics (IAPCM) by Jia Baolin in 1988., and was officially established two years later. The primary work is the compilation, evaluation, storage and recommendation of the atomic data and molecular data for x-ray and fusion research applications. ALADDIN management system is used for the data exchange and manipulation. Data files are the principle part in the database. Besides, the reference files and the dictionary files are included in the database. Up to date, million of data are stored in the database.

1. Purpose for the Database

The database is set up for the purpose of X-ray laser and fusion research applications. The database is constructed at the Institute of Applied Physics and Computational Mathematics, the head unit of China Research Association For A+M Data (CRAAMD).

The following processes and data are mainly considered at the present time: electron collision excitation; electron collision ionization; dielectronic recombination; photoionization; levels; wavelengths; oscillator strengths; Slater-type orbitals parameters etc..

2. Support Institutes, Staff and Installation

Members of CRAAMD are support Institutes for the database, they are: Fudan University, China Univ. of Science and Technology, Ins. of Low Energy Physics of Beijing Normal Univ., Ins. of A+M Physics Jilin Univ., Chang Sha Univ. of Science and Technology, Ins. of Physics Academia Sinica, Ins. of Chengdu Univ. of Science and Technology, etc.. They will supply experimental or theorectical calculation results. At IAPCM, two groups are engaged in the calculation of atomic structure and atomic collision proecsses. A group of five is responsible for the database. One associate professor in full-time services takes responsibility for data compiling, evaluating and recommending, another associate professor in part-time services takes responsibility for data compiling. The other three members are included in this group. A Sun386i pc with a 327 MB hard disk and 3.5 inch 1.44 MB driver is special for the database. It is linked with Sun390 and Sun490 mainframe.

3. Constituents of the database

Three kinds of files are included in the database:

1) Data files. This is the main part of the database. These files are devided into two parts, i.e., database A and database B. The original data are stored in the database A, the evaluated data and the fitting coefficients of analytical formula are stored in the database B. The database consists of a series of files classified according to the types of reactions.

They are electron collision excitation, electron collision ionization, energy levels of ions, photoionization, dielec-tronic recombination etc. All of the files are independent of each other.

2) Dictionary files. They are directional files. In these files we can find the meaning for all of the reactions and notations. From which, the names of research institutes and journals in abbreviation can be found as well.

3) References files. They give the names of authors, titles, journals, date, elements and data type etc., from which the atomic and molecular data are selected.

A flow chart outlining the organization of the database is presented in Fig. 1

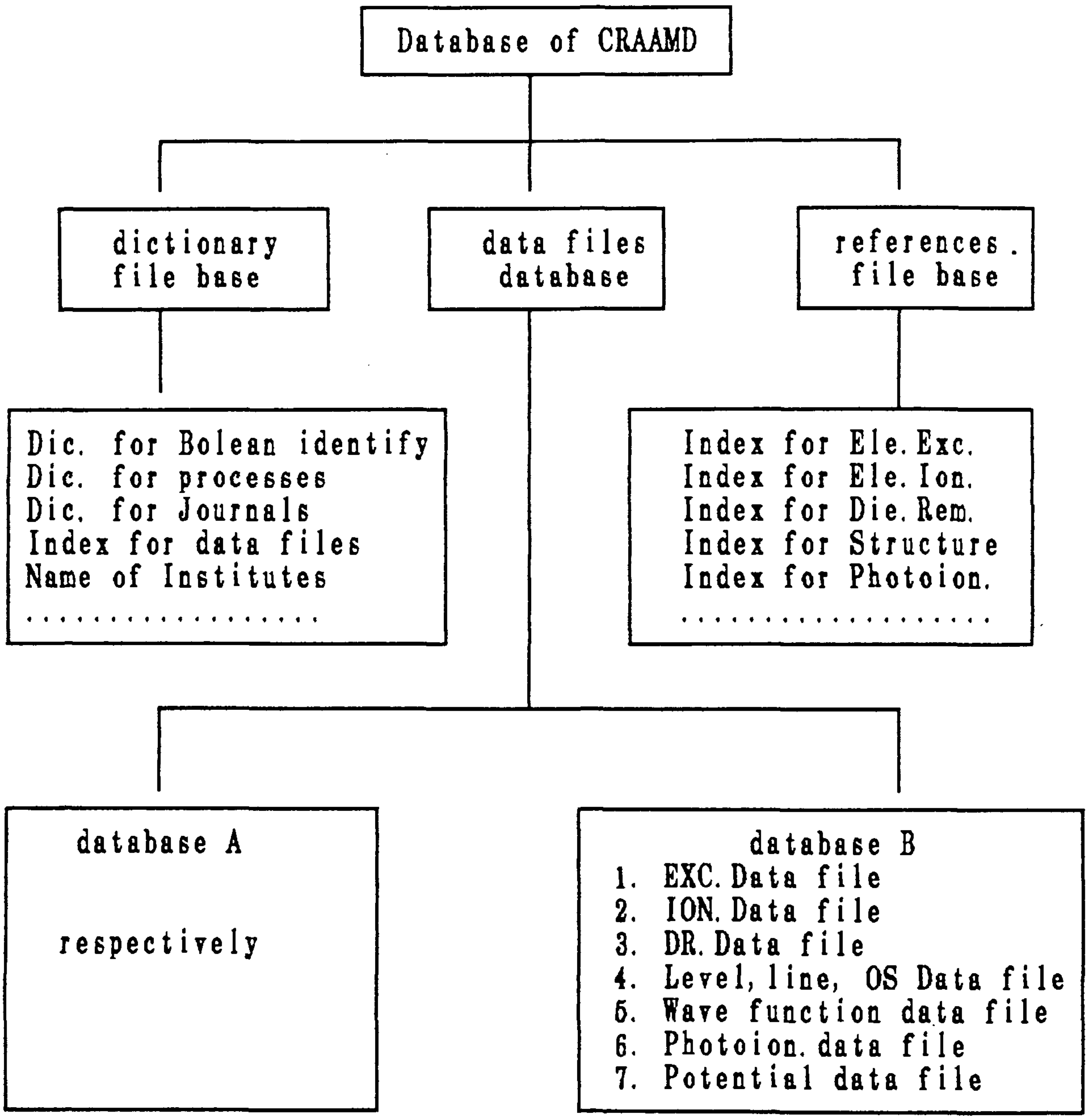

Fig. 1 Schematic Illustration of the Database of CRAAMD

4. Atomic data management and exchange system

ALADDIN management and exchange system is used in our database. Some softwares are added for the purpose of the applications.

A. ALADDIN software

1) ALADDIN.FOR is the drive code, it is an interactive system and by a ' IF...THEN...ELSE...' loop, one can complete a series of operations such as search for, display, evaluate and write out entry data. One can also do other operations as needs change by adding other command lines.

2) ALPACK.FOR is a standard interface subroutine package. This is an inherent routine of ALADDIN. Data in the data files are read by calling this routine. ALPACK.FOR involves 5 subroutines, which can be used to access and retrieve data from ALADDIN files. details can be found in the ALADDIN manual (IAEA-NDS AM-19).

3) ALFLIB.FOR is a fitting form subroutines library. According to the physical problem and different processes, various fitting functions are ALADDIN formatted and the fitting parameters are stored.

4) ALEV.FOR subroutine supports the 'EV' command line. The original subroutine ALEV. FOR is to be called for obtaining tabulated values of the fitting functions. In order to add a new data type to the 'EV' command, it is necessary to add an additional 'ELSE...IF...' loop chain.

B. ALADDIN Data files

Each ALADDIN data file has its name corresponding to one kind of the atomic process. A data file consists of series of entries.

An entry is the basic unit of ALADDIN data files and is independent of each other. An entry contains all the information neccessary to define the physical signification of the stored data. Each ALADDIN entry contains: Hierarchical labels, Boolean labels, Optional free-form comment lines and Numerical data. An entry begins with a symbol '$'.

C. Supplement by IAPCM

1) By a 'IF...THEN...ELSE...' loop, we add some command lines for calling the fitting routine and search for matching.

2) For the fitting of collision excitation cross sections, three kinds of formula are used and subroutines are added respectively.

3) The subroutines for the fitting formula are stored in the evaluation function library.

4) Some kinds of references files are added as well.
For example, An ALADDIN formatted reference file for charge transfer process is considered. The original file is written by T. Kato, but it has not been ALADDIN formatted. We have ALADDIN formatted this file now.

ALADDIN formatted reference files for electron impact excitation and ionization are added as well.

5) Routine for the graphs drawn is added.

A flow chart outlining the organization of the database is presented in Fig. 2

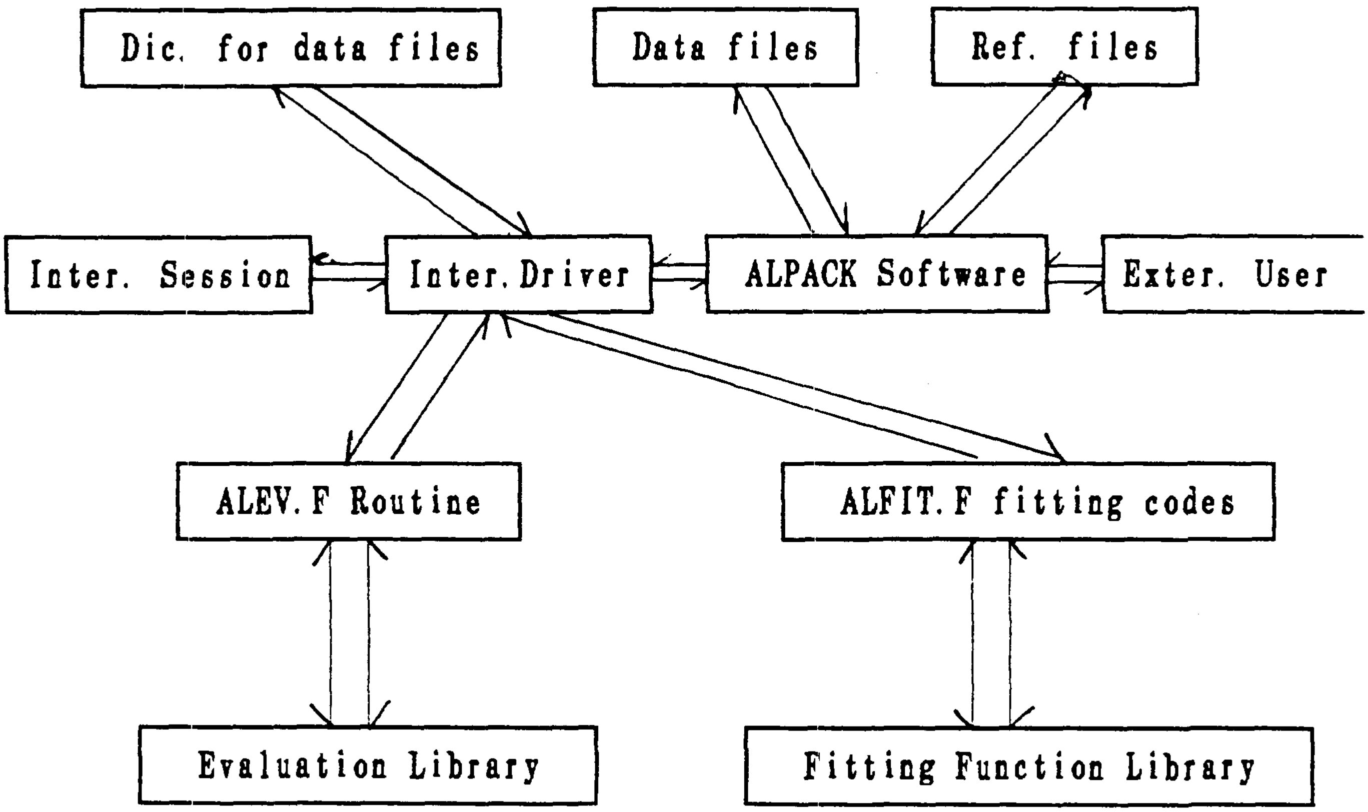

Fig. 2 ALADDIN System Structure

6. Storage and retrieval of the data

1) Compilation

The first step is to compile data. The original data are to be selected from various journals and are received from other data centres as well. Some of which are calculated by ourself and members of CRAAMD.

2) Evaluation

Having the data in hand, theoretical and experimental results, we study these data and compare with each other. We choose the best results and store them in the computer by manpower.

3) Fitting

For the convenience of application, the discrete values are fitted into an analytical formula by the least square method. The parameters of the fitting formula are given.

4) ALADDIN formatted

All of the numerical data are ALADDIN formatted, the original data are stored in database A and the fitted parameters are stored in database B.

5) retrieval of the data

The interactive system can be used to access ALADDIN formatted data files and has a number of commands that provide for the basic manipulation and processing of entries.

When using the interactive system, the interactive system prompts the user for the name of the formatted data file and the dictionary file to be used. Any command can be entered after the ">>" prompt.

Then any ALADDIN formatted entry can be retrieved.

6. Data available up to date

Since Sep. 1989 we have had an amount of million data (23, 412, 717 bytes). Most of the data are concerned with electron collision excitation. The data are evaluated and the recommend data are given. Besides, the data about dielectronic recombination, electron collision ionization, levels etc. are selected. Reference files for electron collision excitation, electron collision ionization and charge transfer are constructed as well. (See Tab. 1)

7. Future improvement and development of the database

1) At the present time we are only interested in the x-ray laser and fusion research application. The potential of the ALADDIN system is, however, such that it can also be used in other atomic data application areas. So we are going to extend the field of the atomic data.

2) To improve and to add ALADDIN softwares. For conveninent of applications, it is evident a numbers of softwares must be added, for example, the evaluation functions and subroutines respectively. The code for graph drawn is added.

3) To link our database with the user program.

4) To publish bulletin.

5) To strength cooperation with other data centres.

Atomic Collision Cross Sections Data Center
at the
Joint Institute for Laboratory Astrophysics
(Boulder, Colorado, USA)

J. Broad

Areas of Activity

Atomic and Molecular Collisions and Optical Physics

Staff

Full time:	John Broad	atomic theorist
	Stephan Krog	programmer
Part time:	Visiting scientists	
	Students	
	P. Ruttenberg	consultant

Equipment

Hardware:	Dec 5000 Workstation	32MB Cpu, 1.36B disc
	386 PC	8MB Cpu, 80MB disc
	486 PC	8MB Cpu, 200MB disc

Software: INGRES for Workstation
CLARION for PC

Projects

1. Maintenance of Atomic Collisions Database

repository for data for reviews
17MB bibliography classified by collision partners
15MB cross section tables

now on DEC-5000 Workstation under INGRES
as a relational database

Resource for reviews, modelling etc
Interest in importing and exporting data

2. Atomic Collisions Projects

In progress:

"Collisional Alignment + Orientation of Atomic Outer Shells"
Vol II: N. Andersen, E.C. Campbell, J.W. Gallagher and I.V. Hertel
Vol III: N. Andersen, K. Bartschat
"Multichannel Quantum Defect Theory"
C.H. Greene, M. Aymar

Planned

"Collisional Data for Aeronomy"
J. Dutton, S. Solomon (NATO)
"Atomic Collision Data for the Reference Dicharge Cell"
N. Petrovic, O. van Brunt
"Electron-Impact Excitation of Atomic Ions"
D. Hummer, M. Shull (NASA)
Supports OPACITY + IRON projects

3. Optical Physics

Gas Laser Database
M. Weber, editor of CRC
Handbook of Laser Science and Technology

Wavelengths, species, transitions and operating conditions of gas laser with full bibliography

PC Database in CLARION
Menu-driver with pop-op + scrolling tables and contact sensitive help screens

Planned

Solid state lasers, optical materials reviews and databases

Questions

1. Sharing resources among data centers
2. Critical Evaluation
3. Funding

STANDARD REFERENCE DATA PROGRAM AT NIST

J.W. Gallagher (NIST, Gaithersburg)

The activities concentrate in the following disciplines:

Analytical Chemistry — mass spectral, surface analysis, crystallographic, and electron diffraction data for chemical identification.

Atomic Physics — atomic energy levels, transition probabilities and collision data used for diagnostics, wavelengths, and modeling.

Biotechnology — data on important groups of molecules, such as lipids, and biological macromolecules, such as proteins, nucleic acids, and viruses.

Chemical Kinetics — rate data on gas-phase reactions.

Materials Properties — structure and characterization of materials, performance properties, including tribology and mechanical corrosion, and phase equilibria.

Molecular Structure and Spectroscopy — evaluated molecular data at microwave and infrared frequencies and; for transient molecules, vibrational and electronic energy levels.

Thermodynamics and Thermochemistry — reliable, widely-used tables of organic and inorganic species.

Thermophysical Properties of Fluids — thermophysical and transport properties of pure and mixed fluids, including refrigerants, that are of great importance to industry.

SRD Atomic Databases

NIST Electron and Positron Stopping Powers of Materials

NIST X-Ray and Gamma-Ray Cross Section and Attenuation Coefficients

NIST Atomic Transition Probabilities Data Files (Scandium through Nickel)

NIST Spectroscopic Properties of Atoms and Atomic Ions

SRD Major Publications in Atomic Data

1986 CODATA Recommended Values of the Fundamental Physical Constants

Atomic Transition Probabilities

Atomic Energy Levels Publications

SRD Analytical Chemistry Databases

Mass Spectra

NIST/EPA/NIH Mass Spectral Database

NIST/EPA/NIH Mass Spectral Database: PC Version

NIST Mass Spectral Database of Common Compounds

Surface Data

NIST X-Ray Photoelectron Spectroscopy Database

Diffraction Data

NIST/Sandia/ICDD Electron Diffraction Database

NIST Crystal Data Identification

Spectrum Analysis

NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database

SRD Major Publications in Analytical Chemistry

The Wiley/NBS Registry of Mass Spectral Data

Crystal Data Determinative Tables (6 vols.)

Elemental and Interplanar Spacing Index

NIST Materials Properties Databases

NIST Structural Ceramics

NACE-NIST Corrosion Performance Databases
COR*SUR 1 - Corrosion Rate Data for Metals
COR*SUR 2 - Corrosion Rate Data for Non-Metals

NIST Crystal Data

NIST/Sandia/ICDD Electron Diffraction

NIST X-Ray Photoelectron Spectroscopy

NIST Tribomaterials I (ACTIS)

Phase Diagrams for Ceramists

SRD Major Publications in Materials Properties

Journal of Phase Equilibria (formerly Bulletin of Alloy Phase Diagrams)

Phase Diagrams for Ceramists

Binary Alloy Phase Diagrams, 2nd edition

SRD Thermochemical Databases

NIST Structures and Properties

NIST Chemical Thermodynamics

NIST Thermophysical Properties of Water

NIST JANAF Thermochemical Tables

DIPPR Data Compilation of Pure Compound Properties

NIST Positive Ion Energetics

NIST Negative Ion Energetics

NIST Estimation of Thermodynamic Properties for Organic Compounds at 298.15 K

NIST Molten Salts

NIST Thermophysical Properties of the Elements

SRD Major Publications in Thermochemistry

NBS Tables of Chemical Thermodynamic Properties

JANAF Thermochemical Tables

Gas-Phase Ion and Neutral Thermochemistry

SRD Fluids Properties Databases

NIST Thermophysical Properties of Hydrocarbon Mixtures

NIST Thermophysical Properties of Fluids

NIST Mixture Property Program

NIST Thermophysical Properties of Refrigerants and Refrigerant Mixtures

Department of Computer Science
The Queen's University of Belfast

Belfast Data Centre

Report on Activities in the Year 1991/92

Prof. F.J. Smith

Unfortunately support for the Data Centre in Belfast from the Culham Laboratory has not been renewed since 31 March 1991; so inevitably the level of activity at Belfast has been substantially reduced.

The Data Centre should have been able to continue with part-time work from the University from that data. Dr. Marguerite Lennon left the University at the same time as the Culham support came to an end and Dr. Michael Higgins replaced her as the member of staff at the University who was assigned to the project. He, however, left the University at the end of 1991. Dr. Shah Saadat, who did experimental work on atomic collisions with Professor Gilbody, was then assigned to the Data Centre on a part-time basis and he has been maintaining the Data Centre over the last few months.

Work has been carried out on the curve fitting of data on the recommended electron excitation rates for iron ions. Previous fits to this data had been unsatisfactory and new fits were produced to the data more accurately than the previous set. A report is near completion. Some sample pages of the draft report are enclosed.

Some more work has also been carried out on electron ionization of molecules, producing more accurate fits of earlier collected data. A report on this work will take some time to complete with current manpower.

Draft

17 July 1992

RECOMMENDED ELECTRON EXCITATION RATES FOR IRON IONS

M A Lennon, A E Kingston, M J Higgins and F J Smith

School of Physics and Mathematical Sciences
The Queen's University of Belfast
Northern Ireland

ABSTRACT

Experimental and theoretical data for the electron impact excitation of Fe I to FE XXVI have been assessed. Based on our assessments, a set of recommended rates has been produced for each species and is presented in the form of a table of polynomial fit coefficients. Using the recommended data an estimate has been made of the line radiative power loss due to Fe in the temperature range 0.1 - 32 keV and the results presented in graphical and tabular form. An estimate of the accuracy is given for each recommended data set and a bibliography for each ion species is supplied.

Figure 5 Weighted radiative power loss per charge state of Fe

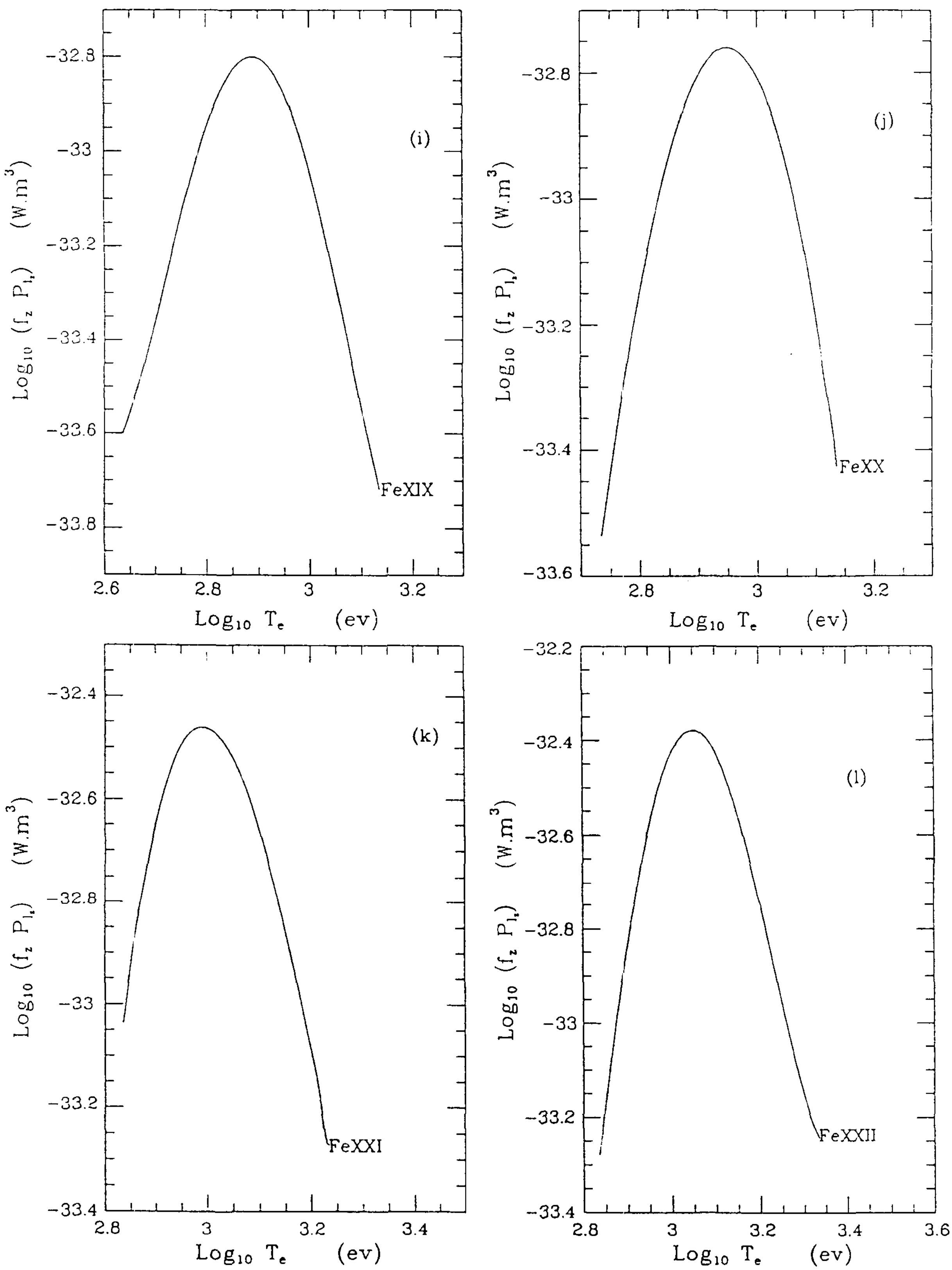

Figure 5 Weighted radiative power loss per charge state of Fe

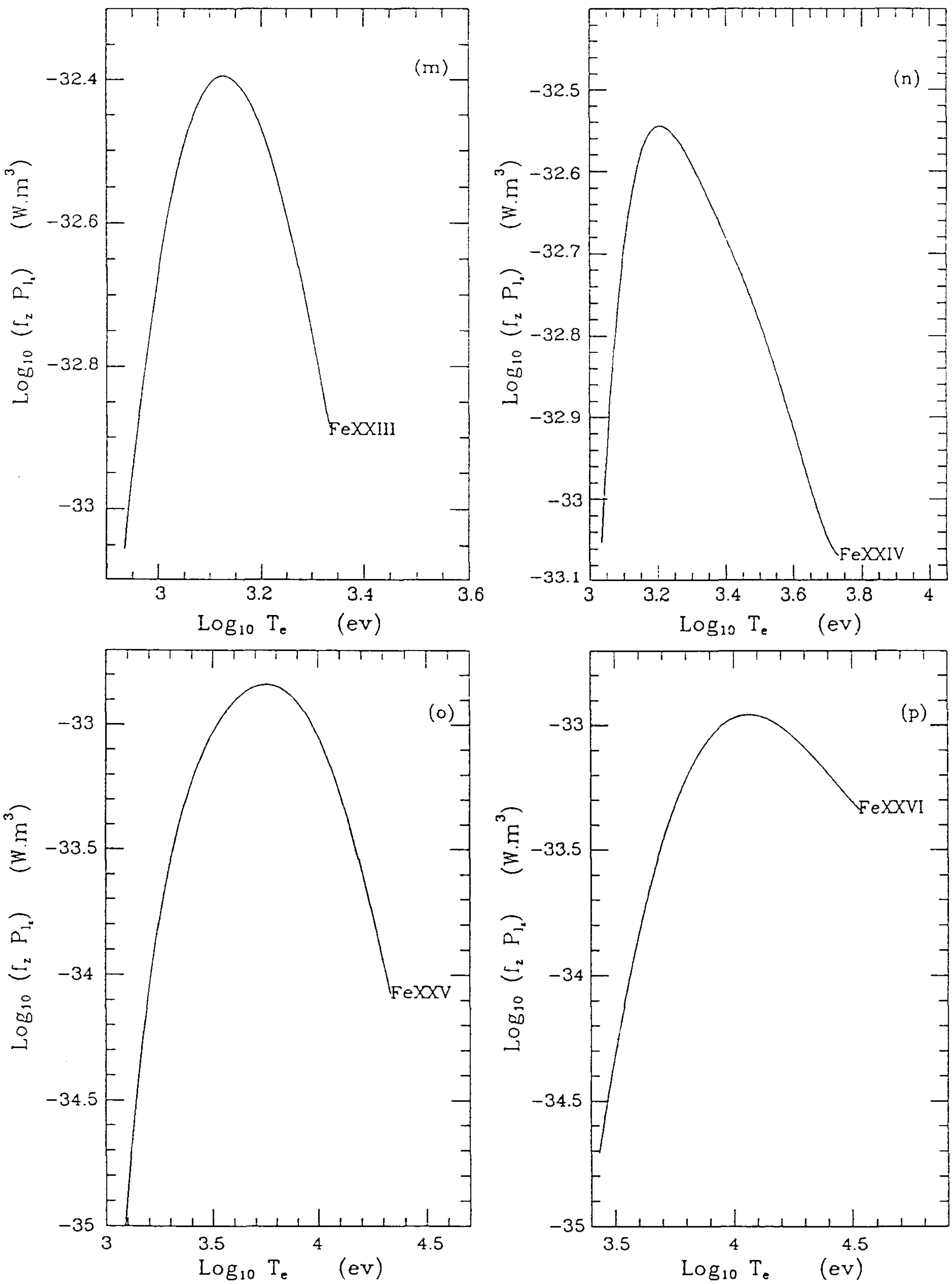

Figure 6 Weighted Radiative Power Loss $f_z P_{l_z}$ (W m^3) as a function of electron temperature T_e (eV)

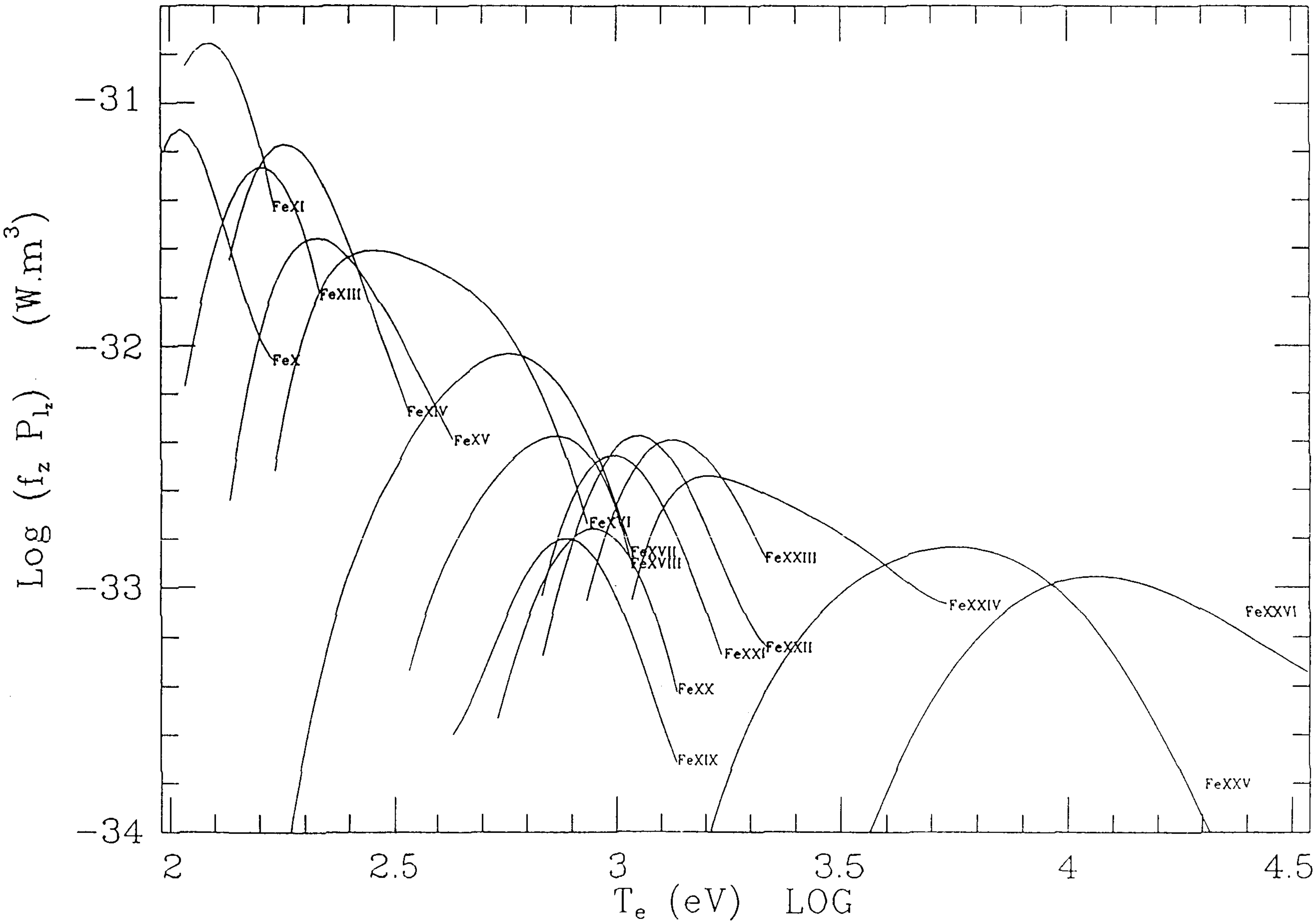

Figure 7. Radiative Power Loss due to Fe

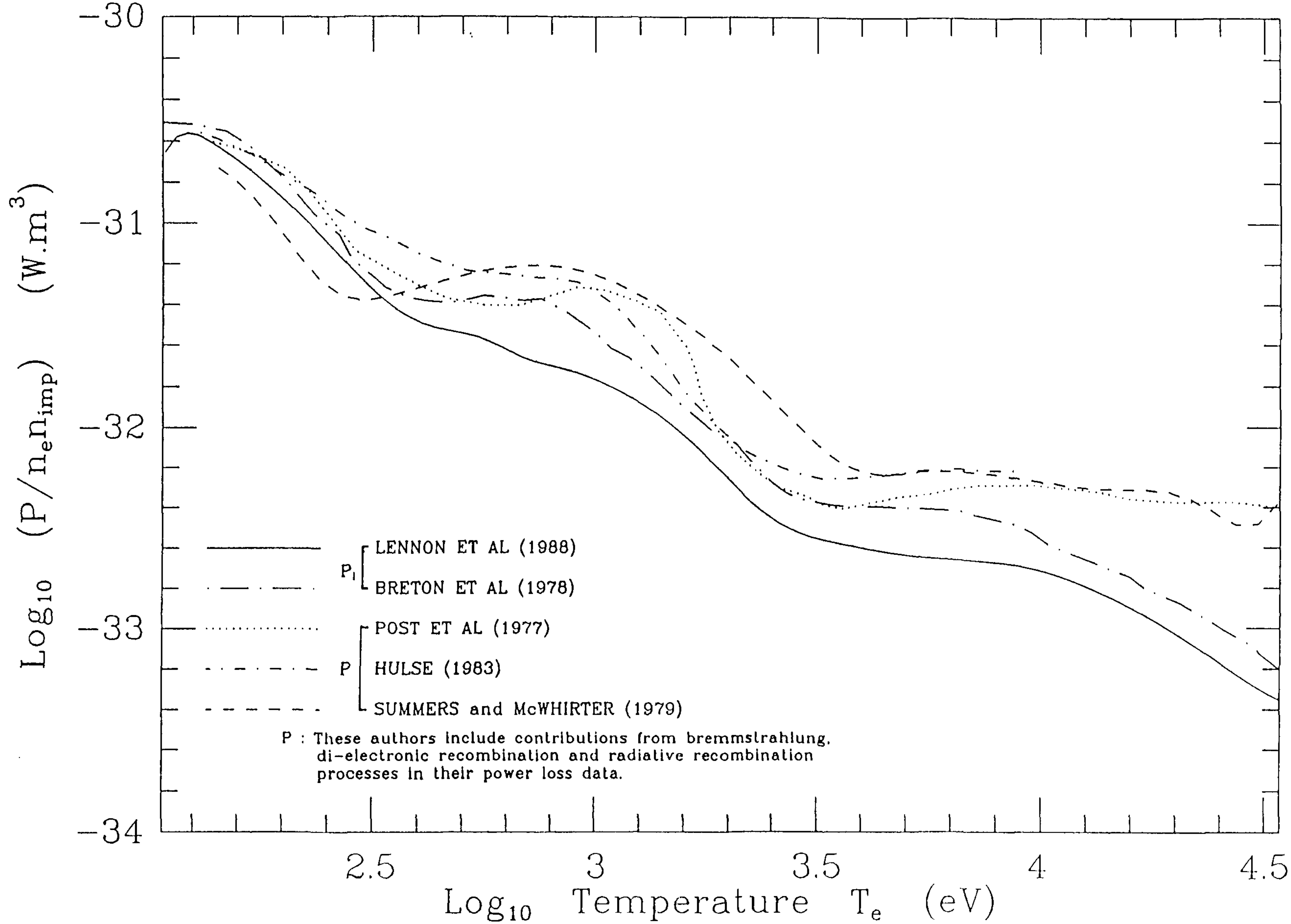

Table 2. Values of Weighted Line Radiative Power Loss per charge state of Fe as a function of temperature.

Charge State:	T_e (eV)	$f_Z P_{lZ}$ (Wm^3)
Fe X	100.0	7.150E-32
	110.0	7.435E-32
	120.0	5.520E-32
	130.0	3.542E-32
	140.0	2.216E-32
	150.0	1.463E-32
	160.0	1.067E-32
Fe XI	110.0	1.487E-31
	120.0	1.747E-31
	130.0	1.673E-31
	140.0	1.369E-31
	150.0	9.959E-32
	160.0	6.598E-32
Fe XIII	110.0	7.647E-33
	120.0	1.715E-32
	130.0	2.963E-32
	140.0	4.210E-32
	150.0	5.113E-32
	160.0	5.457E-32
	170.0	5.237E-32
	180.0	4.602E-32
	190.0	3.753E-32
	200.0	2.876E-32

Table 2. cont.

Charge State:	T_e (eV)	$f_Z P_{lZ}$ (Wm^3)
Fe XIV	140.0	2.746E-32
	150.0	4.267E-32
	160.0	5.602E-32
	170.0	6.470E-32
	180.0	6.776E-32
	190.0	6.599E-32
	200.0	6.081E-32
	210.0	5.383E-32
	220.0	4.627E-32
	230.0	3.897E-32
	240.0	3.240E-32
	250.0	2.671E-32
	260.0	2.196E-32
	270.0	1.806E-32
	280.0	1.489E-32
	290.0	1.235E-32
	300.0	1.031E-32
	310.0	8.680E-33
	320.0	7.379E-33
	330.0	6.336E-33
Fe XV	140.0	3.217E-33
	160.0	1.155E-32
	180.0	2.131E-32
	200.0	2.690E-32
	220.0	2.751E-32
	240.0	2.495E-32
	260.0	2.127E-32
	280.0	1.757E-32
	300.0	1.433E-32
	320.0	1.167E-32
	340.0	9.528E-33
	360.0	7.829E-33
	380.0	6.477E-33
	400.0	5.391E-33

Table 2. cont.

Charge State:	T_e (eV)	$f_Z\ P_{IZ}$ (Wm^3)
Fe XVI	200.0	1.153E-32
	250.0	2.305E-32
	300.0	2.442E-32
	350.0	2.265E-32
	400.0	2.039E-32
	450.0	1.795E-32
	500.0	1.533E-32
	550.0	1.261E-32
	600.0	9.972E-33
	650.0	7.597E-33
	700.0	5.599E-33
	750.0	4.024E-33
	800.0	2.840E-33
Fe XVII	200.0	2.210E-34
	250.0	1.121E-33
	300.0	2.530E-33
	350.0	4.179E-33
	400.0	5.877E-33
	450.0	7.410E-33
	500.0	8.569E-33
	550.0	9.182E-33
	600.0	9.200E-33
	650.0	8.713E-33
	700.0	7.831E-33
	750.0	6.747E-33
	800.0	5.620E-33
	850.0	4.552E-33
	900.0	3.601E-33
	950.0	2.801E-33
	1000.0	2.164E-33

Table 2. cont.

Charge State:	T_e (eV)	$f_Z\ P_{IZ}$ (Wm^3)
Fe XVIII	350.0	5.250E-34
	400.0	1.067E-33
	450.0	1.692E-33
	500.0	2.331E-33
	550.0	2.939E-33
	600.0	3.471E-33
	650.0	3.880E-33
	700.0	4.125E-33
	750.0	4.172E-33
	800.0	4.012E-33
	850.0	3.674E-33
	900.0	3.191E-33
	950.0	2.632E-33
	1000.0	2.062E-33
Fe XIX	450.0	2.849E-34
	500.0	4.331E-34
	550.0	6.612E-34
	600.0	9.424E-34
	650.0	1.230E-33
	700.0	1.454E-33
	750.0	1.570E-33
	800.0	1.570E-33
	850.0	1.468E-33
	900.0	1.298E-33
	950.0	1.104E-33
	1000.0	9.111E-34
	1050.0	7.343E-34
	1100.0	5.851E-34
	1150.0	4.665E-34
	1200.0	3.724E-34
	1250.0	2.985E-34
	1300.0	2.436E-34

Table 2. cont.

Charge State:	T_e (eV)	$f_Z\ P_{IZ}$ (Wm^3)
Fe XX	550.0	3.151E-34
	600.0	5.460E-34
	650.0	8.258E-34
	700.0	1.121E-33
	750.0	1.387E-33
	800.0	1.591E-33
	850.0	1.710E-33
	900.0	1.734E-33
	950.0	1.675E-33
	1000.0	1.556E-33
	1050.0	1.393E-33
	1100.0	1.204E-33
	1150.0	1.013E-33
	1200.0	8.335E-34
	1250.0	6.682E-34
	1300.0	5.257E-34
Fe XXI	700.0	1.085E-33
	750.0	1.716E-33
	800.0	2.334E-33
	850.0	2.878E-33
	900.0	3.264E-33
	950.0	3.444E-33
	1000.0	3.452E-33
	1050.0	3.335E-33
	1100.0	3.128E-33
	1150.0	2.858E-33
	1200.0	2.551E-33
	1250.0	2.239E-33
	1300.0	1.945E-33
	1350.0	1.683E-33
	1400.0	1.452E-33
	1450.0	1.243E-33
	1500.0	1.057E-33
	1550.0	9.011E-34
	1600.0	7.800E-34
	1650.0	6.547E-34

Table 2. cont.

Charge State:	T_e (eV)	$f_Z\ P_{IZ}$ (Wm^3)
Fe XXII	700.0	6.158E-34
	750.0	1.030E-33
	800.0	1.532E-33
	850.0	2.121E-33
	900.0	2.740E-33
	950.0	3.300E-33
	1000.0	3.738E-33
	1050.0	4.023E-33
	1100.0	4.160E-33
	1150.0	4.161E-33
	1200.0	4.034E-33
	1250.0	3.801E-33
	1300.0	3.502E-33
	1350.0	3.173E-33
	1400.0	2.844E-33
	1450.0	2.529E-33
	1500.0	2.233E-33
	1550.0	1.964E-33
	1600.0	1.724E-33
	1650.0	1.514E-33
	1700.0	1.332E-33
	1750.0	1.176E-33
	1800.0	1.043E-33
	1850.0	9.330E-34
	1900.0	8.417E-34
	1950.0	7.662E-34
	2000.0	7.036E-34
	2050.0	6.514E-34
	2100.0	6.081E-34

Table 2. cont.

Charge State:	T_e (eV)	$f_Z P_{IZ}$ (Wm^3)
Fe XXIII	900.0	1.201E-33
	950.0	1.659E-33
	1000.0	2.156E-33
	1050.0	2.641E-33
	1100.0	3.074E-33
	1150.0	3.433E-33
	1200.0	3.712E-33
	1250.0	3.905E-33
	1300.0	4.010E-33
	1350.0	4.029E-33
	1400.0	3.977E-33
	1450.0	3.869E-33
	1500.0	3.719E-33
	1550.0	3.540E-33
	1600.0	3.340E-33
	1650.0	3.128E-33
	1700.0	2.911E-33
	1750.0	2.696E-33
	1800.0	2.487E-33
	1850.0	2.287E-33
	1900.0	2.097E-33
	1950.0	1.920E-33
	2000.0	1.756E-33
	2050.0	1.603E-33
	2100.0	1.464E-33
Fe XXIV	1500.0	2.802E-33
	2000.0	2.551E-33
	2500.0	2.095E-33
	3000.0	1.748E-33
	3500.0	1.457E-33
	4000.0	1.213E-33
	4500.0	1.026E-33

Table 2. cont.

Charge State:	T_e (eV)	$f_Z P_{IZ}$ (Wm^3)
Fe XXV	1500.0	5.921E-35
	2000.0	2.841E-34
	2500.0	5.832E-34
	3000.0	8.591E-34
	3500.0	1.080E-33
	4000.0	1.244E-33
	4500.0	1.356E-33
	5000.0	1.422E-33
	5500.0	1.450E-33
	6000.0	1.446E-33
	6500.0	1.416E-33
	7000.0	1.365E-33
	7500.0	1.300E-33
	8000.0	1.226E-33
	8500.0	1.145E-33
	9000.0	1.061E-33
	9500.0	9.773E-34
	10000.0	8.948E-34
	10500.0	8.156E-34
	11000.0	7.407E-34
	11500.0	6.709E-34
	12000.0	6.064E-34
	12500.0	5.470E-34
	13000.0	4.926E-34
	13500.0	4.429E-34
	14000.0	3.977E-34
	14500.0	3.568E-34
	15000.0	3.200E-34
	15500.0	2.872E-34
	16000.0	2.580E-34
	16500.0	2.321E-34
	17000.0	2.092E-34
	17500.0	1.889E-34
	18000.0	1.707E-34
	18500.0	1.544E-34
	19000.0	1.398E-34
	19500.0	1.267E-34
	20000.0	1.148E-34
	20500.0	1.041E-34
	21000.0	9.469E-35

Table 2. cont.

Charge State:	T_e (eV)	$f_Z P_{IZ}$ (Wm^3)
Fe XXVI	3000.0	3.513E-35
	3500.0	8.069E-35
	4000.0	1.489E-34
	4500.0	2.366E-34
	5000.0	3.377E-34
	5500.0	4.451E-34
	6000.0	5.521E-34
	6500.0	6.544E-34
	7000.0	7.480E-34
	7500.0	8.307E-34
	8000.0	9.014E-34
	8500.0	9.602E-34
	9000.0	1.008E-33
	9500.0	1.045E-33
	10000.0	1.071E-33
	10500.0	1.089E-33
	11000.0	1.099E-33
	11500.0	1.102E-33
	12000.0	1.101E-33
	12500.0	1.095E-33
	13500.0	1.072E-33
	14000.0	1.057E-33
	14500.0	1.039E-33
	15000.0	1.020E-33
	15500.0	1.000E-33
	16000.0	9.797E-34
	16500.0	9.584E-34
	17000.0	9.369E-34
	17500.0	9.153E-34
	18000.0	8.938E-34
	18500.0	8.726E-34
	19000.0	8.517E-34
	19500.0	8.312E-34
	20000.0	8.113E-34
	20500.0	7.918E-34
	21000.0	7.729E-34
	21500.0	7.545E-34
	22000.0	7.366E-34
	22500.0	7.193E-34

Table 2. cont.

Charge State:	T_e (eV)	$f_Z P_{IZ}$ (Wm^3)
Fe XXVI	23000.0	7.025E-34
	23500.0	6.863E-34
	24000.0	6.707E-34
	24500.0	6.556E-34
	25000.0	6.411E-34
	25500.0	6.271E-34
	26000.0	6.136E-34
	26500.0	6.007E-34
	27000.0	5.883E-34
	27500.0	5.764E-34
	28000.0	5.650E-34
	28500.0	5.540E-34
	29000.0	5.435E-34
	29500.0	5.333E-34
	30000.0	5.236E-34
	30500.0	5.142E-34
	31000.0	5.052E-34
	31500.0	4.966E-34
	32000.0	4.883E-34
	32500.0	4.803E-34
	33000.0	4.727E-34
	33500.0	4.653E-34

Table 3. Values of Line Radiative Power Loss for Fe as a function of temperature.

T_e (keV)	P_l (Wm^3)
0.5	2.863E-32
1.0	1.709E-32
1.5	1.004E-32
2.0	5.485E-33
2.5	3.511E-33
3.0	2.871E-33
3.5	2.644E-33
4.0	2.492E-33
4.5	2.379E-33
5.0	2.297E-33
5.5	2.243E-33
6.0	2.208E-33
6.5	2.184E-33
7.0	2.163E-33
7.5	2.139E-33
8.0	2.109E-33
8.5	2.072E-33
9.0	2.026E-33
9.5	1.974E-33
10.0	1.917E-33
10.5	1.857E-33
11.0	1.796E-33
11.5	1.735E-33
12.0	1.674E-33
12.5	1.614E-33
13.0	1.555E-33
13.5	1.499E-33
14.0	1.444E-33
14.5	1.392E-33
15.0	1.341E-33
15.5	1.293E-33
16.0	1.246E-33
16.5	1.202E-33
17.0	1.159E-33
17.5	1.118E-33
18.0	1.079E-33

Table 3. cont.

T_e (keV)	P_l (Wm^3)
18.5	1.041E-33
19.0	1.005E-33
19.5	9.708E-34
20.0	9.378E-34
20.5	9.062E-34
21.0	8.759E-34
21.5	8.470E-34
22.0	8.194E-34
22.5	7.930E-34
23.0	7.678E-34
23.5	7.437E-34
24.0	7.208E-34
24.5	6.989E-34
25.0	6.781E-34
25.5	6.583E-34
26.0	6.394E-34
26.5	6.215E-34
27.0	6.045E-34
27.5	5.883E-34
28.0	5.731E-34
28.5	5.586E-34
29.0	5.450E-34
29.5	5.321E-34
30.0	5.199E-34
30.5	5.085E-34
31.0	4.978E-34
31.5	4.878E-34
32.0	4.784E-34
32.5	4.697E-34
33.0	4.616E-34
33.5	4.542E-34