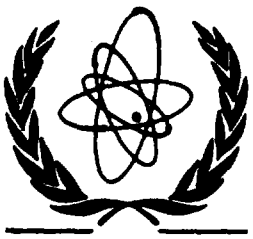
INDC(NDS)-377



International Atomic Energy Agency

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (14th Meeting of the A+M Data Centres and ALADDIN Network)

21-22 July 1997, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared By J. A. Stephens

January, 1998

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

We regret that some of the pages in this report may not be up to the proper legibility standards, even though the best possible copy was used for scanning

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Abstract

The proceedings of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange (14th Meeting of A+M Data Centres and ALADDIN Network)", held on July 21-22, 1997 in Vienna, Austria are briefly described. The meeting conclusions and recommendations on the priorities in A+M data compilation and evaluation, and on the technical aspects of data processing and exchange are also presented.

Reproduced by the **IAEA** in Austria
January, 1998

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1 Introduction

On July 21-22, 1997, the IAEA organized the regular Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Exchange and Processing (14th Meeting of the Atomic and Molecular (A+M) Data Centres and ALADDIN Network)" with the objectives of reviewing the progress in the A+M data related activities in the data centres, the methods and procedures applied in the data processing and exchange, developments in the ALADDIN system, and to co-ordinate the working plans for the next period. The meeting was attended by 14 participants from 12 data centres (**see Appendix 1**). The data centre at the Laboratory for Quantum Optics (Korea Atomic Energy Research Institute) was represented for the first time in this series of Advisory Group Meetings. Additionally, atomic and molecular scientists and data specialists from the Queen's University of Belfast, the Lebedev Physical Institute, the Weizmann Institute of Science, and the Astronomical Observatory in Belgrade attended the conference. The 20th International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC), was held in the Vienna International Centre just following the Advisory Group Meeting. Several AGM participants attended this conference as well.

2 Meeting Proceedings

The Meeting was opened by **Dr. Douglas Muir** (Section Head of the Nuclear Data Section, RIPC) and **Dr. R. K. Janev** (Head of the Atomic and Molecular Data Unit, RIPC). They stressed the necessity of strengthening the communication and collaboration among the data centres and the importance of having ALADDIN as the international format for data exchange, and the timeliness of new Internet and World-Wide-Web (WWW) developments which have occurred since the 13th AGM in 1995.

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

1. Current Activities of the A+M Data Centres,
2. Data Generation and Priorities in Data Compilation and Evaluation,
3. Data Processing and Exchange,
4. Meeting Conclusions and Recommendations.

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

In Session 1, progress reports on the activities of individual data centres during the period July 1995-June 1997 were presented. These reports, which are reproduced in **Appendix 3**, describe the work of the data centres on A+M data compilation, evaluation and generation, WWW developments, the data centre publications during the reporting period, the status of ongoing programmes and the plans for immediate future work in this area. The presentations in this session demonstrate 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, USA) and **Dr. H. Tawara** (NIFS, Japan), who described the ongoing work on establishing A+M databases in their respective centres. Dr. Wiese reported recent work on compilation and evaluation of data for wavelengths of Ar, Ga, Kr V-XXXVI and Be I; for energy levels of Zn, Ga, Ar, Be I; and transition probabilities for all spectra of C, N and O. Work in progress at the NIST data centre includes data compilation and evaluation for the wavelengths of Si I, Be II, F I, He I and Cl; the energy levels for Si I, Cl, Be II, F I and He I; and the transition probabilities of H, D, He, Li, Be, B, F, Ne, Na, Mg, Al and Si. Dr. Wiese described the current databases on the WWW (http://physics.nist.gov) which include annotated bibliographic databases and numerical databases. He also described the programme for the first International Conference on the Atomic and Molecular Data and Their Applications (ICAMDATA), which was subsequently held at NIST (Gaithersburg, USA), September 29-October 2, 1997.

Dr. H. Tawara reported that relocation of their laboratory to Toki city (30 km north of the previous location in Nagoya) was completed. He reported on the recent A+M data compilation, evaluation and recommendation activities, which include: calculations and analysis of the $n\ell$ distributions of the electron-transferred states in He^{2+}-He collisions; heavy particle collisions involving vibrationally-excited hydrogen, e.g. He-$H_2(v_i)$ collisions including fragmentation processes; electron-ion collisions (e.g. C II-C IV and Be-like ions) and electron impact data; surface interactions in divertors, particularly control of formation of vibrationally-excited H_2 by collisions with the surface. Dr. Tawara's data centre has now switched to to using UNIX and are reconstructing their databases using a relational database system. The retrieval system is now accessible through the WWW (http://dbshino.nifs.ac.jp).

Session 1 continued with the presentation of **Dr. D. Schultz** (ORNL, USA) from the Controlled Fusion Atomic Data Center (CFADC). He reported that CFADC now maintains the only US location for the JET/Strathclyde Atomic Data and Analysis Structure (ADAS, a suite of codes and data collection for extracting fundamental and derived atomic data and modelling radiating properties of atoms and ions in plasmas). CFADC now uses the WWW to maintain their bibliographic data compilation, and have also established on-line access to ALADDIN-formatted numerical A+M databases. The ORNL 'Redbooks' have also been digitally scanned and placed on CFADC's homepage. Current atomic data production efforts at CFADC include: an elastic scattering database for edge and divertor modelling; charge transfer and ionization in slow collisions of H+H, H^++He, C^++H; inelastic processes in collisions of Be, Ne, Ar ions with H, H_2, and He over a wide energy range.

The report of the A+M activities at the Nuclear Data Center of the Japan Atomic Energy Research Institute was presented by **Dr. T. Shirai**. He reported current fusion data evaluation work on: analytical fits for dissociation and particle interchange in collisions of H, H_2, He, Li atoms and ions with atoms and molecules; calculations of cross sections for excitation and ionization of excited helium atoms in collisions with bare ions in the

Glauber and CDW-EIS approximations; ion-molecule collision cross sections in the H_3^+ system (e.g. $D^+ + H_2$, and other possible variants); vibrational excitation and dissociative recombination in collisions of electrons with H_2^+ and HD^+; state-selective electron-capture by Be^{2+} and Be^{3+} ions. Compilations of spectral data for the highly-ionized species of Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr and Mo have been made, due to their importance in fusion research.

Dr. J L. Delcroix (GAPHYOR, Orsay) described new developments and surveyed all features offered in the current GAPHYOR database system. Developments on the WWW for GAPHYOR have developed very rapidly since the 13th AGM meeting. He described their homepage (http://gaphyor.lpgp.u-psud.fr) and the main query form, links, and search criteria used for bibliographic and numerical data retrievals. User statistics for the GAPHYOR centre were discussed.

The data activities of the A+M Data Centre at the Scientific Research Centre "Kurchatov Institute" (Moscow) were presented by **Dr. V. Abramov**. The main activities reported were: collection of the A+M bibliography from Russian publications, compilation of cross sections for processes involving Be ions, calculations of the radiative cooling rates for Be and Ne-seeded plasmas, evaluation of excitation cross sections for different metallic ions. Dr. Abramov briefly reviewed the physics of the core plasma, although he indicated that study of the divertor processes have more priority. He indicated that the accuracy of A+M data for ITER must be high, and that such data can only become more important.

Dr. A. Godunov (Troitsk Institute of Innovation and Fusion Research, Troitsk, Moscow region) presented data activities from the Troitsk Atomic Data Group (TADG). He discussed the advantages and features of the TADG HiBase System used for atomic data storage and retrieval. The TADG has also addressed one of the priorities recommended in the 13th AGM meeting, namely, the compilation, evaluation, and generation of comprehensive data on all processes relevant to fusion for Ne and its ions. These include ionization by electron impact (with recommended analytic fits), and suggesting a new analytic formula with less parameters than the now-used ALADDIN evaluation function BELI. Advantages and disadvantages of the new exponential fitting formula for ionization were discussed, and results for Ne ionization cross sections presented. Dr. Godunov promoted formation of a world-wide A+M Data Centre Network, covering all aspects of data handling (software and data exchange, linked Web sites, data representation, forms, etc.).

Dr. W. Eckstein (IPP, Garching) reported on data production, collection and evaluation at IPP-Garching. The main area of the data activities at IPP are kinetic reflection and sputtering of bombarding species. New divertor designs require sputtering data for hydrogen isotopes and by noble gas species, including self-sputtering. New data is being generated by computer simulation using the binary collision program TRIM.SP for sputtering yields and efficiency. Particle and energy reflection coefficients for a large number of projectile-target combinations over a wide rage of energies and angles were reported for H, D, T, N, Ne and Ar, and can be retrieved from their UNIX system with 'afs'. Tables for the mean depth of implanted atoms can also be produced from this data.

Dr. Y. Rhee (KAERI, Taejon) presented data centre activities at the Laboratory for Quantum Optics, which supports several atomic, molecular, and optical (AMO) physics programmes. He specifically reviewed the objectives and scope of the AMO data management at the centre. These objectives include fusion research. Data production and evaluation in the fusion area has been initiated for energy levels, reaction cross sections, and electron impact excitation, including an AMO bibliographic database. AMODS is the database system and is accessible on the Web (http://amods.kaeri.re.kr).

Dr. Y. Ralchenko (Weizmann Institute, Rehevot) reviewed atomic data activities at his plasma research laboratory. Data production here is for plasma diagnostic needs including collisional cross sections, photoionization cross sections, and oscillator strengths. These include atoms and ions relevant to fusion data needs, e.g., H-like, Li-like, and Be-like ions. A comprehensive list of atomics physics resources and Websites on the Internet is included on their homepage (http://plasma-gate.weizmann.ac.il). There are 30 atomic databases and 6 plasma databases. A database of for excitation and ionization cross sections currently available for H I, He I, He II and Be I, computed using the convergent close-coupling (CCC) method (in collaboration with Dr. I. Bray). The homepage now includes Web interfaces for the interactive generation of atomic data using Cowan's Hartree-Fock code for atomic energy levels and oscillator strengths, and Vainshtein's Coulomb-Born-exchange code for calculation of electron-impact excitation cross sections of atoms.

Dr. Sun Yongsheng presented a progress report of the A+M data activities at CRAAMD, Beijing. The CRAAMD centre has now completed a project which has generated and evaluated electron-impact excitation cross section data for Ne and Ne ions published up to mid-1996. The data has been ALADDIN formatted, and was submitted to the A+M Data Unit's for storage and implementation in its databases. Electron impact ionization data for Ne and Ne ions has also been collected and stored in the ALADDIN format, including rate coefficients for Ne^{q+} ($q = 1-9$). This effort strongly compliments the work of Godunov's data centre on Ne and its ions.

At the close of Session 1 **Dr. J. Stephens** (IAEA, A+M Data Unit) presented a report of activities of the IAEA A+M Data Unit. The activities were divided into three areas: database development, data evaluation and recommendation, and Co-ordinated Research Programmes (CRPs). The status of the A+M Data Unit's database system AMDIS (Atomic and Molecular Data Information System) was reviewed. AMDIS contains the Data Unit's on-line service for the ALADDIN numerical databases, and AMBDAS, the IAEA A+M Bibliographic Database. Favorable usage statistics (since activation in June 1995) indicate its usefulness as a database system and effective interface to the ALADDIN databases. A WWW homepage has been written (http://www.iaea.org/programmes/amdis) which describes the Data Unit's activities and also provides access to the AMDIS system and the ALADDIN databases. In data evaluation and recommendation, a database on the chemical erosion of Be, C and W has been evaluated following conclusion of a five-year CRP, and will be published in **Nucl. Fus. Suppl.** in two volumes. A critical assessment of electron impact cross sections for Be and B plasma impurity ions has been made (with K. Bartschat, K. Berrington, and I. Bray). An ALADDIN collisional database

for Lithium-beam interactions (previously prepared by J. Smith and R. Janev) has been added to the on-line ALADDIN databases.

2.2 Session 2: Data Generation and Priorities in Data Compilation and Evaluation (Chairman: Dr. Y. Rhee)

Dr. K. Berrington (Queen's University of Belfast, UK) briefly reviewed the Opacity project and then discussed in-depth the "P-Cl" project. This latter project will yield a systematic study and database of bound-bound oscillator strengths and photoionization cross sections for atoms and ions P^{q+}-Cl^{q+}, using R-matrix techniques with multi-state and inner-shell excitations. The Iron Project is generating a database of collision strengths for the electronic excitation of Fe^{q+} (mainly Fe^{+1}). Dr. Berrington reviewed the results and conclusions of an IAEA Consultants' Meeting on the "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions". At the close of the presentation, Dr. Berrington expressed the view that the IAEA should define the essential data needs, coordinate tasks and deadlines for data productions, and organize user/producer collaborations.

Dr. L. Presnykov (Lebedev Physical Institute, Moscow) reviewed the atomic data generation efforts at three Russian Research Centres: the Lebedev Physical Institute (RAS), the Institute of Spectroscopy (RAS), and the Institute for Physico-Technical Measurements: VNIIFTRI. Focusing mainly on activities at the Lebedev Institute, Dr. Presnykov described the theoretical methods and computer codes used for data production. The main codes are ATOM and MZ (radiative and electron collision processes), ION-COL (ion-atom and ion-ion processes), and GKU (level populations and intensities), and there are estimated accuracies available for output from the three codes. Dr. Presnykov mentioned that a goal of their database activities is to store methods for calculation and final formulas instead of data itself. Dr. Presnykov briefly discussed activities at the Institute of Spectroscopy and VNIIFTRI; the former centre concentrates on the systematic study of spectra of many-electron ions and bibliographic data, the latter centre on x-ray spectroscopy of multicharged ions and the SPECTR database.

The last presentation of Session 2 was given by **Dr. M. Dimitrijević** (Astronomical Observatory, Belgrade), who discussed experimental and theoretical studies of the spectroscopy of many elements (e.g. Fe II, Ca II, and Be II) within the astrophysical context. The data from this work is available via their STARK database, accessible by a telnet session (mesi@a.obspin.fr, user: stark).

Following lunch there was a demonstration of data centre WWW pages, and software demonstrations by **Dr. Y. Ralchenko** (Weizmann Institute), and **Dr. J. Stephens** (IAEA) in Room A23-41.

Session 2 was concluded with an open discussion led by **Dr. R. Janev** on priorities in A+M data compilation and evaluation. It was agreed that most of the priorities summarized in Section 3.4 and Appendix 4 of the Summary Report for the 13th AGM Meeting remain valid. It was agreed that needs for the core plasma were satisfied. New or adjusted data priorities which were identified during the 14th AGM are summarized

in Section 4 below.

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

This session was devoted to a discussion on the ALADDIN implementation, World-Wide-Web developments and use, and future DCN activities. There were open discussions with contributions from all meeting participants. The ALADDIN data format is recognized as the internationally adopted format for atomic, molecular, particle-surface interaction and material properties data exchange among data centres themselves and among data centres and the fusion community.

Although the importance of the ALADDIN format for collaboration among different data centers was acknowledged, the desire to further identify what the fusion modellers really need was stressed repeatedly. Three members of the Data Centre Network (Drs. Schultz, Godunov and Ralchenko) volunteered to to approach the problem of identifying the needs of the fusion modeller, with coordination and assistance by the A+M Data Unit. It was further suggested that the ALADDIN concept be extended to new regimes, with a more flexible format and user interface to the ALADDIN programs themselves. The ALADDIN programs and concept needs to be fully integrated using the WWW as the main interface with users in the future, with "user friendliness" kept in mind. A Web link to the Opacity and Iron Projects (and the ADAS database) was suggested at relevant atomic physics and fusion science Web database sites.

It was pointed out that there is an important difference bewteen database "mirroring" and "subsuming", i.e. the latter process occurring without **proper credit** assigned to the database originators. The latter situation is obviously deemed unacceptable within the DCN community.

It was suggested that a new document be created to list priorities in fusion research; such a document could be sent around or maintained on a WWW page. The A+M Data Unit will be responsible for this document and its distribution. It was also agreed that a News page should be set up on the A+M Data Unit's WWW homepage and contributed to on a regular basis by members of the Data Centre Network. This will facilitate communication and make collaboration among all Data Centres much easier.

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

The presentations and discussions at the 14th Advisory Group Meeting regarding the A+M, PSI and data-related activities in the A+M Data Centre Network, the data processing, management and exchange methodology, present and future use of the World-Wide-Web, the ALADDIN system implementation and development, and the priorities in A+M data compilation and evaluation work have resulted in the following conclusions and recommendations.

2.5 Conclusions

2.6 Status of Data Generation and Priorities in Data Compilation and Evaluation

1. It was concluded that the comprehensive summary of data needs and priorities presented at the 13th AGM are still valid. This list of priorities are presented in the IAEA report INDC(NDS)-339, prepared by Dr. J. Botero following the 13th AGM (copies are available from the A+M Data Unit).
2. The IAEA experts' meetings, consultants' meetings, co-ordinated research programmes and individual consultants make a significant contribution to the data evaluation effort. The IAEA also needs to help "enforce" the quality control of atomic and molecular data for fusion research. A list of approved sites where A+M data for fusion can be obtained needs to be created.
3. The Advisory Group observes an increase of data generation activities in the A+M Data Centre Network more of which is freely available on the Web. The strengthening of this effort in terms of quality, direction and organization (in terms of fusion research) is highly encouraged and needed.

2.7 Data Processing and Exchange (ALADDIN)

1. The implementation of ALADDIN in the data exchange among the A+M data centres is well established. Yet with new Web capabilities the need for an improved user interface and technical extensions of ALADDIN are desirable. A common exchange format such as employed by ALADDIN guarantees compatibility among all data centres which have an interface of their own system to ALADDIN formatted data. Thus the need for such a common data exchange mechanisms remains highly desirable. Increasing the advantages of employing ALADDIN using a Web interface is highly desirable. One data centre (CFADC) has implemented a working model for a WWW interface of the ALADDIN programs. The A+M Data Unit's Web site also has available all ALADDIN programs and formatted data available for downloading.
2. In order to improve the communication and data exchange among data centres, a News page will be implemented on the A+M Data Unit's WWW site, with list of data activities provided by the data centres. This list and description will be updated quarterly.
3. The Advisory Group concluded that the efforts on data compilation and ALADDIN formatting of data have to be strengthened by making more contact with the fusion modeller user community to identify desirable improvements in the use of ALADDIN.
4. There is a valid need for mirroring (at authorized Web sites) atomic and molecular databases in Europe, North America, and elsewhere. This will decrease

access times and downloads between the regions. Specific sites for mirroring are to be identified, and insofar as possible, implemented before the 15th AGM.

2.8 Priorities in Data Compilation, Evaluation and Generation

A comprehensive list of priorities has been presented in the IAEA report INDC(NDS)-339 (prepared by Dr. J. Botero) following the 13th AGM in 1995, and is available from the A+M Data Unit. The 14th Advisory Group adopted the following additions and additional emphasis to the list presented in INDC(NDS)-339:

1. Plasma-core region
   (a) Cross sections for electron impact (excitation, ionization, radiative and di-electronic recombination) and charge exchange processes involving incompletely stripped ions, particularly those of Be, C, and B. Energy range: from a few keV to 30 keV.
   (b) Charge exchange collision cross sections of X^{q+} (X = Be, C, and B) with H, H^+ and He_2^+. Energy range: from 1 eV (or threshold) to 500 eV.
2. Plasma-edge region
   (a) A complete collisional database for N, N_2, Ne and Ar is needed.
   (b) Studies of collision processes of the ions H_2^+, H_3^+ with e^-, H, H^+, H_2, H_2^+, He, He^+, He_2^+ and other projectiles (relevant to proposed radiative cooling scheme of divertors).

2.9 Recommended Actions

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

1. Continue the efforts on the co-ordination of data compilation, evaluation and recommendation by the Data Centre Network along the lines presented in the conclusions of this meeting (see previous section).
2. Form a Task Group to further define what interface fusion data users really desire, and investigate questions of how ALADDIN can and should be advanced from a user perspective. Members of this Task Group presently include of Drs. D. Schultz, Y. Ralchenko and A. Godunov, with co-ordination by the A+M Data Unit.
3. Utilize the World-Wide-Web by providing at its site a Links page to other fusion laboratories and Data Centres, as well as a News page providing a description of on going data activities at the data centres.
4. Strengthen its efforts on the coordination of data generation projects through its Co-ordinated Research Programmes in order to meet the evolving A+M and PSI data needs of the fusion community, in particular those for ITER.

5. Create a new document to list the data priorities in fusion research and distribute this to the Data Centre Network, e.g., on its WWW site and by regular mail, on a semi-annual basis.

Appendix 1

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(14th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

21-22 July 1997, IAEA Headquarters, Vienna, Austria

LIST OF PARTICIPANTS

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Appendix 2

IAEA Advisory Group Meeting on
"Technical Aspects of Atomic and Molecular Data Processing and Exchange
(14th Meeting of the Atomic and Molecular Data Centres and ALADDIN Network)"

21-22 July 1997, IAEA Headquarters, Vienna, Austria

PROPOSED MEETING AGENDA

Monday, July 21 — **Meeting room: C-07-V**

09:30 - 09:45	- Opening (R.K. Janev, Head A+M Data Unit) - Adoption of Agenda
Session 1.	Current Activities of the A+M Data Centres
Chairman:	Abramov
09:45 - 10:45	Reports from Data Centres: Wiese (NIST), Tawara (NIFS)
10:45 - 11:00	**Coffee break**
11:00 - 12:00	Reports from Data Centres: Schultz (ORNL), Shirai (JAERI)
12:00 - 14:00	**Lunch**
Session 1.	(Cont'd.)
Chairman:	Wiese
14:00 - 15:30	Reports from Data Centres: Delcroix (GAPHYOR), Abramov (Kurchatov Institute), Godunov (ITI-Troitsk)
15:30 - 16:00	**Coffee break**
16:00 - 17:30	Reports from Data Centres: Eckstein (Max-Planck-Institute, Garching), Rhee (KAERI) Ralchenko (Weizmann Institute)

Tuesday, July 22

Session 1.	(Cont'd.)
Chairman:	Tawara
09:30 - 10:30	Reports from Data Centres: Yongsheng (CRAAMD, Bejing), Stephens (IAEA)
10:30 - 11:00	**Coffee break**
Session 2.	Data Generation and Priorities in Data Compilation and Evaluation
Chairman:	Rhee
11:00 - 11:30	New "Converged" Collisional Data for Atoms and Ions Berrington (Queen's University of Belfast)
11:30 - 12:00	Atomic Data Generation at Lebedev Physical Institute and other Research Centres Presnykov (Lebedev Institute)
12:00 - 12:30	Stark Broadening Data for Fusion, Laboratory and Astrophysical Plasmas. Present Status and Perspectives. Dimitrijević (Astronomical Observatory, Belgrade)
12:30 - 14:00	**Lunch**
Session 2.	(Cont'd.)
14:00 - 14:30	Priorities in A+M Data Compilation and Evaluation (Janev)
Session 3.	Data Processing and Exchange
Chairman:	Delcroix
14:30 - 16:00	- ALADDIN Implementation and Developments; Possibilities for Technical Improvements: Comments from all Data Centres (all participants) - Mirror Sites for AMDIS/ALADDIN
16:00 - 16:30	**Coffee break**
16:30 - 17:00	Plan of DCN Activities for the Near Future (coordination: Janev)
Session 4:	Meeting Conclusions and Recommendations
Chairman:	Stephens
17:00 - 17:30	Formulation of Meeting Conclusions and Recommendations
17:30 -	**Adjourn of the Meeting**

Appendix 3

Data Centres Report of Activities

Activities of the Atomic Spectroscopy Data Centers at the National Institute of Standards and Technology (NIST) 1995-1997

W. L. Wiese

Data Center	Director	Staff
Atomic Energy Levels and Wavelengths	W. C. Martin	J. Sugar (retired, contractor), A. Musgrove
Atomic Transition Probabilities	W. L. Wiese	D. E. Kelleher J. R. Fuhr
Spectral Line Shapes and Shifts	W. L. Wiese	No permanent workforce; Occasional contractors, guest scientists

Compilations of Numerical Data*

	Recent Work	In Progress
Wavelengths	Ar, Ga, Kr V-XXXVI, Be I	Si I, Be II, F I, He I, Cl
Energy Levels	Zn, Ga, Ar, Be I	Si I, Cl, Be II, F I, He I
Transition Probabilities	All spectra of C, N O	H, D, He, Li, Be, B, F, Ne, Na, Mg, Al, Si

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

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

1. Annotated Bibliographic databases:

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

2. Numerical databases:

   An interactive searchable database with wavelengths, energy levels and transition probabilities for a limited number of chemical elements and spectra is currently available (version 1.1). A much more comprehensive tabulation, covering such spectroscopic data for all light elements up to Ni (Z = 28) and also including wavelength material on the heavier elements (Z = 99), is in the final testing stage, with a planned release date of Fall 1997.

   Also, two user-friendly databases have been developed for PC users with DOS operating

Also, two user-friendly databases have been developed for PC users with DOS operating systems:

1. NIST Spectroscopic Properties of Atoms and Atomic Ions, J. W. Gallagher, Standards Reference Database 38

2. NIST Database for Atomic Spectroscopy, D. E. Kelleher, Standard Reference Database 31

NIST Spectroscopic data publications 1995-1997:

1. "Energy Levels of Zinc, Zn I through Zn XXX," J. Phys. Chem. Ref. Data **24** 1803 (1995).

2. "Spectral Data for Highly Ionized Krypton, Kr V through Kr XXXVI," J. Phys. Chem. Ref. Data **24**, 1577 (1995.

3. "Wavelengths and Energy Level Classifications for the Spectra of Gallium (Ga I through Ga XXXI)," J. Phys. Chem. Ref. Data, submitted (1997).

4. "Spectral Data for Highly Ionized Atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo," J. Phys. Chem. Ref. Data Monograph **8** (1997).

5. "Atomic Transition Probabilities for Carbon, Nitrogen and Oxygen, A Critical Data Compilation," J. Phys. Chem. Ref. Data Monograph **7** (in press 1996).

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

7. "Wavelengths and Energy Level Classifications for the Spectra of Argon (Ar I through Ar XVIII)," J. Phys. Chem. Ref. Data, submitted (1997).

Progress Report on AM Data Activities at NIFS (1995-1997)

H. Tawara (1997.7.21-22)

This spring, NIFS has finished the relocation of the Institute to Toki city, 30 km north of Nagoya, the former location for 30 years.

The address of our new site is
National Institute for Fusion Science
Toki 509-52, Japan
H. Tawara :
fax (81)-52-789-4200 till the end of March, 1998
(81)-572-58-2628
e-mail : tawara@nifs.ac.jp

Due to this, we have to change the whole system of our data handling.

I) Topics of activities

1) Diagnostics for high temperature plasmas

(a) Electron transfer data at high energies in He^{2+} + He collisions :

We have calculated and analyzed the (*nl*) distributions of the electron-transferred states in

$He^{2+} + He \rightarrow He^{+}(nl) + He^{+}$.

which are relevant to diagnostics of the burning plasmas. In particular, those calculated with CDW-EIS for *nl*=4s, 4p, 4d and 4f have been found to reproduce the observed results by Folkerts et al. (1994) reasonably well down to 20 keV/amu.

More systematical calculations for the (*nl*) distributions in this process have also been performed over a wide range of the collision energy (20 keV/amu-500 keV/amu) and the results are going to be published soon in NIFS-Data report (under the collaboration of R.Rivarola, Rosario, Argentina).

2) Processes related with divertor plasmas

(a) Collisions involving low-energy heavy neutral particles :

These, relevant to the divertor design physics, are being pursued theoretically based on the quantum mechanical calculation. The main topics covers the collisions :

$He + H_2(v_i) \rightarrow He + H_2(v_f)$

$\rightarrow He + H + H$

with various initial vibrational excitation v_i.

We plan to publish our survey of the data for such low-energy heavy particle collisions involving hydrogens and heliums (with the collaboration of K.Onda, Tokyo Univ. Sci. and T.Shirai, JAERI) soon.

(b) Electron-ion collisions :

Systematic calculations of the dielectronic recombination processes for relatively low-charged ions such as C II-C IV and Be-like ions, which are relevant to the gas divertors, have been performed (under the collaboration of U.Safronova, Moscow).

(c) The evaluation of electron impact data :

The evaluation work involving various atoms and molecules under electron impact is in progress. The data of total scattering, elastic as well as inelastic (excitation, ionization dissociation) scattering are being included (under the collaboration of M.Hayashi, GEI, Nagoya).

3) Surface interactions in divertors
(a) Some important issues in low energy molecule-surface collisions have been reviewed with the emphasis on the mechanisms of formation of hydrogen molecules. One of the important findings is the fact that we can control the formation or fraction of the vibrationally excited hydrogen molecules by choosing the surface materials or their temperatures, depending on whether they really play an important role in the gas divertors. This result is going to be published soon in Comm. At. Mol. Opt. Phys. (under the collaboration of K.Snowdon, Newcastle).

II) Data management
Our whole computer system has been changed to UNIX system and, thus, we are going to reconstruct our databases using the relational database (DB) managing system (dbshino) on the new computer.
Now our data retrieval system can be accessible through WWW on
http://dbshino.nifs.ac.jp/
The users are required to have their ID which can be obtained by asking
dbmaster@dbshino.nifs.ac.jp
Some reconstructions have been finished and it is now possible to look at our demonstration on
http://amdata.nifs.ac.jp/amdata/
This reconstruction work is still under way. The whole DB system is expected to become accessible this fall.
We are also constructing our mirror-site of ORNL DB under the new computer system which will be opened soon.

For more detailed information on DB, please ask the followings :
takako@dpkato.nifs.ac.jp
murakami@dpkato.nifs.ac.jp

III) International collaboration
1) On the occasion of International Conference of Physics of Highly Charged Ions, Ohmiya, Japan, we have organized a small "International Symposium on Atomic and Molecular Processes in Fusion Plasmas" at NIFS over September 17-19, 1996. About 60 scientists including atomic and molecular physicists as well as plasma physicists had joined this symposium to discuss the present situations of atomic and molecular data for fusion and their applications. The summaries of the invited talks and posters have been published in NIFS-DATA-39.

2) We had some visitors under our collaboration programs :
Prof. R. Rivarola, Rosario, Argentina
Prof. J. Dubau, Observatoire, Meudon, France

IV) Activity reports
Our activities in the past years are summarized in the following NIFS-DATA series reports published (1995-1997):

NIFS-DATA-30 T. Nishikawa, T. Kawachi, K. Nishihara and T. Fujimoto, *Recommended Atomic Data for Collisional-Radiative Model of Li-like Ions and Gain Calculation for Li-like Al Ions in the Recombining Plasma;* Sep. 1995

NIFS-DATA-31 Y. Yamamura, K. Sakaoka and H. Tawara, *Computer Simulation and Data Compilation of Sputtering Yield by Hydrogen Isotopes ($^1H^+$, $^2D^+$, $^3T^+$) and Helium ($^4He^+$) Ion Impact from Monatomic Solids at Normal Incidence;* Oct. 1995

NIFS-DATA-32 T. Kato, U. Safronova and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CII from CIII; Feb. 1996

NIFS-DATA-33 K.J. Snowdon and H. Tawara,
Low Energy Molecule-Surface Interaction Processes of Relevance to Next-Generation Fusion Devices; Mar. 1996

NIFS-DATA-34 T. Ono, T. Kawamura, K. Ishii and Y. Yamamura,
Sputtering Yield Formula for B_4C Irradiated with Monoenergetic Ions at Normal Incidence; Apr. 1996

NIFS-DATA-35 I. Murakami, T. Kato and J. Dubau,
UV and X-Ray Spectral Lines of Be-Like Fe Ion for Plasma Diagnostics; Apr. 1996

NIFS-DATA-36 K. Moribayashi and T. Kato,
Dielectronic Recombination of Be-like Fe Ion; Apr. 1996

NIFS-DATA-37 U. Safronova, T. Kato and M. Ohira,
Dielectronic Recombination Rate Coefficients to the Excited States of CIII from CIV; July 1996

NIFS-DATA-38 T. Fujimoto, H. Sahara, G. Csanak and S. Grabbe,
Atomic States and Collisional Relaxation in Plasma Polarization Spectroscopy: Axially Symmetric Case; Oct. 1996

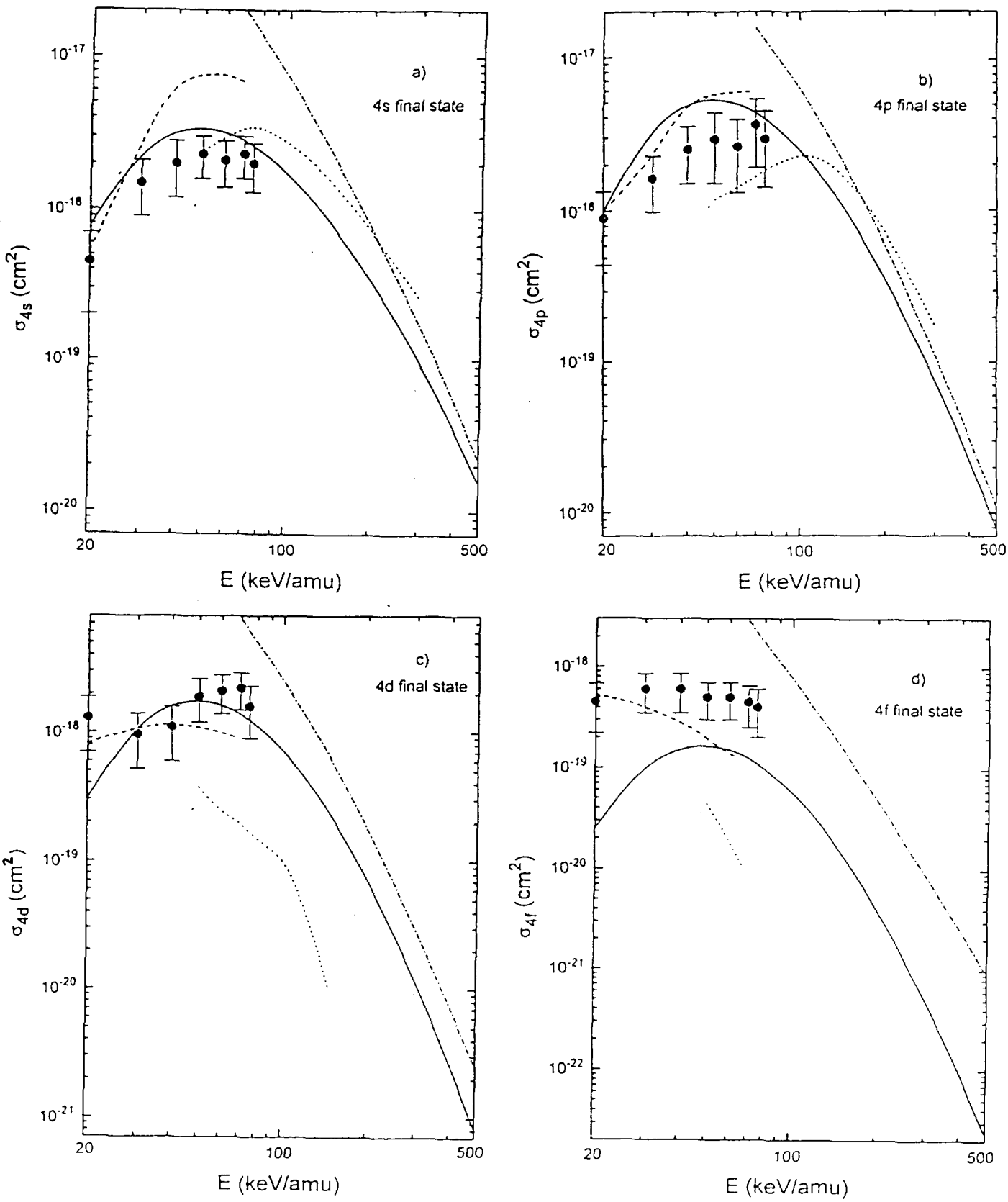
NIFS-DATA-39 H. Tawara (Ed.)
Present Status on Atomic and Molecular Data Relevant to Fusion Plasma Diagnostics and Modeling; Jan. 1997

NIFS-DATA-40 Inga Yu. Tolstikhina,
LS-Averaged I/Z Method as a Tool of Studying the Interactions of Highly Charged Ions with a Metal Surface; Jan. 1997

NIFS-DATA-41 K. Moribayashi and T. Kato,
Atomic Nuclear Charge Scaling for Dielectronic Recombination to Be-like Ions; Apr. 1997

NIFS-DATA-42 H. Tawara,
Bibliography on Electron Transfer Processes in Ion-ion / Atom / Molecule Collisions -Updated 1997 -; May 1997

He^{2+} + He -> $He^{+}(nl)$ + He^{+}



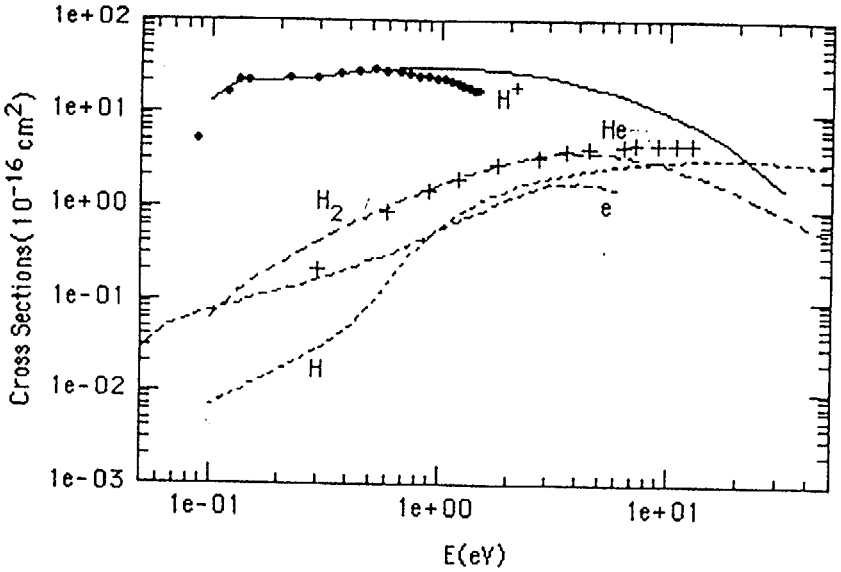


Figure 1. Rotational Excitation of H_2(J=0->2)

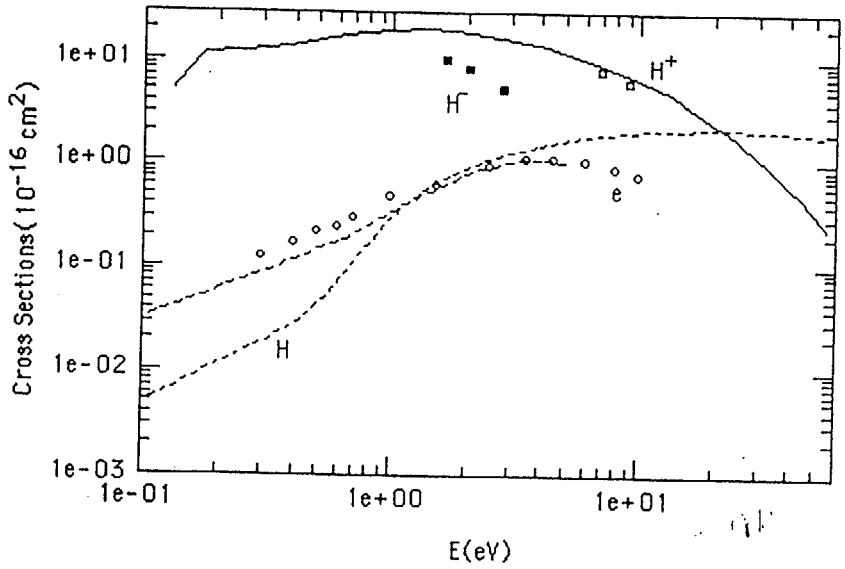


Figure 2. Rotational Excitation of H_2(J=1->3)

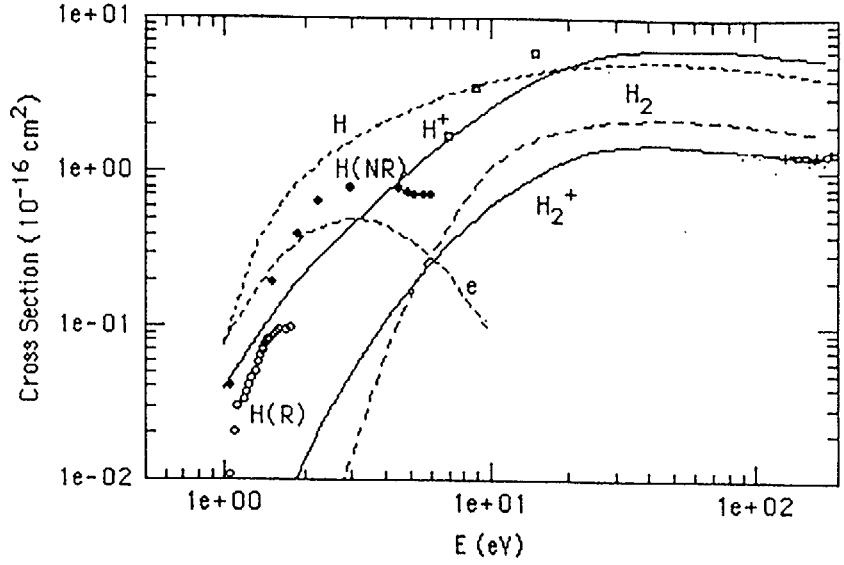


Figure 3. Vibrational Excitation of H_2 (v = 0->1)

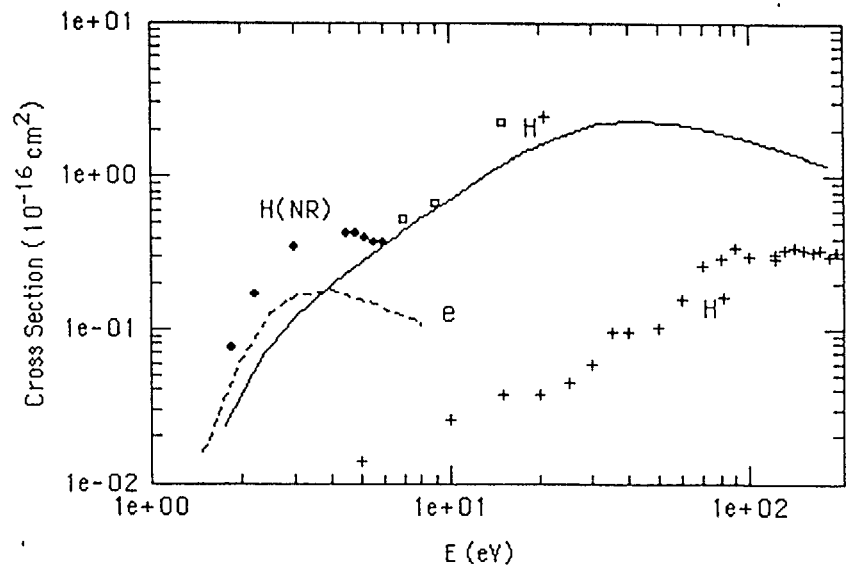
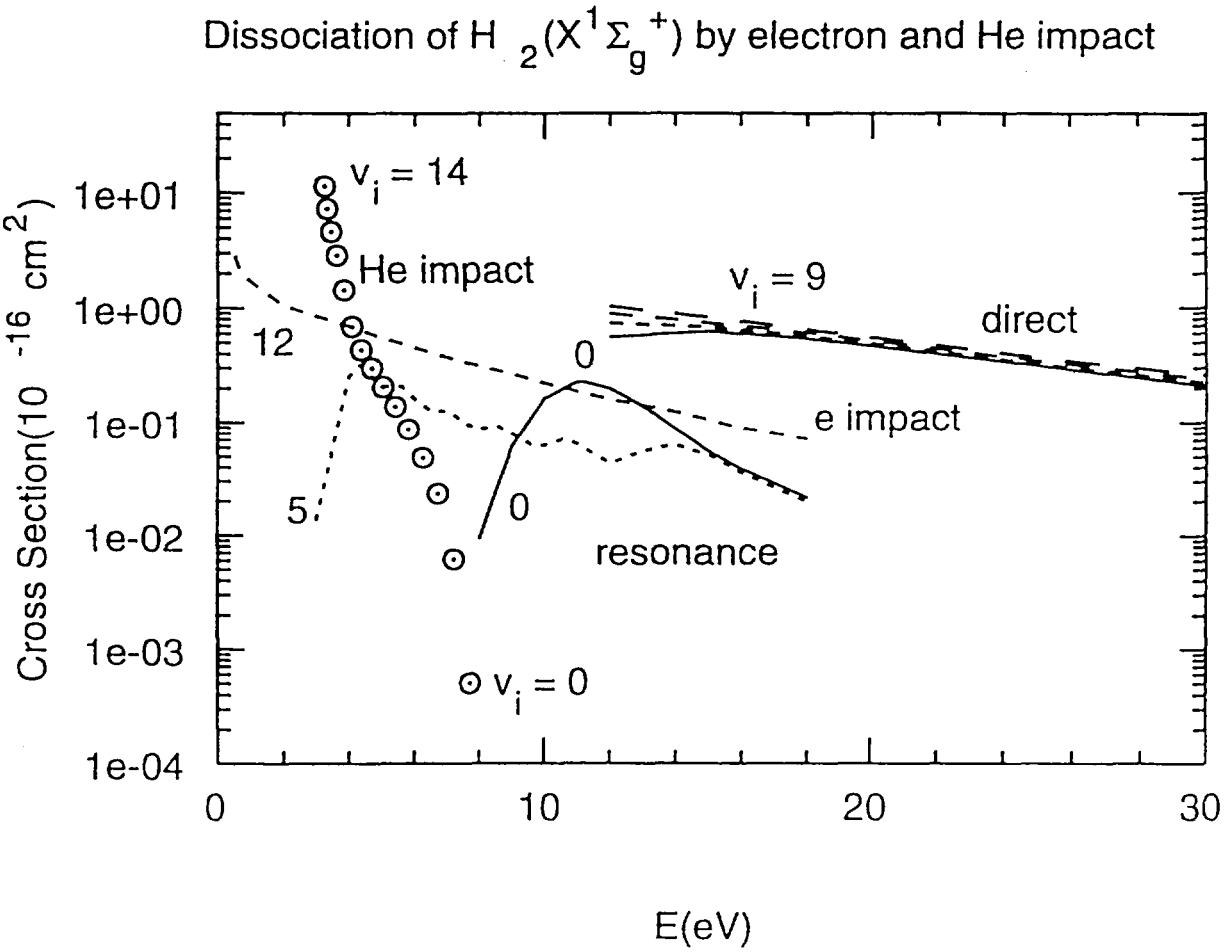


Figure 4. Vibrational Excitation of H_2 (v=0->2)


Dissociation of H 2(X1Σg+) by electron and He impact
Cross Section(10 -16 cm2)
1e+01
1e+00
1e-01
1e-02
1e-03
1e-04
0
10
20
30
E(eV)
vi = 14
He impact
vi = 9
direct
12
0
e impact
5
0
resonance
vi = 0

The ORNL Controlled Fusion Atomic Data Center

Progress Report: 1997

Staff

David Schultz, Predrag Krstić, Edmund Mansky, Phillip Stancil, Weihong Liu, David Jeffery, Fay Ownby

ORNL Consultants

Fred Meyer, Charlie Havener, Mark Bannister

External Consultants

Brian Gilbody, Earl McDaniel, Ed Thomas, Tom Morgan, Mitch Pindzola

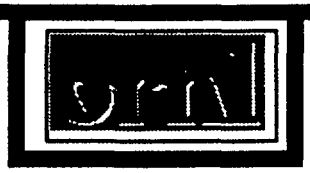
Summary

- World Wide Web used to leverage limited manpower as interface to external users
  - ⋆ ALADDIN, Bibliography, Redbooks
- US site of the JET/Strathclyde Atomic Data and Analysis Structure (ADAS)
- Plans/work underway on a unified data interface – ALADDIN, Bibliography, Redbooks, JILA database, ADAS, ORNL Multicharged Ions Research Facility data, potential collaborations with NIFS
- Propose expanded role for CFADC within atomic physics application community (e.g. astrophysics)
- Various atomic data production projects carried out, e.g.
  - ⋆ Elastic scattering database for edge and divertor modeling'
  - ⋆ Charge transfer and ionization in slow collisions, $H + H$, $H^+ + He$, $C^+ + H$
  - ⋆ Inelastic processes in collisions of Be, Ne, Ar ions with H, H_2, and He over a wide range of energies

The Controlled Fusion Atomic Data Center

More information regarding the hyperlinks below

ALADDIN	BIBLIOGRAPHY	REDBOOKS	MIRF	ASTROPHYSICS
LINKS	TAMOC	ADNDT	E-PRINTS	PHYSICS DIVISION



The mission of the Controlled Fusion Atomic Data Center (CFADC) is to compile, evaluate, recommend, and disseminate atomic and molecular collision data relevant to fusion energy research and development. The CFADC is supported through the U.S. Department of Energy, Office of Fusion Energy Sciences, and is part of the Oak Ridge National Laboratory's Physics Division.

This World Wide Web site is intended to serve as an electronic interface between the Data Center's resources and the fusion energy community. Access to these databases and other tools will be an ongoing development. through the links below.

Further infomation on the history, funding and staff of the CFADC is available.

Last Modified: *January 14, 1997.*

ALADDIN

ALADDIN is a database management system accepted by the International Atomic Energy Agency for the exchange of atomic and molecular data of interest in fusion energy research and development.

- Introduction: More information about who wrote ALADDIN and what it is

---

- Files: The data files that are available in ALADDIN format

- Programs: The data ALADDIN codes and dictionary files

- Run ALADDIN: Interactive search of ALADDIN data files

Last Modified : Thursday July 6, 1995.

Return to CFADC Home Page

ALADDIN programs and dictionary files

The ALADDIN program is a sequence of FORTRAN programs including the main search program and evaluation functions. The recommended data has been fit to certain functional forms which require these evaluation functions. In addition, dictionary files are required by some of the files listed below. All files can be accessed on-line at the IAEA. To reach them telnet to *ripcrs01.iaea.or.at* and use the username *aladdin* . You can also download them directly through your browser from this site. For example, if you are using NCSA Mosaic, single click on the file number below and your browser will view the appropriate *.txt* file. You can then pull down on the *File* widget of the browser and use *Save as* to download the file to your local host.

Basic ALADDIN programs

- 1. The main ALADDIN code (23935 bytes).
- 2. The ALADDIN common block sub-code (3071 bytes).
- 3. The ALADDIN Standard Interface Subroutine Package ALPACK (2223 bytes).
- 4. The ALADDIN Fitted Form Subroutine Library ALFLIB (18229 bytes).
- 5. The ALADDIN common block for ALPACK (21095 bytes).

ALADDIN evaluation functions

- 3. The basic set of ALADDIN evaluation functions (30822 bytes).

ALADDIN dictionary files

- 4. The general ALADDIN dictionary file (3003 bytes).
- 5. Data dictionary of hierarchycal labels for atomic and molecular collisions (9594 bytes).
- 6. Dictionary of evaluation functions and references (35377 bytes).

Last Modified: October 24, 1995.

ALADDIN data files

The list of recommended databases is given below. Those marked by an asterisk (*) are in ALADDIN format and can be accessed on-line at the IAEA. Connect to the IAEA via telnet to:

```
telnet:  ripcrs01.iaea.or.at
account name:   aladdin
```

You can also download them directly through your browser from this site. For example, if you are using NCSA Mosaic, single click on the file number below and your browser will view the appropriate *.txt* file. You can then pull down on the *File* widget of the browser and use *Save as* to download the file to your local host.

A+M Collisional Databases

● 1.* "Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions" K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, F. J. Smith. J. Phys. Chem. Ref. Data 12, 891 (1983). *[This file contains databases 1 and 5]*

● 2.* "Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions" Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M. S. Pindzola, D. H. Crandall. At. Data Nucl. Data Tables (ADNDT) 33, 149 (1985).

● 3.* "Recommended Data on Atomic Collision Processes Involving Iron and Its Ions" C. Bottcher, D. C. Griffin, H. T. Hunter, R. K. Janev, A. E. Kingston, M. A. Lennon, R. A. Phaneuf, M. S. Pindzola, S. M. Younger. Nucl. Fusion, Special Supplement (1987).

● 4.* "Collisions of Carbon and Oxygen Ions with Electrons, H, H2 and He." Atomic Data for Controlled Fusion Research, Vol. V. R. A. Phaneuf, R. K. Janev, M. S. Pindzola (Editors). Report ORNL-6090/V5, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831 USA (1987).

● 5.* "Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions: Fluorine to Nickel." M. A. Lennon, K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, M. J. Murray, F. J. Smith. J. Phys. Chem. Ref. Data 17, 1285 (1988). *[This file contains databases 1 and 5]*

● 6.* "Recommended Data for Excitation Rate Coefficients of Helium Atoms and Helium-like Ions by Electron Impact." T. Kato and S. Nakazaki. At. Data Nucl. Data Tables (ADNDT) 42, 313 (1989).

● 7.* "Elementary Processes in Hydrogen-Helium Plasmas" R. K. Janev, W. D. Langer, K. Evans, Jr., D. E. Post, Jr., Springer-Verlag (1987).

● 8.* "Collisions of H, H2, He and Li Atoms and Ions with Atoms and Molecules." Vol. 1. C. F. Barnett (Editor). Report ORNL-6086/VI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA (1990).

● 9.* "Atomic and Molecular Data for Fusion, Part III. Recommended Cross Sections and Rates for Electron Ionization of Atoms and Ions: Copper to Uranium." M. J. Higgins, M. A. Lennon, J. G. Hughes, K. L. Bell, H. B. Gilbody, A. E. Kingston, F. J. Smith. Culham Report, CLM-R294, Abingdon, Oxfordshire, U.K. (1989).

● 10. "Collisional Processes of Hydrocarbons in Hydrogen Plasmas." A. B. Ehrhardt, W. D. Langer. Report PPL-2477, Plasma Physics Laboratory, Princeton University, Princeton, New Jersey, USA (1988).

● 11.* "Recommended Cross Sections for Collision Processes of Hydrogen Ground-State and Excited Atoms with Electrons, Protons and Multiply Charged Atoms." R. K. Janev, J. J. Smith. Atomic and Plasma-Material Data for Fusion, a supplement to the journal Nuclear Fusion, Vol.4 (1993).

● 12. Volume 3 of the Atomic and Plasma-Material Interaction Data for Fusion, a supplement of the journal Nuclear Fusion (1992), contains several articles with recommended data for different atomic collision processes of helium atoms and of beryllium and boron atoms and ions.

Particle-Surface Interaction Databases

● 1. "Energy Dependence of Ion-Induced Sputtering Yields of Monatomic Solids in the Low Energy Region." N. Matsunami, Y. Yamamura, N. Itoh, H. Tawara, T. Kawamura. Report IPPJ-AM-52, Institute of Plasma Physics (National Institute for Fusion Science), Nagoya, Japan (1987).

● 2. "Energy Dependence of the Yields of Ion-Induced Sputtering of Monatomic Solids." N. Maksunami, Y. Yamaura, Y. Itikawa, N. Itoh, Y. Kazumata, S. Miyagawer, K. Morita, R. Strimizu, H. Tawara. Report IPPJ-AM-32, Institute of Plasma Physics (National Institute for Fusion Science), Nagoya, Japan (1988).

● 3.* "Particle Reflection from Surfaces - A Recommended Data Base." E. W. Thomas, R. K. Janev and J. J. Smith. Report IAEA INDC(NDS)-249, July 1991.

● 4.* "Sputtering Data." W. Eckstein, C. Garcia-Rosales, J. Roth and W. Ottenberger. Max-Plank-Institute fur Plasmaphysik Report IPP9/82 (1993).

● 5.* "An Evaluated Database for Sputtering." E. W. Thomas, R. K. Janev, J. Botero, J. J. Smith and Y. Qiu. Report IAEA INDC(NDS)-287 (1993).

Last Modified : Tuesday July 18, 1995.

Return to Aladdin Home Page

```
$ ION e H  [+0] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-7  #BELI
  13.6  0.185  -0.019   0.123  -0.190   0.953

$ ION e He [+0] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-5  #BELI
  24.6  0.572  -0.344  -0.523   3.445  -6.821   5.578
$ ION e He [+1] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-10  #BELI
  54.4  0.185   0.089   0.131   0.388  -1.091   1.354

$ ION e Li [+0] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-10  #BELI
   5.4  0.085  -0.004   0.757  -0.178
$ ION e Li [+1] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-12  #BELI
  75.6  0.722  -0.149  -1.301   1.944
$ ION e Li [+2] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-10  #BELI
 122.4  0.400

$ ION e Be [+0] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
   9.3  0.924  -0.770   0.362
$ ION e Be [+1] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
  18.2  0.269   0.389  -1.836   3.939  -2.275 0.0
   92.82   18.2  0.753  -0.582   0.643  -0.966
$ ION e Be [+2] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
 153.9  0.796  -0.500   0.884
$ ION e Be [+3] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
 217.7  0.400

$ ION e B  [+0] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
   8.3  1.106  -1.069  -0.088
$ ION e B  [+1] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
  25.1  0.907  -0.477   0.197
$ ION e B  [+2] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
  37.9  0.393  -0.082  -0.303   0.263
$ ION e B  [+3] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
 259.4  0.796  -0.500   0.884
$ ION e B  [+4] (G)
& XS REC ACC-B BELFAST DOC-JPCRD-88-17/3 ERROR-%-20  #BELI
 340.2  0.400

$ ION e C  [+0] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-5  #BELI
  11.3  2.114  -1.965  -0.608
$ ION e C  [+1] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-10  #BELI
  24.4  1.082  -0.161  -0.856   0.906
$ ION e C  [+2] (G)
& XS REC ACC-A BELFAST DOC-JPCRD-88-17/3 ERROR-%-10  #BELI
  47.9  0.715  -0.041   0.175
$ ION e C  [+2] (*)
```

The CFADC Bibliography

Through a network of expert consultants the CFADC maintains a catagorized bibliography of atomic and molecular collision references relevant to fusion energy research and development. Since the data center's inception in 1958, over 100 journals have been regularly searched and over 60,000 individual entries have been accumulated. Presently, the bibliography may be queried on-line regarding the entries since 1978 (approximately 26,000). The archival entries dating from *c.*1950 to 1977 will be added in the near future.

- Categories: The major categories and subcategories used in the bibliography

---

- Search-category: Initiate a search of the CFADC Bibliographic Database by reaction category

---

- Search-author: Initiate a search of the CFADC Bibliographic Database by author

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- Journals: The journals which have been searched over the last decade

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Return to CFADC Home Page

Last Modified: August 30, 1995.

CFADC Bibliographic Search

Instructions

Enter CFADC Catagory: A06 Example: A06 , E03 , H07

Enter Reactant #1: He Example: He , e , h

Enter Charge of Reactant #1: 1 Example: 2 , -1 , 0

Enter Reactant #2: H_2 Example: H , Be , H_2

Enter Charge of Reactant #2: 0 Example: 0 , 1 , 4

Year Range (limits 78-96) 78 to 96

Begin Search Clear Search

Return to Master Search Page

Last Modified : July 1, 1996.

The Results of Your Search Are:

RECORD NUMBER: 74
EXPERIMENT OR THEORY: E-
ENERGY RANGE: 1.5-3.0 keV
REACTANTS: A03: He^+ + H_2
A06: He^+ + H_2
JOURNAL: Phys. Rev. A
REFERENCE: 17, 1296 (1978)
AUTHOR(S): Eriksen, F. J.
Jaecks, D. H.
TITLE: He(3^3P) excitation in 1.5- and 3.0-keV He^+ + H_2 collisions.

RECORD NUMBER: 900
EXPERIMENT OR THEORY: T-
ENERGY RANGE: 0.005-0.28 eV
REACTANTS: A04: He^+ + H_2
A06: He^+ + H_2
JOURNAL: J. Chem. Phys.
REFERENCE: 68, 13 (1978)
AUTHOR(S): Preston, R. K.
Thompson, D. L.
McLaughlin, D. R.
TITLE: A theoretical prediction of vibrational enhancement for dissociative ch
arge transfer in the HeH_2^+ system.

RECORD NUMBER: 3308
EXPERIMENT OR THEORY: E
ENERGY RANGE: 25-90 keV
REACTANTS: A03: He^+ + H_2
A03: He^+ + Na
A06: He^+ + H_2
A06: He^+ + Na
JOURNAL: Phys. Rev. Lett.
REFERENCE: 42, 440 (1979)
AUTHOR(S): Horsdal Pedersen, E.
TITLE: Metastable-atom population of fast, neutral helium beams.

RECORD NUMBER: 4717
EXPERIMENT OR THEORY: T-
ENERGY RANGE: 1-4 eV
REACTANTS: A02: He^+ + H_2
A06: He^+ + H_2
JOURNAL: Chem. Phys. Lett.
REFERENCE: 67, 491 (1979)
AUTHOR(S): Schneider, F.
Zulicke, L.
TITLE: Approximate diatomics-in-molecules potential energy surfaces and non-ad
iabatic coupling for He^+ + H_2.

CFADC Bibliographic Search – Author Search

Instructions

Enter Author Last Name: Dunn

Examples: Smith von Hellman DeLeone

Enter Author First Initial: d

Examples: M Dz YY *

Enter Author Second Initial: *

Examples: M Dz YY *
(Any third initial is ignored)

Year Range (limits 78-96) 78 to 96

Begin Search Clear Search

Return to Master Search Page

Last Modified : July 1, 1996.

The Results of Your Search Are:

RECORD NUMBER: 76
EXPERIMENT OR THEORY: E-
ENERGY RANGE: 0.065-2.0 eV
REACTANTS: E06: e + NH_4^+
JOURNAL: Phys. Rev. A
REFERENCE: 17, 1314 (1978)
AUTHOR(S): DuBois, R. D.
Jeffries, J. B.
Dunn, G. H.
TITLE: Dissociative recombination cross sections for NH_4^+ ions and electrons

---

RECORD NUMBER: 1759
EXPERIMENT OR THEORY: E-
ENERGY RANGE: 61-162 eV
REACTANTS: E03: e + Li^+
JOURNAL: Phys. Rev. A
REFERENCE: 18, 1353 (1978)
AUTHOR(S): Rogers, W. T.
Olsen, J. O.
Dunn, G. H.
TITLE: Absolute emission cross section for electron-impact excitation of Li^+
to the (2 ^3P) level.

RECORD NUMBER: 3879
EXPERIMENT OR THEORY: E-
ENERGY RANGE: 4-50 eV
REACTANTS: E03: e + N^4^+
JOURNAL: Phys. Rev. A
REFERENCE: 20, 410 (1979)
AUTHOR(S): Gregory, D. C.
Dunn, G. H.
Phaneuf, R. A.
Crandall, D. H.
TITLE: Absolute cross sections for 2s-2p excitation of N^4^+ by electron impac
t.

RECORD NUMBER: 6100
EXPERIMENT OR THEORY: E-
ENERGY RANGE: 500 eV
REACTANTS: E03: e + He
JOURNAL: Proc. XI ICPEAC, Kyoto,
REFERENCE: p.174, North-Holland (1979).
AUTHOR(S): van Zyl, B.
Dunn, G. H.
Heddle, D.W.O.
Chamberlain, G. E.
TITLE: Benchmark cross sections for electron impact excitation of n^1S levels

Atomic Data for Fusion. Volume 1: Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules (C. F. Barnett ed.), ORNL-6086 (1990).

Last Modified: April 25, 1997

Return to CFADC Home Page

Atomic Data for Fusion. Volume 1: Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules (C. F. Barnett ed.), ORNL-6086 (1990).

A. Electron Capture Collisions

Electron Capture by Neutral H

Electron Capture by H^+

Electron Capture Cross Sections for
$H + H_2 \rightarrow H^-$

Energy (eV/amu)	Velocity (cm/s)	Cross Section (cm^2)
4.0E+01	8.79E+06	1.05E-18
7.0E+01	1.16E+07	1.78E-18
1.0E+02	1.39E+07	2.52E-18
1.4E+02	1.64E+07	3.08E-18
2.0E+02	1.96E+07	2.74E-18
4.0E+02	2.78E+07	1.70E-18
7.0E+02	3.68E+07	1.24E-18
1.0E+03	4.39E+07	1.31E-18
2 0E+03	6.21E+07	5.28E-18
4 0E+03	8.79E+07	1.46E-17
7 0E+03	1.16E+08	2.18E-17
1 0E+04	1.39E+08	2.32E-17
2 0E+04	1.96E+08	1 91E-17
4 0E+04	2.78E+08	9 93E-18
7 0E+04	3.68E+08	4 07E-18
1 0E+05	4.39E+08	1 68E-18
2 0E+05	6.21E+08	1.72E-19
4 0E+05	8.78E+08	6.12E-21
4 6E+05	9.42E+08	2.97E-21

References: 26, 27, 28, 29, 30, 31, 32, 33, 35, 396

Accuracy: 25%

Note: The quoted results are believed to be accurate to within 25%, although the data presented in some of the references may deviate by 50-60%.

For a Chebyshev fit of the above cross sections it is necessary to use the following parameters.
E_{min} = 4.0E+01 eV/amu, E_{max} = 4.6E+05 eV/amu

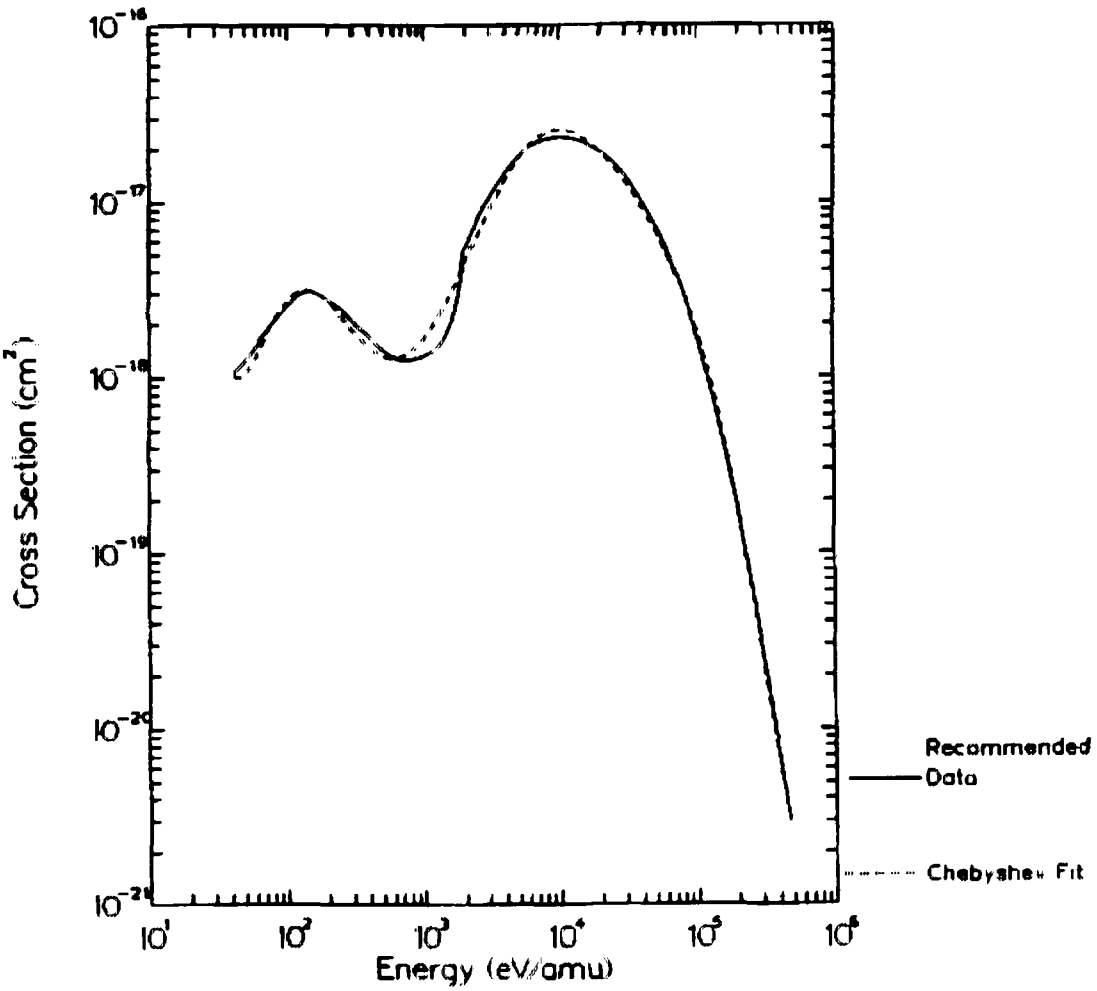
Chebyshev Fitting Parameters for Cross Sections

A0	A1	A2	A3	A4	A5	A6	A7	A8
-81.8133	-1.65457	-2.60606	-1.53878	-.368649	.0135120	-.165702	-.127116	.256041

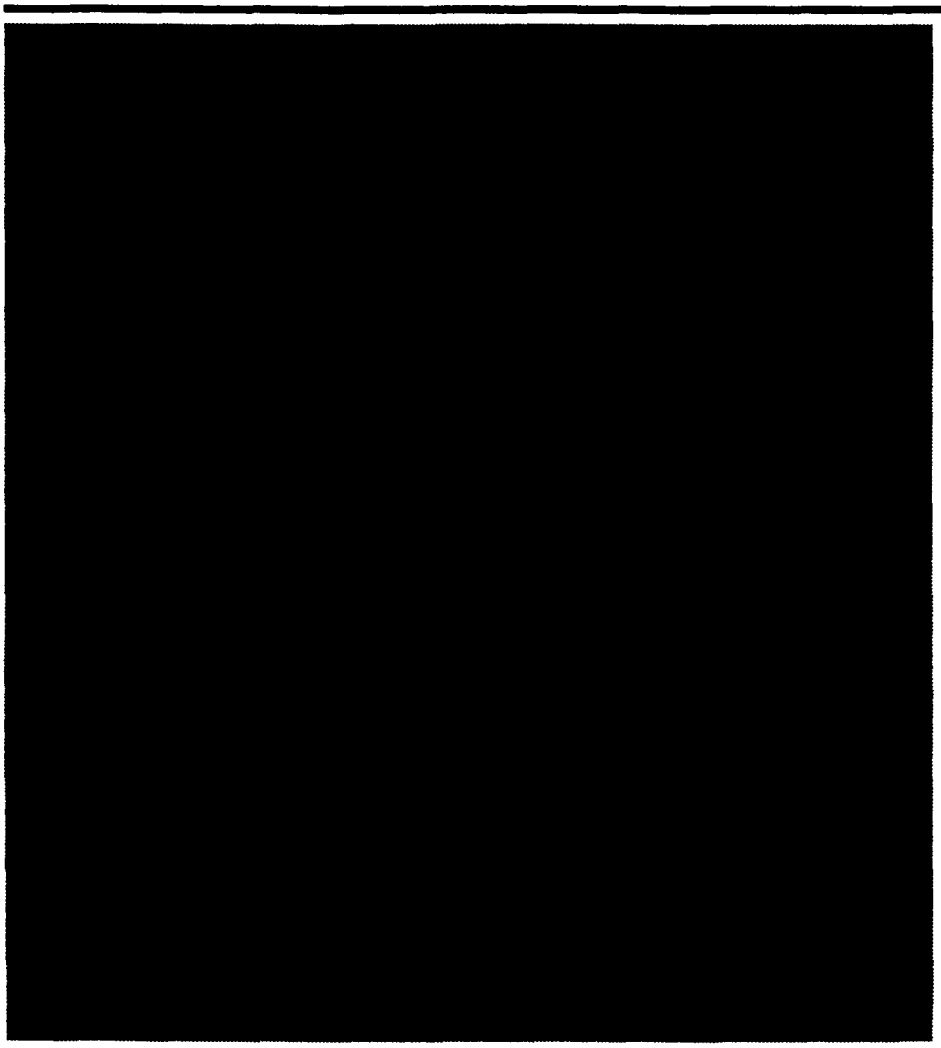
The fit represents the above cross sections with an rms deviation of 9.5%.
The maximum deviation is 26.2% at 1.0E+03 eV/amu.
See appendix for Chebyshev fit details.

$$H + H_2 \rightarrow H^-$$

Cross Section vs. Energy



Welcome to ORNL Multicharged Ion Research Facility (MIRF)



CFADC | ECR SOURCE | ION ION EXP | USER PORT
ELECTRON-ION CROSSED BEAM EXP | ION-ATOM MERGED BEAM EXP
ELECTRON-ION MERGED EXP | ION SURFACE EXP | FEEDBACK

Last modified by Frank Yan on *December 4, 1996*

Question, Comments, and Feedback

Electron–Impact Ionization of Multicharged Ions at ORNL

Presented here are experimental ionization cross sections measured using the Electron–Ion Crossed Beams apparatus in the Physics Division at Oak Ridge National Laboratory (ORNL). The data are given in both graphical and tabular form along with the reference to the original publication of the experimental results. Also presented in the figures are theoretical cross sections supporting the experiments. For details of the theoretical work, please refer to the original publication given for the particular experiment. These World–Wide Web pages are based primarily on three technical memorandums issued by ORNL.

- D. H. Crandall, R. A. Phaneuf, and D. C. Gregory, *Electron Impact Ionization of Multicharged Ions*, ORNL/TM–7828, Oak Ridge National Laboratory, 1979.
- D. C. Gregory, D. H. Crandall, R. A. Phaneuf, A. M. Howald, G. H. Dunn, R. A. Falk, D. W. Mueller, and T. J. Morgan, *Electron Impact Ionization of Multicharged Ions at ORNL 1980–1984*, ORNL/TM-9501, Oak Ridge National Laboratory, 1985.
- D. C. Gregory and M. E. Bannister, *Electron–Impact Ionization of Multicharged Ions at ORNL 1985–1992*, ORNL/TM–12729, Oak Ridge National Laboratory, 1992.

Also presented are more recent (1993–present) data, both published and unpublished.

These pages are optimized for the Netscape Navigator. Other browsers may not be able to display all the pages as designed. If your browser does not support tables, a list of cross sections is available as an alternative.

METHOD **Experimental Method**

INDEX **Cross Section Index**

HTML 3.0 table for linking to cross sections of interest. If your browswer does not support tables, there is also a list of cross sections.

PUBS **List of Publications**

MIRF **Multicharged Ion Research Facility (MIRF) Home Page**

CFADC **Controlled Fusion Atomic Data Center (CFADC) Home Page**

This research was supported by the Division of Applied Plasma Physics, Office of Fusion Energy Sciences of the U.S. Department of Energy under Contract No. DE–AC05–96OR22464 with Lockheed Martin Energy Research Corp.

Electron–Impact Ionization of Multicharged Ions at ORNL
Table of Cross Sections

Note: If your browser does not support tables, this page may be unusable. Please try the list of cross sections instead.

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INTRO

MIRF

CFADC

Single Ionization

Element	Initial Charge State						
5 B	2+	3+					
6 C	2+	3+	4+				
7 N	2+	3+	4+	5+			
8 O	2+	3+	4+	5+			
9 F	2+						
10 Ne	2+	3+	4+	5+	6+		
13 Al	2+						
14 Si	1+	2+	3+	4+	5+	6+	7+
16 S				4+			
17 Cl	2+			4+	5+		
18 Ar	2+	3+	4+	5+	6+	7+	8+
	2						

Electron-Impact Single Ionization of B^{2+}

INDEX
INTRO
MIRF
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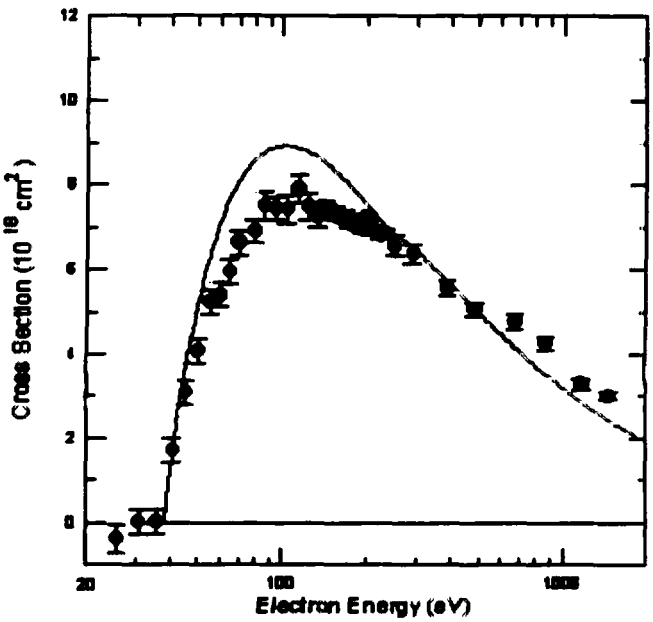
FIG. 1
FIG. 2
TABLE



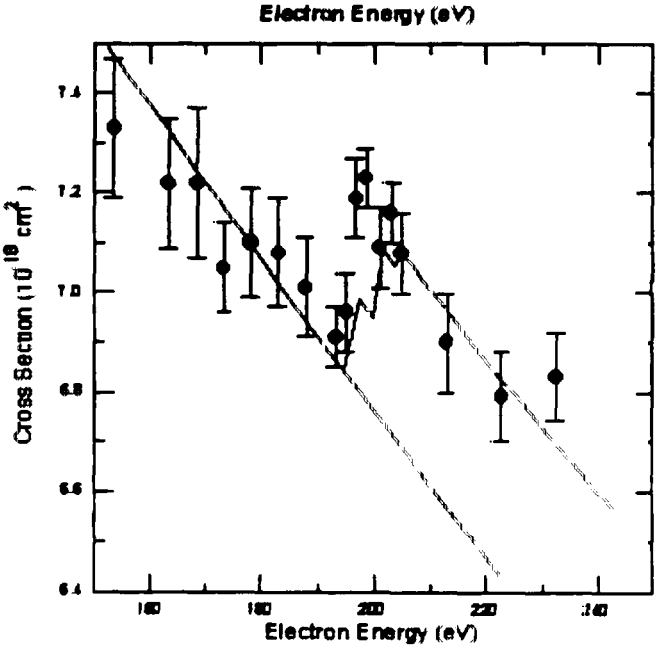
Legend:
Circles – ORNL data
Solid line (red) – Scaled Coulomb-Born direct (ground state)
Dashed line (green) – Lotz formula (ground state)

Reference D H Crandall *et al*, Phys Rev A 34, 1757 (1986)

Absolute uncertainty 8% typical near peak of cross section

Estimated metastable fraction of target ions <1%

Please click here for a tabular listing of the experimental data



Legend:
Circles – ORNL data
Lower solid line (red) – 0.90 x DW direct (ground state)
Upper solid line (purple) – 0.90 x DW direct + EA (ground state)

Please click here for a tabular listing of the experimental data

Ion-Atom Merged-Beams Experiment (Electron-Capture)

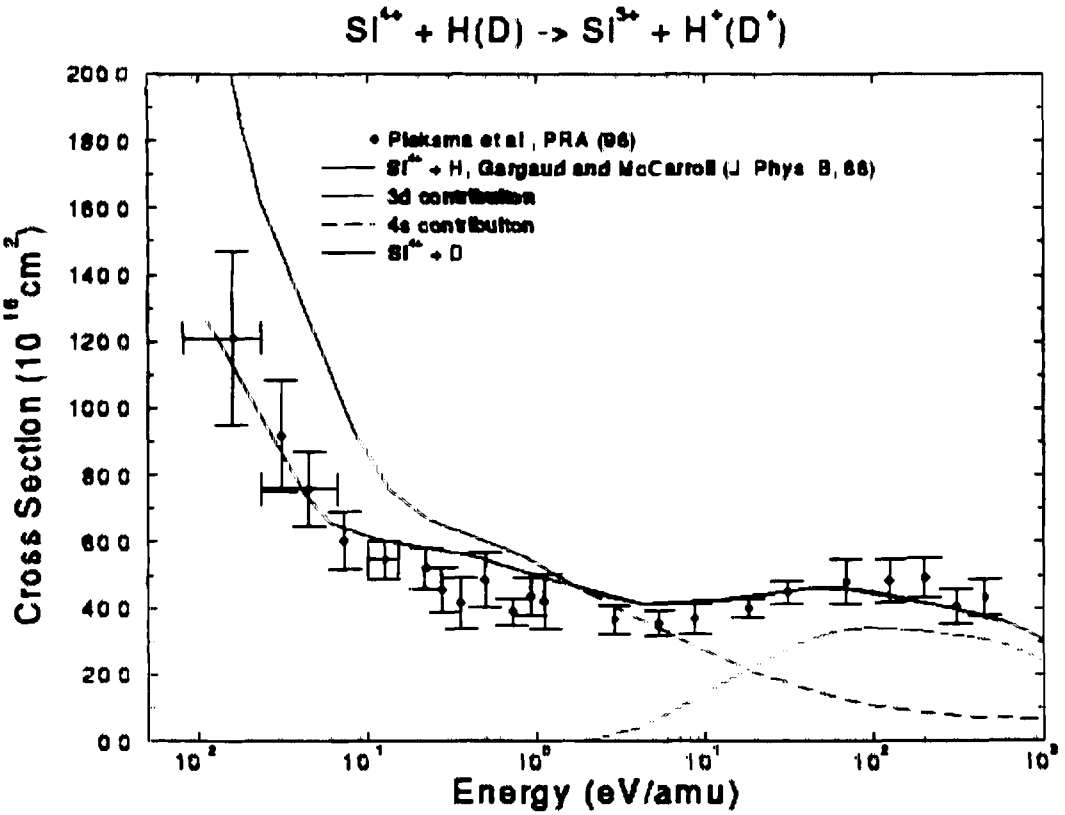
The ORNL ion-atom merged-beams apparatus has been successful in performing benchmark electron capture cross section measurements for the multicharged ions (C^{3+}, C^{4+}, N^{2+}, N^{3+}, N^{4+}, N^{5+}, O^{3+}, O^{4+}, O^{5+}, and Si^{4+}) on H(and D) from 20 meV/amu to 5000 eV/amu, over five orders of magnitude in collision energy (see publication list) In this energy range the relative nuclear motion between collision partners is slow compared to the orbital motion of active electrons in the system. Electrons of the quasimolecule formed in the collision have sufficient time to adjust to the changing interatomic field as the nuclei appraoach and separate. Simple scaling laws which exist at higher collision energies (v ~ 1 a.u.) do not exist at eV/amu energies. Fully quantal coupled- channel molecular-orbital calcualtions are considered most accurate at these energies but are difficult to perform and have only recently been tested in detail.

Merged-beams measurements have provided critical comparison with theory and experiment. A brief summary is given here. Select a collision system of interest from the Index. A brief abstract will be presented after which the data can be viewed in either graph or table format. The graph contains comparsion with other experiment or theory when available.

Apparatus	Publications	Index	MIRF	CFADC

Ion-Atom Merged-Beams Experiment (Electron-Capture)

Index



Abstract | Table | Index | IonAtom | MIRF

Last modified by Charles Havener on *April 23, 1997*

Progress Report on A+M data activities at the NDC/JAERI
July 1995 - June 1997

Toshizo Shirai
Nuclear Data Center (NDC), Japan Atomic Energy Research Institute (JAERI)
Tokai-mura, Ibaraki 319-11, Japan

Compilation and evaluation work has been continued to make the 4th edition of Evaluated Atomic and Molecular Data Library (JEAMDL-4) for fusion in collaboration with the JAERI Research Committee on Atomic and Molecular Data and with researchers of ORNL and NIST under the US-Japan fusion cooperation program. The production of JEAMDL-5 for divertor plasma was undertaken at the beginning of this fiscal year.

Data Activities and Work in Progress

Analytical least-squares fits to the recommended cross sections were made for dissociation and particle interchange in collisions of H, H_2, He, Li atoms and ions with atoms and molecules [1]. All these data sets are stored in the ALADDIN format as a part of JEAMDL. Similar analytical fits were made to the recommended cross sections for collision processes between electrons and hydrocarbon molecules, such as CH_4 and so forth, that occur as impurities in divertor plasma [2]. Further application is now in progress for collision processes between electron and H_2O, CO and CO_2 relevant to edge plasma impurities.

In relation to the injection of energetic neutral beams into moderate and high density plasmas, cross sections were calculated for excitation and ionization of excited helium atoms in collisions with bare ions in the Glauber and CDW-EIS approximations, respectively, besides the Born approximation [3].

For the molecular processes relevant to gas dynamic divertor, some theoretical or experimental studies have been undertaken, which are summarized below.

A theoretical study has been made on ion-molecule reactions in the H_3^+ ($D^+ + H_2$, $D^+ + D_2$, and $H^+ + D_2$) system in the collision energy range of 2.5 to 8.0eV with the trajectory-surface-hopping method on *ab initio* three-dimensional potential energy surfaces [4, 5]. The results agree well with experiments for the production of atomic and molecular ions. For the D_2^+ ion formation above 5 eV, the present calculation overestimated its cross section, but the deviation from the experiments was within a factor of two. We will extend the calculations to the collision processes involving H_2 molecules in ro-vibrational excited states.

Cross sections for state-selective electron-capture by Be^{2+} and Be^{3+} ions in collisions with

He atoms were calculated at low collision energies below 9 keV/u by using the molecular-orbital expansion method modified by inclusion of the electron translation effect [6]. The results show that the Be^{2+} formation becomes more probable, while the Be^{+} formation becomes less probable, as the collision energy decreases.

Theoretical data production has also been carried out for the cross sections for ro-vibrational excitation, dissociative recombination, and dissociative excitation in collisions between electron and H_2^+ (and isotopic variants) within a framework of multi-channel quantum defect theory. For the dissociative recombination of HD^+, the result agrees well with a recent experiment.

Cross sections were measured for electron capture by C^{q+}(q=1-4) ions from H_2, CH_4, C_2H_6, C_3H_8, and CO_2 molecules in the energy range of (1-20)q keV [7]. The measurement is now in progress for Be and Cr ions in collisions with rare gases and carbon-containing molecules.

We also undertook publication of a series of compilations of spectral data for highly ionized atoms: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Kr, and Mo, of special importance for fusion research. All these data will be presented as a monograph [8]. Further data compilation has been made of wavelengths, energy levels, ionization energies, line classifications, intensities and transition probabilities for argon in all stages of ionization.

References

[1] R. Ito, T. Tabata, T. Shirai, and R. A. Phaneuf, JEAERI-Data/Code 96-024.

[2] T. Tabata, T. Shirai, and H. Tawara, ADNDT, to be submitted.

[3] A. Igarashi and T. Shirai, Phys. Scr. T**62**, 95 (1996).

[4] A. Ichihara and K. Yokoyama, J. Chem. Phys. **103**, 2109 (1996).

[5] A. Ichihara, T. Shirai, and K. Yokoyama, J. Chem. Phys. **105**, 1857 (1996).

[6] S. Suzuki, N. Shimakura, T. Shirai, and M. Kimura, XX ICPEAC (Vienna, 1997).

[7] A. Itoh, N. Imanishi, F. Fukuzawa, N. Hamamoto, S. Hanawa, T. Tanaka, T. Ohdaira, M. Saito, Y. Haruyama, and T. Shirai, J. Phys. Soc. Jpn 64, 3255 (1995).

[8] T. Shirai, J. Sugar, and W. L. Wiese, JPCRD Monograph No. 8 (1997) in press.

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[8] T. Shirai, J. Sugar, and W. L. Wiese, JPCRD Monograph No. 8 (1997) in press.

GAPHYOR DATA CENTER 1996-1997
http://gaphyor.lpgp.u-psud.fr

Status Report and Projects

presented at the 14th Atomic and Molecular Data Centers Network Meeting IAEA, Vienna, 21-23 July 1997, Rapport GA-279

J.L. Delcroix, D. Humbert, C. Leprince
Centre de Données GAPHYOR, Laboratoire de Physique des Gaz et des Plasmas, Université Paris-Sud Orsay
e-mail 1 : gaphyor@lpgp.u-psud.fr – e-mail 2 : delcroix@supelec.fr

GAPHYOR (GAz-PHYsics-ORsay) Data Center produces a Database on the properties of atoms, molecules and neutral or ionized gases ; as of June 15th 1997 the GAPHYOR file included about 495 000 entries. GAPHYOR includes now more than 18 000 Numerical Data , completing its traditional bibliographical and factual information.

On-line dissemination through Internet (WWW) has developed rapidly, with a total of 4 807 distinct visitors including 834 effective users, during the last fifteen monthes.

The paper publications are :
- GAPHYOR UPDATE : the last entries (last issue published in January 1997)
- GAPHYOR HANDBOOK : a selection of best entries (last issue published in July 1997)

The future developments include :
- some improvements in our request program (years, authors, journals, ...),
- a better service on-line by increase of our computer power,
- a better coverage of the litterature by association of new experts,
- an increase in volume and quality of Numerical Data,
- an evaluation of possible improvements in our paper publication policy,
- attempts to improve our cooperation with other Data Centers,

Le Centre de Données GAPHYOR (GAz-PHYsique-ORsay) produit une Banque de Données sur les propriétés des atomes, des molécules et des gaz neutres ou ionisés ; au 15 Juin 1997 le fichier GAPHYOR comprenait environ 495 000 enregistrements, avec maintenant plus de 18 000 données numériques, complètant les traditionnelles informations bibliographiques et factuelles.

Le service de consultation en ligne sur Internet (WWW) s'est rapidement développé avec un total de 4 807 visiteurs distincts, incluant 834 utilisateurs effectifs, durant les quinze derniers mois.

Les publications sur papier sont les suivantes :
- *GAPHYOR UPDATE : entrées récentes (dernière parution Janvier 1997)*
- *GAPHYOR HANDBOOK : une sélection des meilleures données (dernière parution Juillet 1997).*

Nos projets de développement portent sur :
- *quelques améliorations de notre programme d'interrogation (année, auteur, journal, ...)*
- *un meilleur service en ligne par augmentation de nos moyens informatiques,*
- *une meilleure couverture de la littérature par association de nouveaux experts,*
- *une augmentation en volume et qualité de nos Données Numériques,*
- *une amélioration éventuelle de notre politique en matière de publications papier,*
- *un développement de notre coopération avec les autres Centres de Données,*

July 18, 1997

Contents

1 Some Statistics

As of 15th of June 1997, the total number of entries in the files was about 495 000 distributed as shown in Table 1. This means that 40 000 new entries (including 18 000 Numerical Data) have been collected during the last two years.

Sections	Structures	Photon coll.	Electron coll.	At./mol. coll.	Macro. prop.	Σ
Factual Data	267 178	26 941	29 743	124 753	32 006	480 621
Numerical Data	6 642	347	1 650	9 010	734	18 383
Σ	272 730	27 244	30 810	132 107	32 642	495 533

Table 1: Statistics of Data (June 15th, 1997)

2 Collection of new Data

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

M. Aubès, A. Ricard *Université Paul Sabatier, Toulouse*
J. P. Booth *Université de Grenoble*
M. Costes, J. Masanet *Université Bordeaux 1*
A.M. Diamy, C. Lalo *Université Pierre et Marie Curie, Paris*
J.L. Delcroix, C. Hellner *Université Paris-Sud*
V. Hrachova, R.Hrach *Karlova Univ., Praha, République Tchèque*
P. Veis *Comenius Univ., Bratislava, Slovaquie*

The origin of Data is shown in Table 2 below.

Rank	Code	Title	References	Entries
1	JCP	J. Chem. Phys.	19343	84882
2	JPC	J. Phys. Chem.	5039	38806
3	PR/A	Phys. Rev. A	7941	31774
4	JRD	J.Phys.Ch.Ref.Data	296	28821
5	JMSC+JMSR	J. Molec. Stuctures	2411	21069
6	CHPL	Chem. Phys. Lett.	6316	20709
7	ADND	Atom. data and nuclear data tables	288	18198
8	JP/B	J. Phys. B	6037	17847
9	IJMS	Int. J. Mass spec. ion. phys.	1184	10798
10	JACS	J. of the Am.Chem.Soc.	1081	10185
11	EACC+EACI	Conf.Phys.elec.atom.Coll.	3151	9871
12	JMSP	J. Molec. Spectroscopy	4649	8733
13	ZP/D	Z. Phys. D	1175	8346
14	NIFD+IPPJ	Nagoya Reports	95	7181
15	CHPH	Chem. Phys.	1966	6919
16	ZFKH	Zh. Fiz Khim.	773	6122
17	MOL	Molecular Phys.	2009	6015
18	NBSS	NBS Special Pub.	63	5476
19	OASK+OAS	Opt. i Spektr.	1723	5264
20	IJQC	Int.J.Quantum Chem.	950	4746
	Σ		66490	351762
	...	...	...	...
	ΣΣ		96242	495533

Table 2: Origin of Data

3 Structure of Data

The structure of Data has suffered only minor changes, with respect to the description given in our 1995 report at our last meeting. Let us mention here only the most significant modifications :

3.1 Chemical elements

We have introduced the following notations to describe the transuranian elements :

9E Np **Pu** *Am* **Cm** Bk Cf *Es* Fm Mv
9F No Lr Rf(104) Db(105) *Sg*(106) Bh(107) Hs(108) Mt(109) Ll(110)

3.2 Numerical Data

The numerical Data are registered in three fields :

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

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

4 Paper publications

The HANDBOOK and the UPDATE philosophies have been described in detail in the Progress Report presented at the 13th meeting of our Data Center Network. Let us summarize them quickly.

4.1 Handbook

The HANDBOOK presents a selection taken from the whole GAPHYOR Database. The selection criteria depend on quality and actuality of data. More precisely the selection is made as follows :

- **Assigning a value index** (cf. Annex 1) to every GAPHYOR record. Note that the indexes are chosen so as to *include in the Hanbook all the Numerical Data.*
- **Multiplets.** A catalog of the "multiplets" included in the Base is then produced. A multiplet is the set of entries describing the same process : same values of elements, reactants, processes.
- **Separation in two volumes.** Volume 1 includes Standard Data, i.e. those related to atoms and small molecules. Volume 2 covers Special Data related to some fields extending the general scope of GAPHYOR :
  1. Multicharged ions

2. Iso-electronic series
3. Clusters
4. Gas-Surface interactions

- **Selection.**
  - For every multiplet one selects the entry having the highest value index. One registers moreover the multiplicity MULT i.e. the number of entries in the multiplet.
  - To decrease the global volume of the selection one eliminates all the entries whose value index is smaller than a given minimum value. The minimum value in Handbook 97 has been fixed at 52 in Volume 1 and 43 in Volume 2.

Finally, Table 3 shows some statistics linking together the Handbook 97 and the whole Database. The average multiplicity is about 2.2 in Volume 1 and 1.6 in Volume 2. For Sections 3 and 4, describing Collisions and Reactions, the Handbook covers only 17% (in Volume 1) and 60% (in Volume 2) of the topics (multiplets) included in the Base. The coverage in Sections 1 (structures), 2 (photonic collisions) and 5 (macroscopic processes) are much smaller, especially in Volume 1. This was a deliberate choice in this 1997 Handbook.

Sections	1	2	3	4	5	Σ
BASE (Vol 1)						
Entries	231 779	24 661	23 009	110 053	26 722	416 224
Multiplets	83 644	13 736	8 266	68 163	12 421	186 230
Multiplicity	2.8	1.8	2.8	1.6	2.2	2.2
HANDBOOK (Vol 1)						
Numerical Multiplets	3 605	265	714	5 708	568	10 860
Selected multiplets (IV≥52)	3 600	1 201	1 473	10 955	568	17 797
Selection (IV≥52)	4%	9%	18%	16%	5%	10%
BASE (Vol 2)						
Entries	39955	2522	7727	21534	5848	77586
Multiplets	20018	2179	4529	16958	5562	49246
Multiplicity	2.0	1.2	1.7	1.3	1.1	1.6
HANDBOOK (Vol 2)						
Numerical Multiplets	1817	28	322	1461	64	3692
Selected multiplets (IV≥43)	1914	541	2937	9285	90	14767
Selection (IV≥43)	10%	25%	65%	55%	2%	30%

Table 3: Statistics of entries and multiplets.

Remark. Note that the selection presented in the Handbook is rather restricted. To get more information, the on-line connection on the Web *(http://gaphyor.lpgp.u-psud.fr)* should be used.

4.2 Update

GAPHYOR UPDATE is now published once a year : It includes the new entries registered during the last year. The last published issue is UPDATE 96 (published in January 1997). This includes about 25 000 entries.

5 Internet server

On-line dissemination through Internet (WWW) has developed rapidly, during the last fifteen monthes. Let us then describe quickly some pages of our server.

5.1 Home Page

The text version of GAPHYOR Home page is shown below, with the various links underlined (external links in italics).

Centre de Données GAPHYOR

A Database for Atoms, Molecules, Gases and Plasmas
Produced by a Group of Research Centers led by *LPGP*, Université Paris-Sud, France.

to French Version

Overview Database Handbook and Update Fees Help Home Contacts

GAPHYOR 3.0 is on line : interrogation on 2 reactants
Last news from the Data Center
GAPHYOR Handbook GAPHYOR Update
Thanks to our sponsors *CEA* *EDF* *Air Liquide*

To be informed of changes on this server, leave here your name and e-mail address.
For more information or any suggestion, please contact : Denis Humbert

LPGP University Lab. *Univ. Paris-Sud* associate to *CNRS* and *Supelec*

5.2 Query Form

The text version of GAPHYOR Query Form is shown below, with links underlined and Search Criteria printed in bold face.

Overview Database Handbook and Update Fees Help Home Contacts
to Old Version

Search Reset

Reactant 1	Formula	Ioniz.	Excit.1	Excit.2	Excit.3	Type	State
Reactant 2	Formula	Ioniz.	Excit.1	Excit.2	Excit.3	Type	State
	Section	Process	Process				

Additionnal Information

Data type	Nature	Energy	Special data
Numerical Data	New Data		

Number of chemical elements involved in the reaction : n = 1 to 4
Selection of 1 to 4 chemical elements Aa Bb Cc Dd

Note that there are two kinds of descriptors :

- Some must be typed by the user :

"Formula"	Examples : Ar1, H2O1 (possibly in lower case)
"Ioniz."	Examples : 0, +, 13+, -
"Process"	Examples : en, ex, in (cf. full list and codes in Annex 2 or process link)
"Elements Aa, Bb, Cc, Dd"	Examples H, He, Ar

- For all other descriptors the user has just to choose in a pull-down menu ∇, multi-choice box ◯ or checked box □, with the following values (explained in an on-line help) :

"Excit.1"	∇	0, *, v, *v, all
"Excit.2"	∇	-, r, p, n, rp, rn, rpn, pn
"Excit.3"	∇	-, y, m, z
"Type"	∇	-, surface, ads.atom, clust.(motif), clust.(core), iso. series
"State"	∇	initial, final
"Section"	∇	structures, hv coll., e coll., at/mol coll., macro.prop.
"Data Type"	◯	-, S, W, K, U, P, <
"Nature"	◯	-, R, E, T, D, X
"Energy"	◯	-, L, J, H
"Special Data"	◯	-, I, /, 8
"Numerical Data"	□	
"New Data"	□	
"Number of chemical elements"	∇	1, 2, 3, 4

Note that all these descriptors are optional.

5.3 Example of Data Search

5.3.1 Intermediate Report

Having reqested for instance new numerical Data about e, H (H, H+, H-) collisions, one gets the following intermediate form as a first report of the search :

You submitted the following request to GAPHYOR :
Reactant 1 (initial state) : H1 all/
Reaction : section=3, numerical values, new data

Reactant 1
◯ 10 data found for H
◯ 2 data found for H -
Sub-total of 12 data

help Now, you can get data
◯ from the whole set of the above data
◯ only from the selected reactant
◯ on screen, sorted by year, the whole set of reactants.
◯ on screen, sorted by year, the nn (pill-down menu) more recent data.

5.3.2 Data output

Zhou S (US MI DW), Li H , Kauooila W E , Kwan C K , Stein T S
Phys. Rev. A, US vol.55 p.361 (1997)

H, e + $\Longrightarrow$ H +, Ps
Ionization (Electronic collisions)
Total cross sections (absolute values)
Thermal energies (E < 10 eV CM system)
Medium energies (10 eV < E < 10 keV CM system)
Experimental data
energies: 6 - 16 - 100 eV
values: 0.2 - 3 - 0.1 E-16 cm2

H, e
Total cross sections (Electronic collisions)
Total cross sections (absolute values)
Thermal energies (E < 10 eV CM system)
Medium energies (10 eV < E < 10 keV CM system)
Experimental data
energies: 1.7 - 300.7 eV
values: 16.83(.17) - 0.89(.06) E-16 cm2

H, e +
Total cross sections (Electronic collisions)
Total cross sections (absolute values)
Thermal energies (E < 10 eV CM system)
Medium energies (10 eV < E < 10 keV CM system)
Experimental data
energies: 1.5 - 16 - 301 eV
values: 0.36(.27) - 5.01(.21) - 1.01(.32) E-16 cm2

Kuang Y R (CD NF SJ), Gien T T
Phys. Rev. A, US vol.55 p.256 (1997)

H, e + $\Longrightarrow$ H +, Ps
Ionization (Electronic collisions)
Total cross sections (absolute values)
Thermal energies (E < 10 eV CM system)
Theoretical data
energies: 7 - 10 eV
values: 0 - 2.5 $\pi(a_0)^2$

H, e + $\Longrightarrow$ H, e +
Elastic collision (Electronic collisions)
Total cross sections (absolute values)
Thermal energies (E < 10 eV CM system)
Theoretical data
energies: 0.1 - 5 - 10 eV
values: 8.5 - 1 - 1.1 $\pi(a_0)^2$

5.4 Some statistics on Users

5.4.1 Global results

The total number of distinct visitors during the last fifteen monthes has been 4 807. Among them we have counted 834 effective users. By effective user we mean a visitor who has effectively extracted Data from the Database. Those numbers have regularly increased, as can be seen in Table 4 below. The slight decrease during the last trimester is due to connexion problems to our computer. Those seem to be related with the installation of a new, more performant (?) network on the Université Paris-Sud ! We are presently trying to improve this paradoxical situation.

	Users	Sessions	Data sets
96-II	158	208	2027
96-III	188	318	2128
96-IV	222	436	2708
97-I	285	614	3290
97-II	256	331	2739
Σ	1109	1907	12892

Table 4: trimesters

5.4.2 Geographical Repartition

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

na	data sets	org.na	data sets	serv.org.na	data sets
fr	6137	u-psud.fr	1133	iwr.uni-heidelberg.de	853
???	2233	uni-heidelberg.de	825	lsmsil.univ-lille1.fr	570
de	1167	univ-lille1.fr	570	naimn3.cnrs-imn.fr	555
us	799	cnrs-imn.fr	555	onera.onera.fr	337
jp	738	cea.fr	496	lpcr.u-psud.fr	298
ru	548	onera.fr	337	lpgp.u-psud.fr	291
com	485	tvt.fr	280	modem3.tvt.fr	280
uk	348	toshiba.jp	271	fr.airliquide.com	242
se	176	jussieu.fr	251	saclay.cea.fr	237
su	131	airliquide.com	242	lpct.u-bordeaux.fr	223
au	124	u-nancy.fr	229	ps.uci.us	196
net	124	ujf-grenoble.fr	197	mines.u-nancy.fr	178
ch	119	univ-mlv.fr	181	bruyeres.cea.fr	177
nl	116	u-bordeaux.fr	179	lcam.u-psud.fr	164
by	111	ups-tlse.fr	171	alpha.univ-mlv.fr	147
mx	99	sandia.us	165	ca.sandia.us	146
at	97	univ-rennes1.fr	164	120.96.172	138
cz	76	ias.fr	155	ext.jussieu.fr	136
pt	60	slu.se	134	stud.slu.se	134
ca	51	mephi.ru	133	zzzzzz.mephi.ru	133
20 na	13739	20 org.	6668	20 serv.	5435
other na	361	363 other org.	7432	678 other serv.	8665
ΣΣ	14100	ΣΣ	14100	ΣΣ	14100

Table 5: Nations, Organizations, Services using GAPHYOR

6 Payments policy

The text version of our "Fees" page is shown below.

Overview Database Handbook and Update Fees Help Home Contacts

* Why we can't afford to stay totally free
* Fees
* How to pay
* Sponsors

Access to database is presently totally free. Our purpose is to leave this access free, offering thus to R&D people a tool which should be as convenient as possible. But GAPHYOR gets only small support from government agencies. This is a world-wide problem : databases on atomic and molecular physics are not supported by any large national or international program (cf. Harvard Meeting 1996). Data Centers should then be supported by their users.

If you find that GAPHYOR is useful, please support it through one of the following channels :

Annual voluntary subscription
* Research organization, company : 2 000 FF. (TTC)
* Research laboratory : 1 000 FF. (TTC)
* Personal : 200 FF. (TTC)

Partnership contract (Sponsors)
* Annual subscription : 25 000 FF. (TTC)
* Additional services will be offered (expert reports, several samples of our publications, advertising, ...)

Publications purchase
* Handbook 97, Volume 1 : 500 FF. (TTC)
* Handbook 97, Volume 2 : 500 FF. (TTC)
* Update 96 (published in January 1997) : 850 FF. (TTC)
* Update 97 (to be published in 1998) : 850 FF. (TTC)
* Update 95 : 300 FF. (TTC)

Expert report
For special requests, you can get an expert report : we make the query for you in the database.
Please send us your requests by e-mail in free text to gaphyor@lpgp.u-psud.fr.
Cost : 200 + 2n FF. (TTC) where "n" is the number of data obtained.
But first, try our web access.

How to pay
* By cheque to the order of GAPHYOR
* By bank transfer to GAPHYOR :

o bank : 18707-0019
o account : 01919161172

To get an invoice, please place your order :
* by e-mail : gaphyor@lpgp.u-psud.fr.
* by fax : (33) 01 69 15 78 44
* by mail : Centre de Donnes GAPHYOR, Universit Paris-Sud, LPGP, Bt. 210, 91405 Orsay Cedex, France.

Our sponsors *CEA* *EDF* *Air Liquide*

7 Future Developments

7.1 Request Program

Up to now we gave priority in our request program to descriptors related to the physico-chemical process, and there is no possibility to search for bibliograpical items like year, author, journal, ... We consider now to introduce these other fields into our request program. This may produce a too complicated query form and we shall make provisions to avoid it (possibly by having two different query forms : one for ordinary users, the other for "expert" users).

7.2 On-line Service

To improve our on-line service we shall first try to get control of the connexion problems related with the network of Université Paris-Sud. But very soon we shall also change our work-station to a new more performant one. At present time our computer facility includes :

- a Spark 10 station, with 64 Mo of RAM and 2.2 Go hard disk. This contains the Database, but it is also used for programs development and Data processing,
- a MacIntosh Quadra 650 for administrative management, as well as preprocessing of Data before integration into the Database
- connexion facilities to the University network with an out-speed of 100 Mbits/s.

We find now a significant over-load of our station, which accomodate with difficulty 3 to 4 simultaneous connexions. This is evidenced by the increasing number of aborted requests (though Internet is also partly responsible of it). With the increasing number of requests we could have a saturation of our station. Also, with the increasing number of entries, our storing capacity become critical, especially for complex operations like large Data sortings.

In conclusion we have decided to install as soon as possible a new work-station. This will be devoted only to the on-line service. The old station will be used for development and as a mirror station.

7.3 Literature Coverage

Our coverage of the literature is not quite satisfactory, as can be seen in Table 6 below. In this table we give for the main journals both the present stock of GAPHYOR entries and a so-called actualisation ratio A. This last ones is the ratio of the new 95-97 entries to the present stock, multiplied by a factor such that A should be unity when the flow of new entries is "normal". One notes that we are in trouble with some journals. Two new experts joined recently our group to solve these problems (see also paragraph 7.5 below).

7.4 Numerical Data

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

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

7.5 International Cooperation

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

	Code	Title	Entries	A
1	JCP	J. Chem. Phys.	84882	0.7
2	JPC	J. Phys. Chem.	38806	1.2
3	PR/A	Phys. Rev. A	31774	2.4
4	JRD	J.Phys.Ch.Ref.Data	28821	0.3
5	JMSC+JMSR	J. Molec. Stuctures	21069	1.0
6	CHPL	Chem. Phys. Lett.	20709	1.1
7	ADND	Atom. data and nuclear data tables	18198	1.5
8	JP/B	J. Phys. B	17847	0
9	IJMS	Int. J. Mass spec. ion. phys.	10798	0.6
10	JACS	J. of the Am.Chem.Soc.	10185	0
11	EACC+EACI	Conf.Phys.elec.atom.Coll.	9871	0
12	JMSP	J. Molec. Spectroscopy	8733	1.2
13	ZP/D	Z. Phys. D	8346	0
14	NIFD+IPPJ	Nagoya Reports	7181	1.7
15	CHPH	Chem. Phys.	6919	0.1
16	ZFKH	Zh. Fiz Khim.	6122	0.6
17	MOL	Molecular Phys.	6015	1.3
18	NBSS	NBS Special Pub.	5476	0
19	OASK+OAS	Opt. i Spektr.	5264	1.0
20	IJQC	Int.J.Quantum Chem.	4746	2.0

Table 6: Actualisation rates of the first 20 journals

8 Annex 1 : Value indexes

One has seen in Section 4.1 that the Handbook is a selection taken from the whole GAPHYOR Database, and that the selection criteria depend on quality and actuality of data. More precisely the selection is made as follows :

- Assigning a value index to every GAPHYOR record
- Production of a catalog of "multiplets" and selection
- Selection of the best entry in every "multiplet"
- Elimination of entries below a minimum value index
- Separation in two volumes

The basic quantity in this program is then the value index assigned to every entry. Let us now define the rules choosen for it : the value index is the sum of six partial indexes as shown in Tables 7 which take account of the quality of bibliographical (Vjo, Van, Vau), factual (Vse, Vin), and numerical (Vnu) data.

Bibliographical						Factual				Numerical	
An	Van	Journal	Vjo	Authors	Vau	Sect.	Vse	Info	Vin	Data	Vnu
97	45	JCP	92	10 aut.	45	2	50	r	10	Energies	25
96	42	JPC	91	9 aut.	40	3	50	e	10	Values	50
...	...	PR/A	90	...	...	4	50	s k <	5	Remarks	25
87	15	CHPL	89	5 aut.	25	5	20	p u l	5		
86	12	JP/B	88	4 aut.	20	1	0	w	2		
85	9	JACS	87	3 aut.	15						
84	6	JRD	86	2 aut.	10						
83	3	...	...	1 aut.	5						
Max	45		92		45		50		25		100

Table 7: Value indexes for the three categories of Data in an entry

9 Annex 2 : Processes list

Section 1. Structures

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

Section 2. Photonic collisions

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

Section 3. Collisions of electrons

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

Section 4. Atomic and molecular collisions

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

Section 5. Macroscopic properties

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

Some remarks about the heavy particles effects for the ITER divertor and core plasmas

V. A. Abramov

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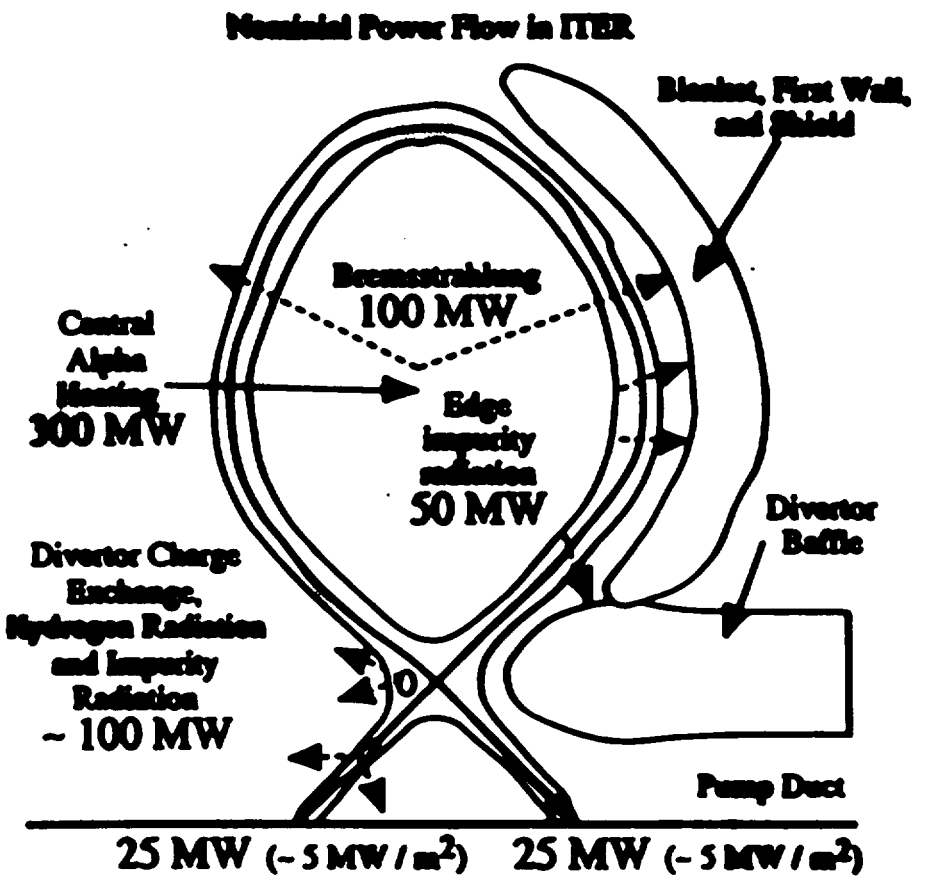
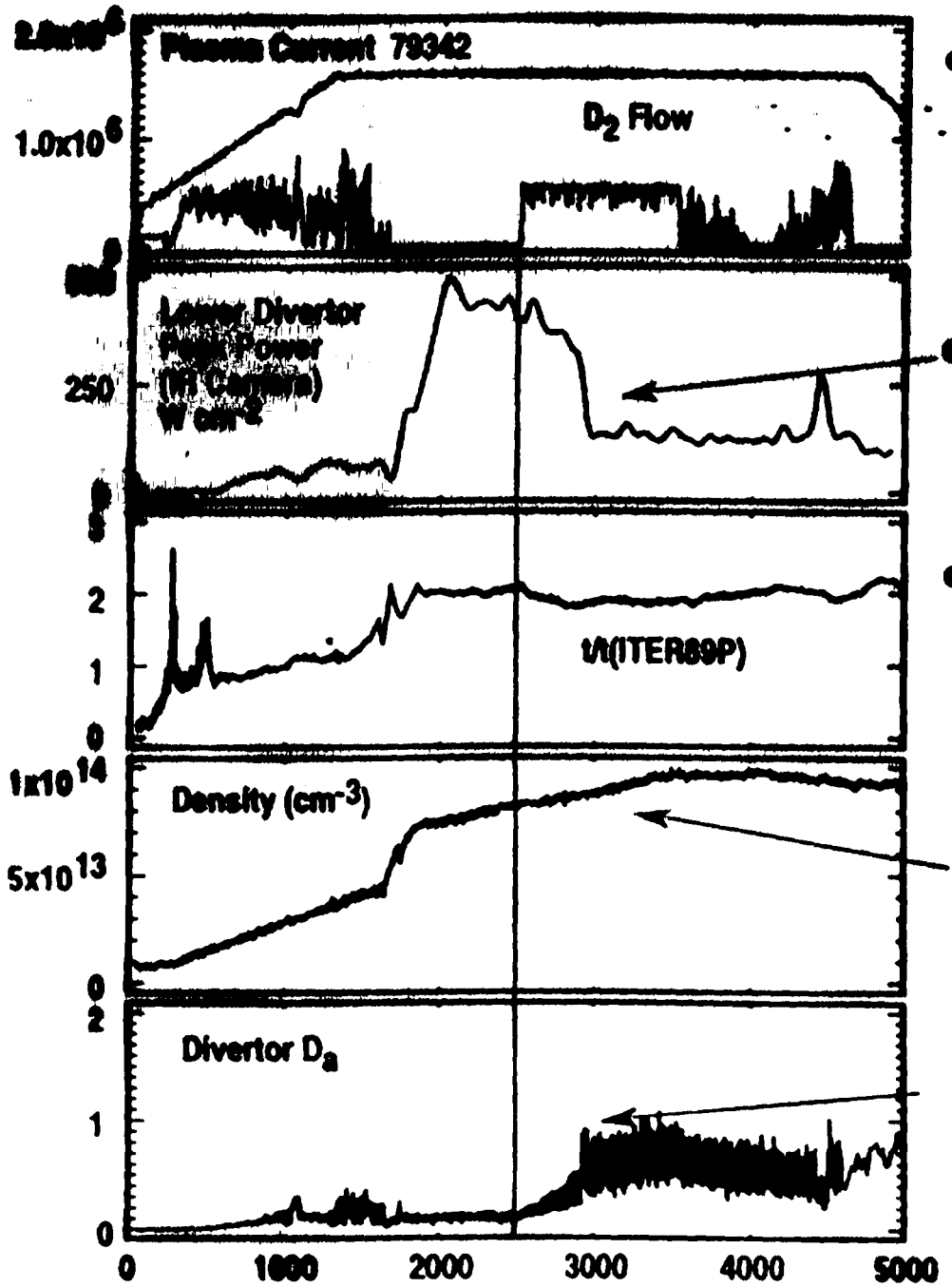
ITER Divertor Concept

- Radiate most of the heating power to the chamber walls before it reaches the divertor plates using intrinsic and injected impurities (e.g. Ne, Ar,..) :

Bremsstrahlung from center	~ 100 MW
Plasma mantle/edge	~ 50 MW
Divertor/SOL	~ 100 MW
Divertor plates	~ 50 MW
Total heating	~ 300 MW



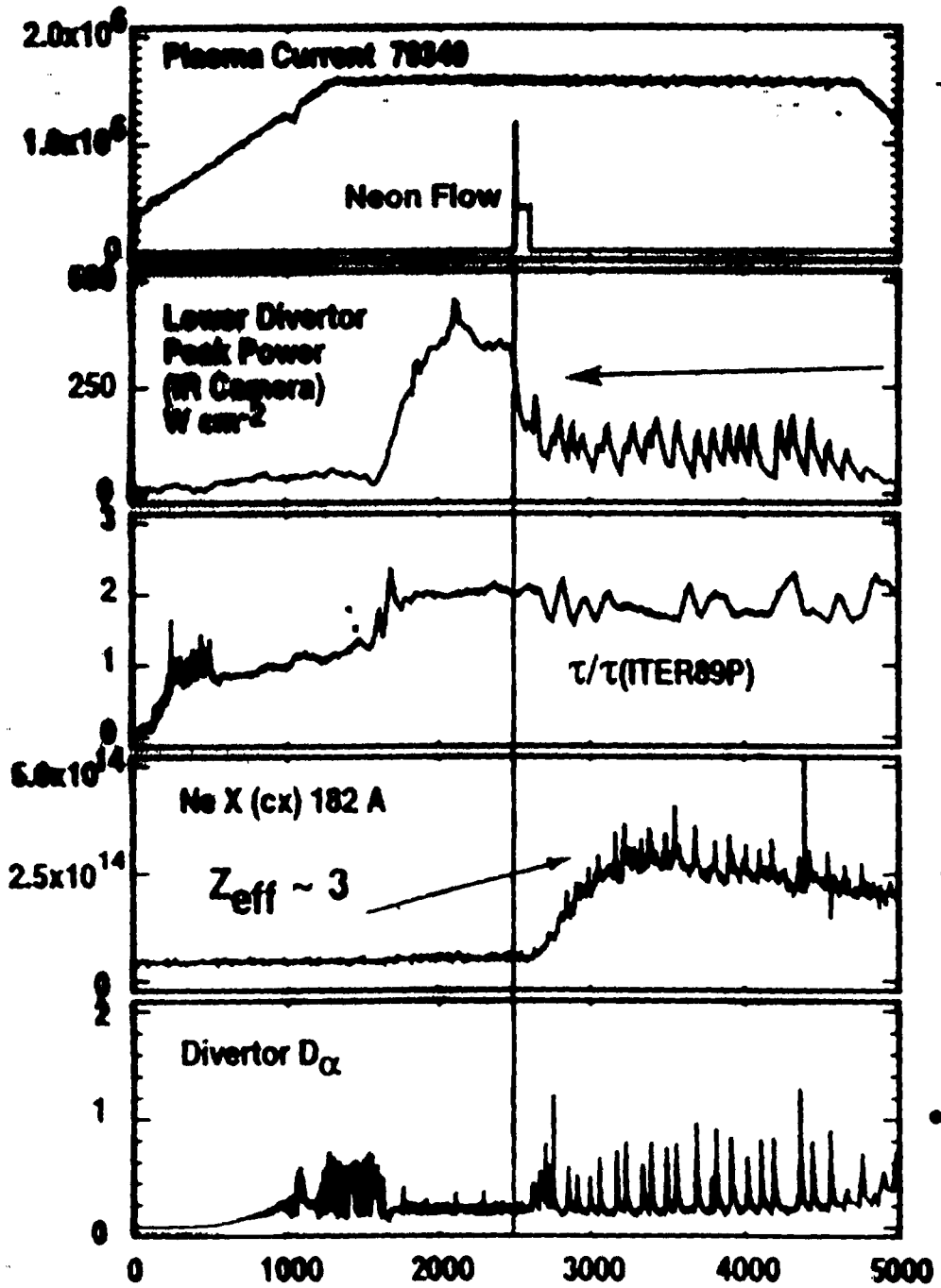
D_2 PUFFING REDUCES DIVERTOR HEAT FLUX BUT INCREASES CORE DENSITY



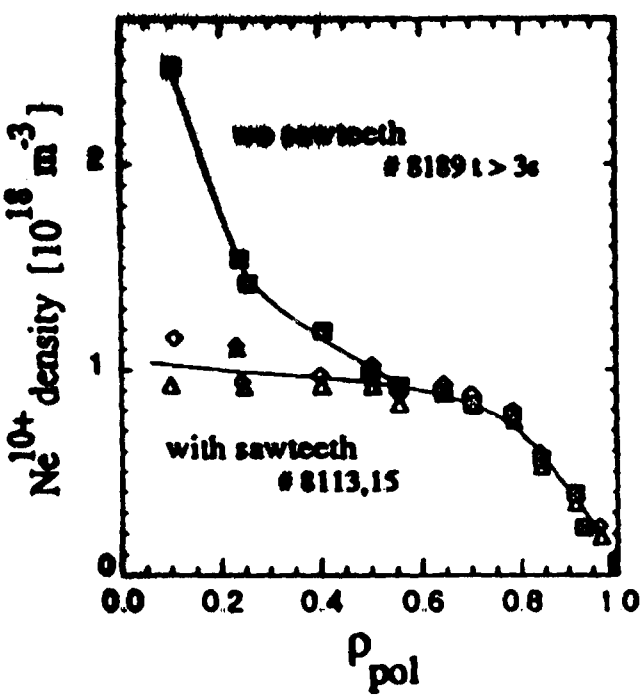
- Beam Power 9 MW
- Heat Flux Reduction
- Small Effect on τ
- Core Density Increases
- ELMs Change

GENERAL ATOMICS

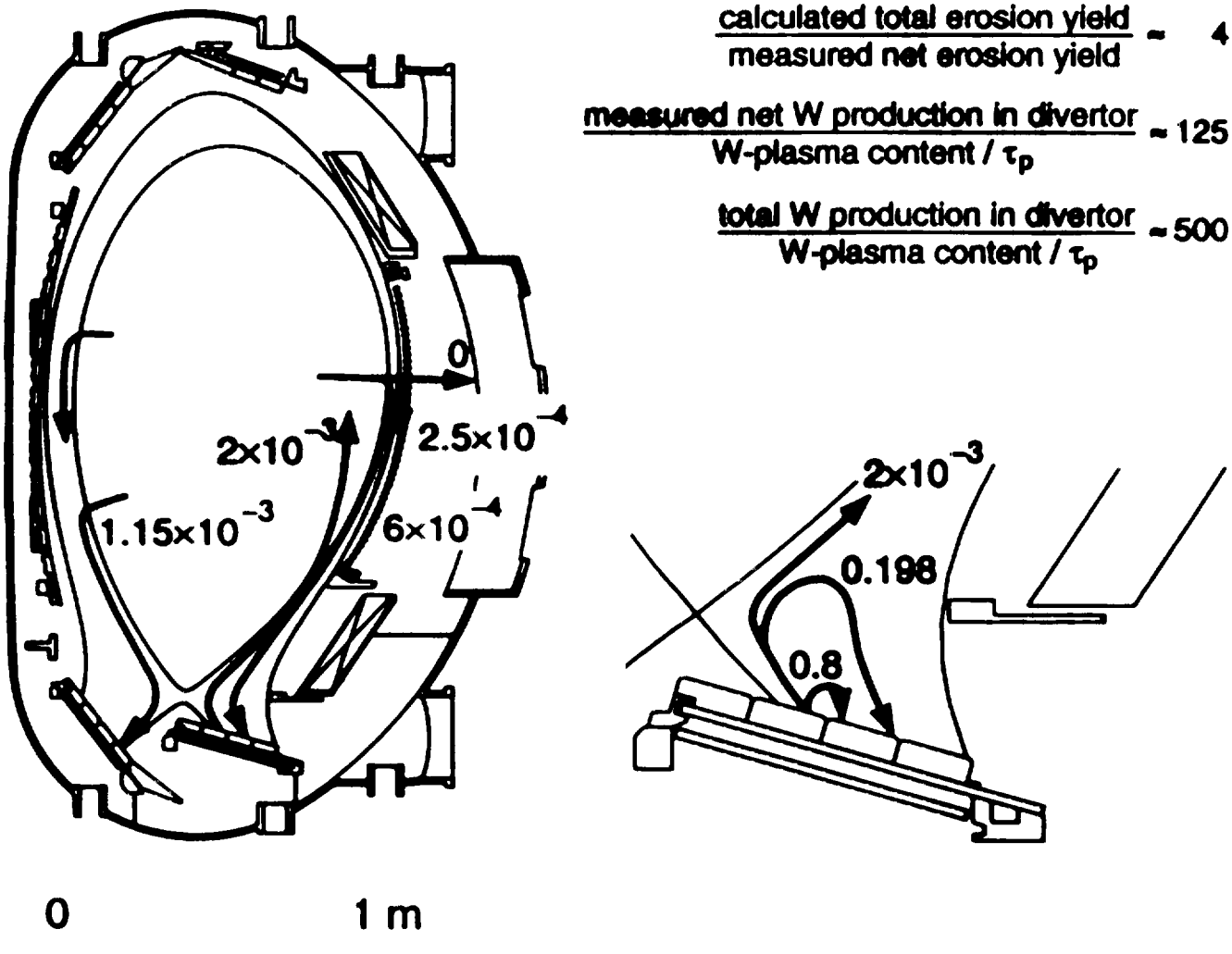
NEON PUFFING REDUCES DIVERTOR HEAT FLUX BUT INCREASES CORE Z_{eff} ~ 3



- Beam Power 9 MW
- Heat Flux Reduction
- Small Effect on τ
- Core Neon Decreasing Z_{eff} ~ 3
- ELMs Change



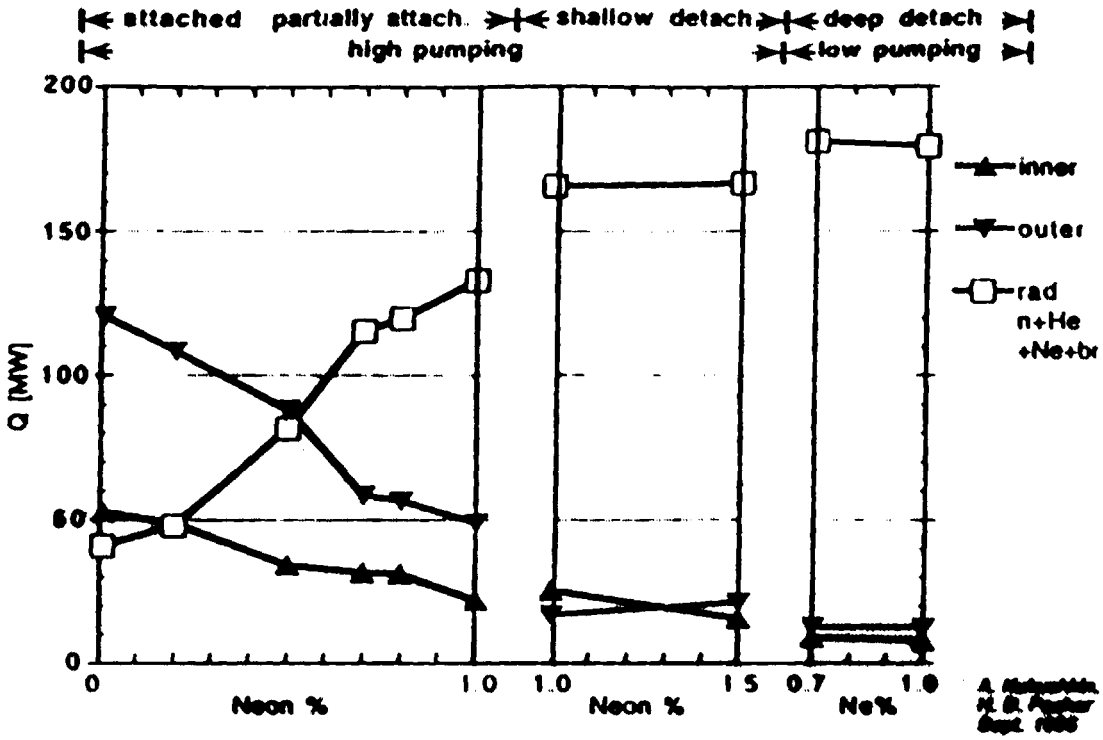
l profiles of fully ionised neon from CXRS for standard CDH and without sawtooth activity. Both discharges have the same the bulk plasma, where the neon-density is rather similiar, but ma dilution is strongly improved with sawteeth.



Typical migration pattern of tungsten in the ASDEX Upgrade vessel for low density Ohmic discharges with $Y_{eff} = 5\times10^{-4}$.

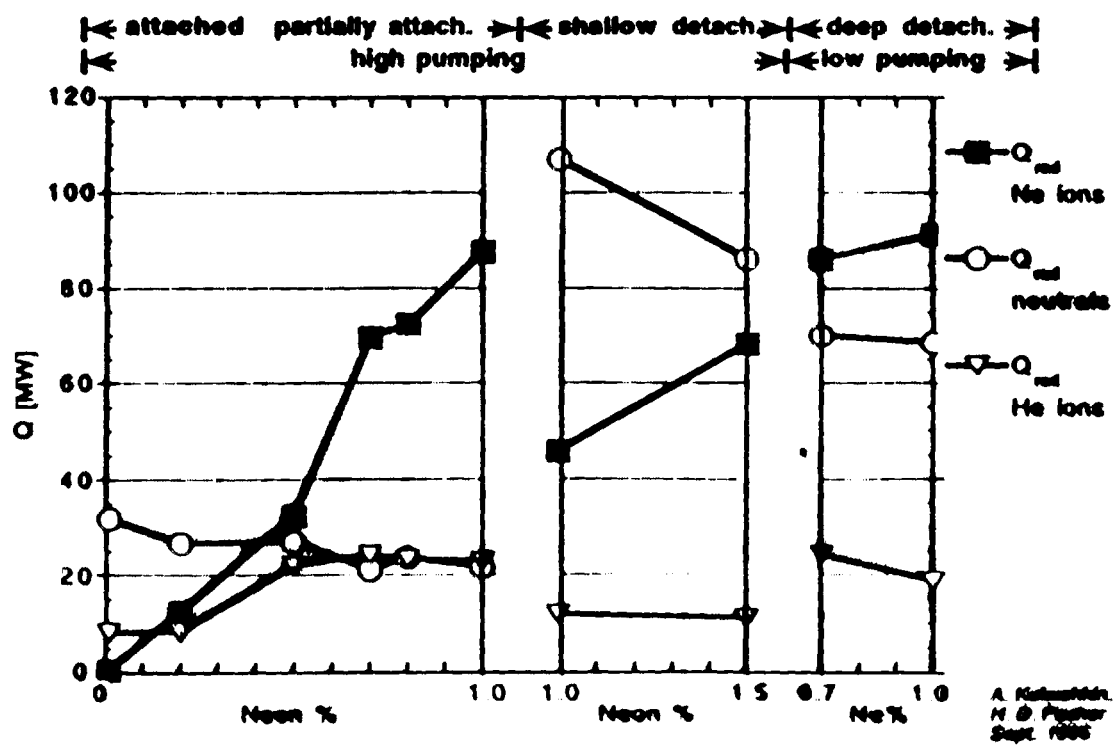
POWER BALANCE

Power to divertors and radiated power

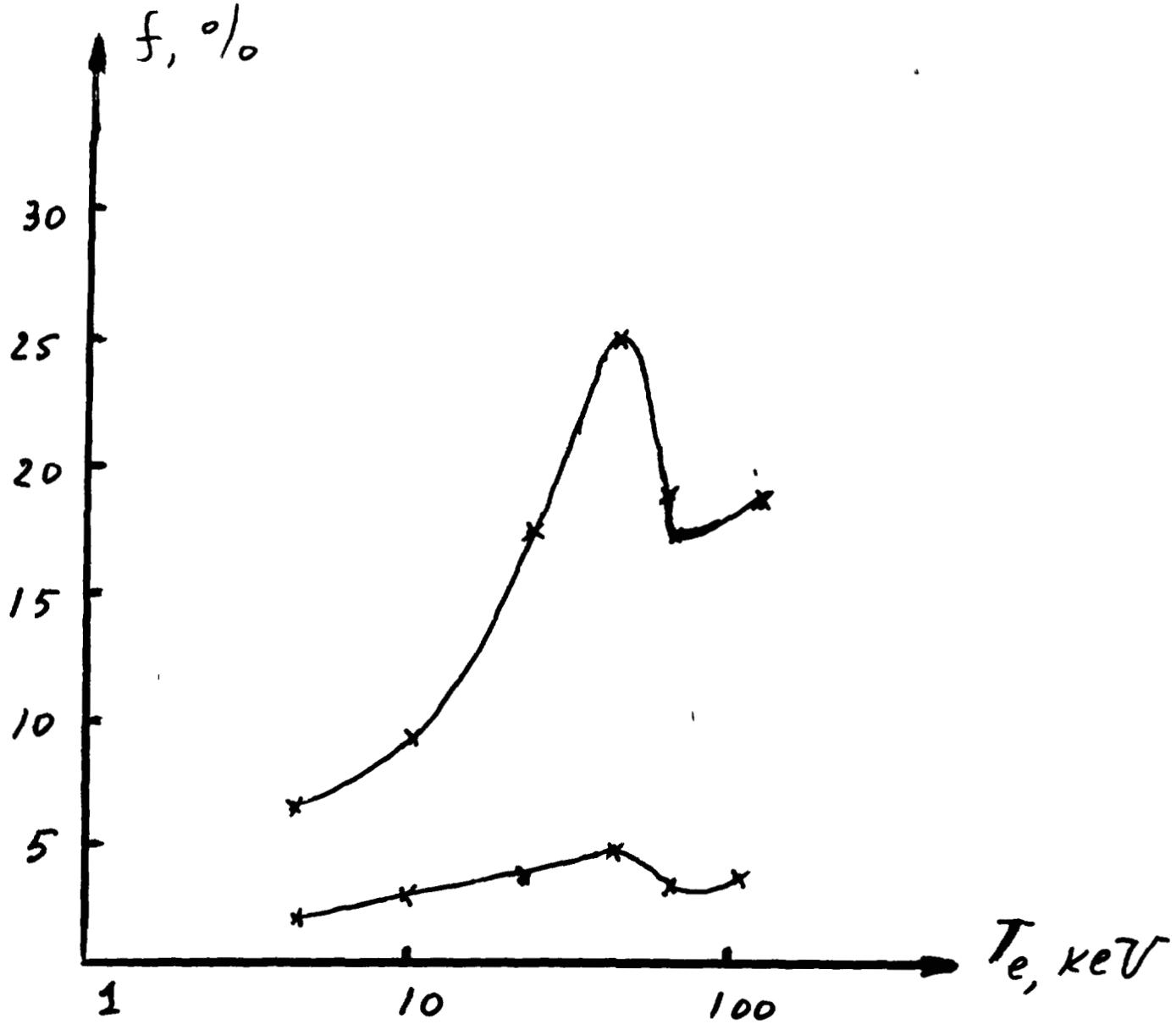


- More than 50% of power can be radiated by partial detachment

Radiation source: Ne or He ions or neutrals

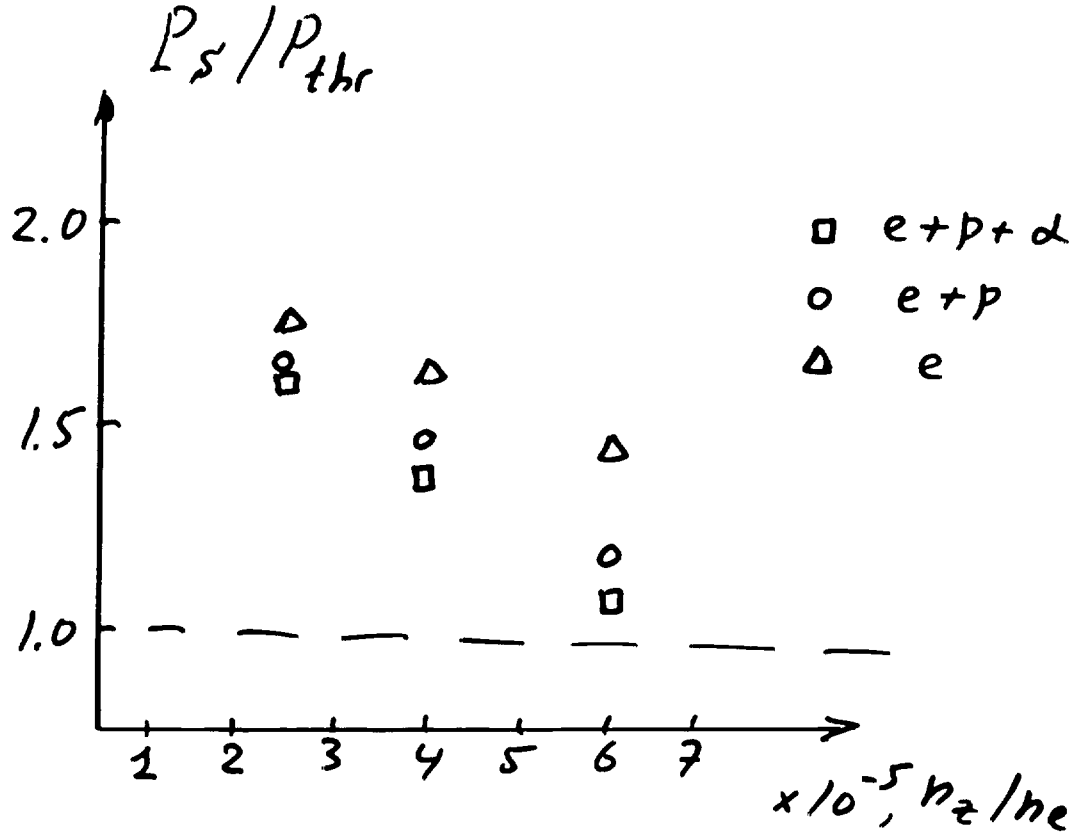


- Helium radiates 6 MW (UEDGE) to ~20 MW (B2)
- Hydrogen radiation significant in detached plasmas

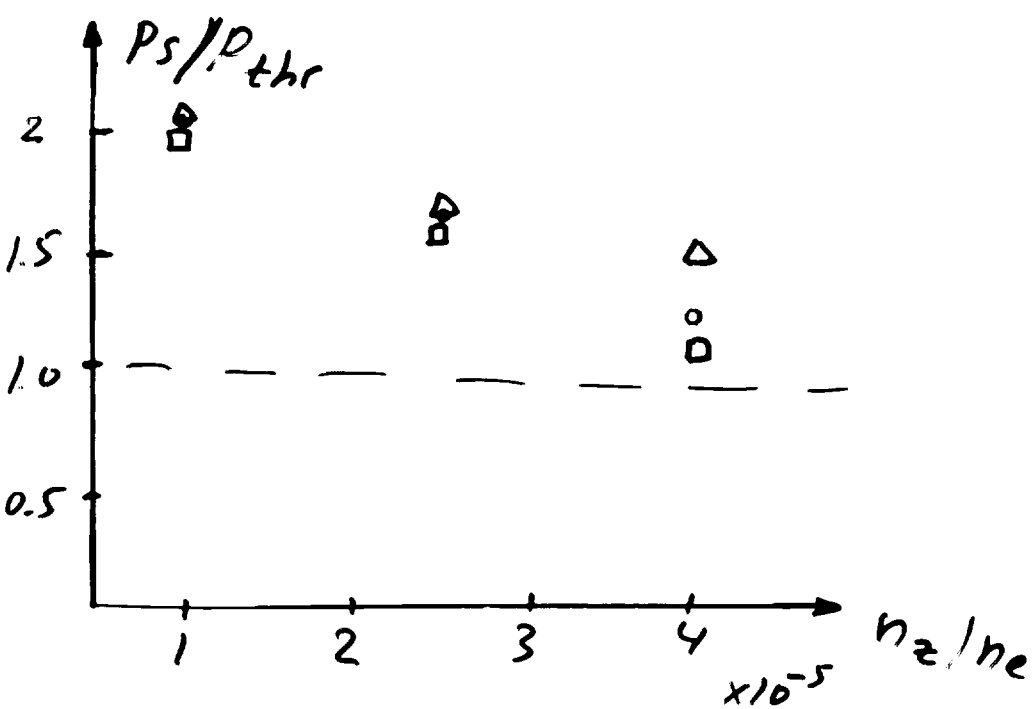


——— $n_z / n_e = 2 \cdot 10^{-4}$

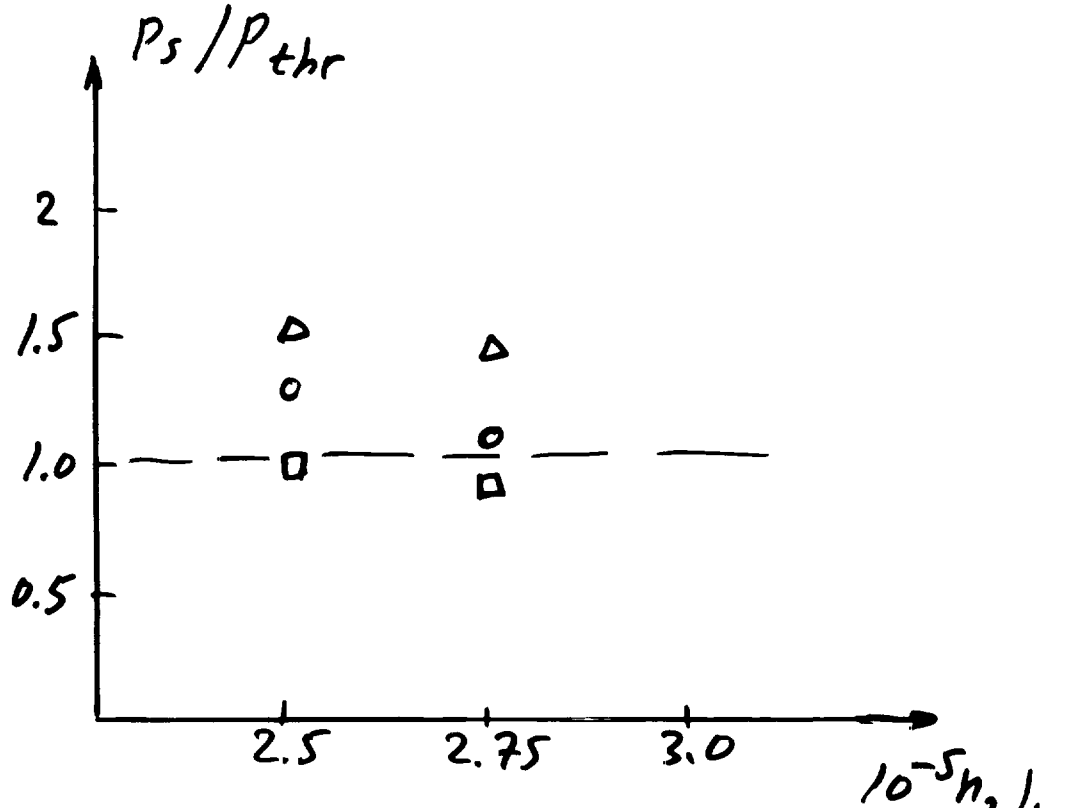
——— $n_z / n_e = 5 \cdot 10^{-3}$



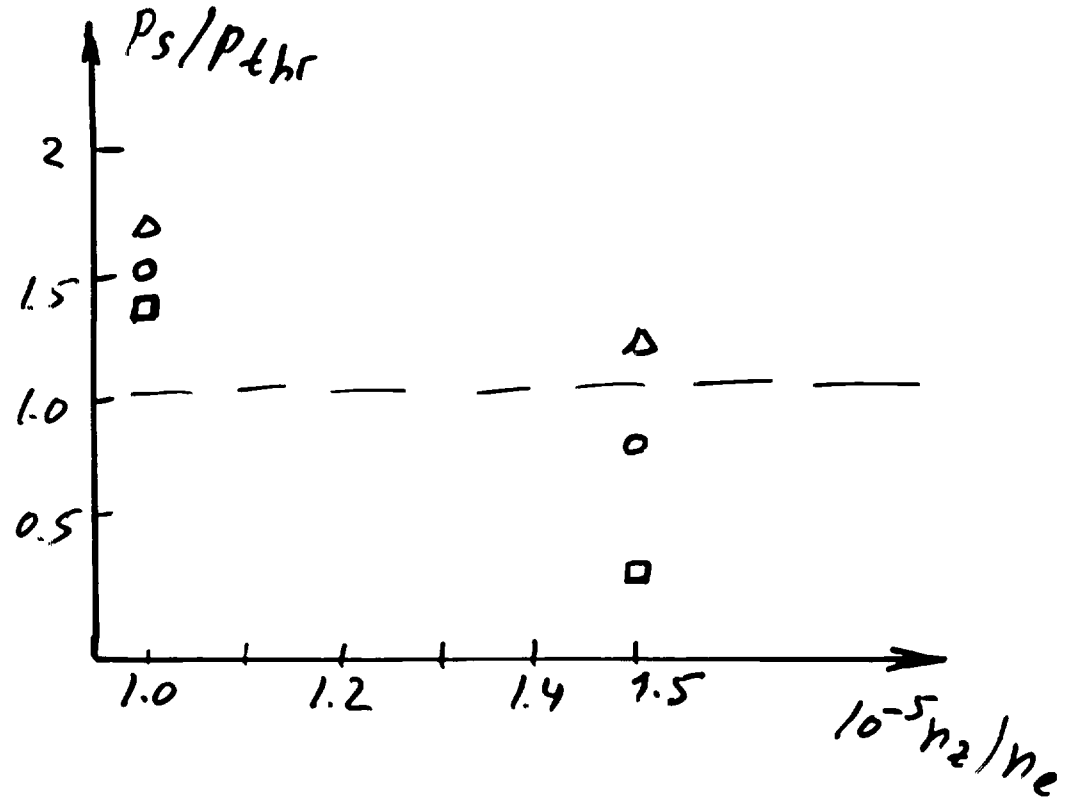
$\bar{n}_e = 6 \cdot 10^{13}\ cm^{-3}$



$\bar{n}_e = 8 \cdot 10^{13}\ cm^{-3}$



$\bar{n}_e = 10^{14}\,cm^{-3}$



$\bar{n}_e = 1.3 \cdot 10^{14}\,cm^{-3}$

$$\sigma_{eff}(E) = \sigma_1(E)\left[\,1 + \sum_{n\geq 2}^{n_{max}} \frac{N_n\,\sigma_n}{N_1\,\sigma_1}\,\right]$$

Be

σ_{eff}/σ_1

n_e / T_e, eV	10^{12}	10^{13}
3	5.5	2.95
50	$2.2\cdot10^{3}$	36.3

Troitsk Atomic Data Group

Troitsk Institute for Innovation and Fusion Research

Troitsk, Moscow region, 142092, Russia

Activities during September 1995 — June 1997

Staff

Alexander L. Godunov	head of the Group *godunov@fly.triniti.troitsk.ru*
Pavel B. Ivanov	system programmer, database supervisor *jones@fly.triniti.troitsk.ru*
Vladimir A. Schipakov	staff member
Yuri K. Zemtsov	associated member
Nadezhda I. Gapotchenko	technical assistant

Main activities

1. Theory of electronic an atomic collisions
   - ⇨ Direct and resonance ionization of atomic systems by charged particle impact, including the effects of strong electron correlations.
   - ⇨ Two-electron transitions in collision of atoms with charged particles. Two-electron excitation and ionization via multiply excited states.
   - ⇨ Dependence of collisional cross sections on the projectile: charge sign effects, mass effects, structured projectiles.
2. Atomic data management
   - ⇨ Development of methods and software for processing diverse atomic data
   - ⇨ Producing compact specialized banks of atomic data (excitation and ionization of atoms and ions by electron impact, autoionization, two-electron transitions in ion-atom collisions)
   - ⇨ Data evaluation and approximation to obtain recommended values (electron-impact ionization of neon and its ions)
   - ⇨ Supplying reliable atomic data for physical models of laboratory and space plasmas
3. Systematic calculations of collisional and spectroscopic characteristics

Hierarchical database management system

HiBase System

A hierarchical database management system (HiBase) has been constructed to satisfy our need for a versatile and easy-to-work tool which would match the specific requirements of atomic data storage and retrieval.

The advantages of hierarchical databases

1. The data structure conforms with the natural organization of the problem area
2. The database does not contain any irrelevant information and empty data fields
3. Search operations do not deal with irrelevant data fields
4. Data of different types may be mixed (text, graphics, binary data, code etc.)
5. Data formats may be independently modified in any branch of the hierarchy

Some features of HiBase

1. The system complies with the requirements of the IAEA.
2. A user-friendly interface requires no preliminary training to get started.
3. The small program size and compact data storage makes the system convenient to install on personal computers.
4. Most data are checked for formal correctness at input.
5. A wide range of search operations is implemented.
6. Many built-in data types, including those specially designed for the application in atomic physics
7. Modular structure permits easily incorporating of new data types and new output formats.

HiBase version 1.99 can be freely requested from Troitsk Atomic Data group.

Project Neon

General Description

Compilation, evaluation and generation of comprehensive data on all the processes of Ne and its ions is one of the priorities recommended by the IAEA Advisory Group Meeting in July 1995.

TADG participation

Cross sections and rates of excitation and single or multiple ionization of Ne and its ions by electron impact:

⇒ Compilation.
⇒ Evaluation.
⇒ Analytic fits.
⇒ Recommendations.

Activities during September 1995 – June 1997

- Compiling experimental and theoretical data on the cross sections of Ne^{q+} ionization by electron impact available in the literature.
- Reassessing earlier data and recommended analytic fits for electron impact ionization cross sections.
- A new analytic formula has been suggested, with less parameters required for the same accuracy.

Earlier approximations

The BELI form as a part of the ALADDIN standard:

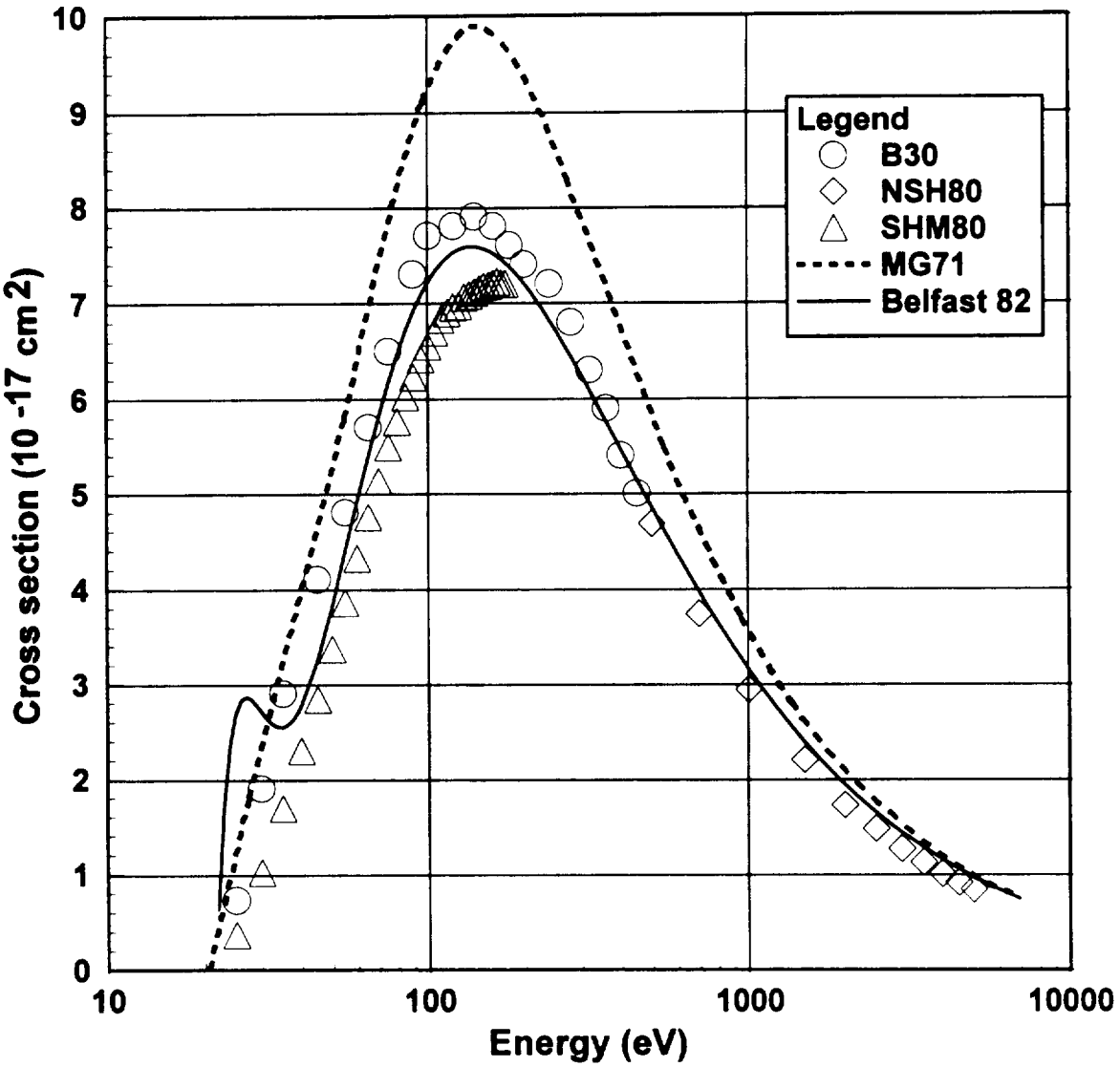
$$\sigma(E) = \frac{1}{IE}\left[A\ln\left(\frac{E}{I}\right) + \sum_{k=1}^{N} B_k\left(1 - \frac{I}{E}\right)^k\right]$$

E — incident electron energy
I — ionization potential
A, B_k —fitting coefficients

M. A. Lennon, K. L. Bell, H. B. Gilbody, J. G. Hughes,
A. E. Kingston, M. J. Murray, and F. J. Smith
J. Phys. Chem. Ref. Data **17**, 1285 (1988)

Main experiments on single ionization of Ne by electron impact

B30	W. Bleakney *Phys. Rev. A*, **36**, 1303 (1930)
ABSK66	B. Adamczyk, A. J. H. Boerboom, B. L. Schram, and J. Kistemaker *J. Chem. Phys.*, **44**, 4640 (1966)
SBK66	B. L. Schram, A. J. H. Boerboom, and J. Kistemaker *Physica*, **32**, 185 (1966)
GH67	A. Gaudin and R. Hageman *J. Chim. Phys.*, **64**, 1209 (1967)
VSV69	M. J. Van Der Wiel, Th. M. El-Sherbini, and L. Vriens *Physica*, **42**, 411 (1969)
SA75	S. G. Shchemelinin and E. P. Andreyev *Zh. Exp. Teor. Fiz.*, **45**, 1490 (1975)
SHM80	K. Stephan, H. Helm, and T. D. Mark *J. Chem. Phys.*, **73**, 3763 (1980)
NSH80	P. Nagy, A. Skutlartz, and K. Helenelund *J. Phys. B*, **13**, 1249 (1980)
WBHF87	R. C. Wetzel, F. A. Baiocchi, T. R. Hayes, and R. S. Freund *Phys. Rev. A*, **35**, 559 (1987)
KS88	E. Krishnakumar and S. K. Srivastava *J. Phys. B*, **21**, 1055 (1988)
AFG95	D. P. Almeida, A. C. Fontes, and C. F. L. Godinho *J. Phys. B*, **28**, 3335 (1995)

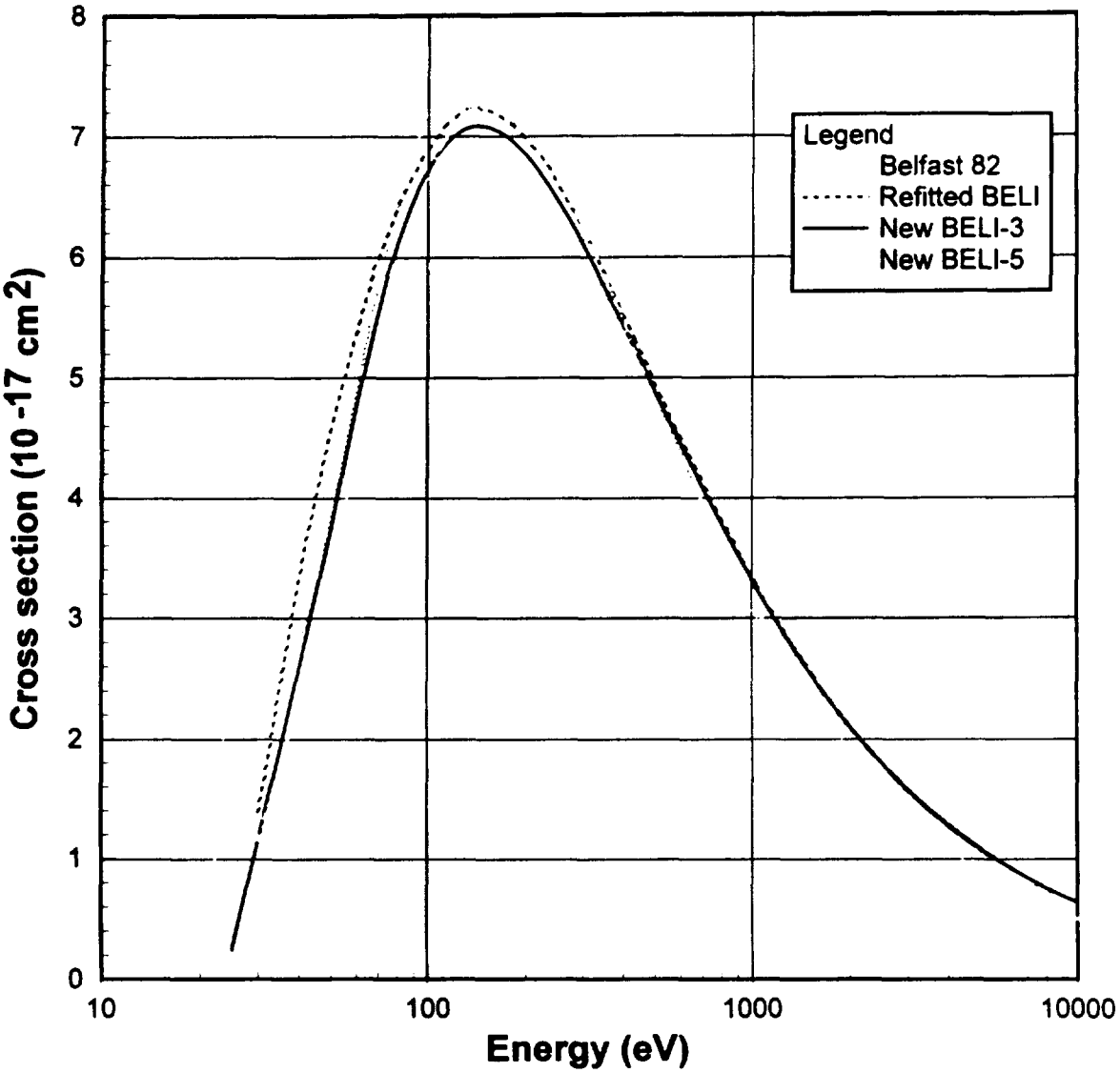


Ne ionization cross sections as recommended by the Belfast group

Fitting coefficients (10^{-16} eV^2 cm^2): $A = 2192$, $B_1 = -447$, $B_2 = -7006$, $B_3 = 5927$

The curve MG71 represents theoretical calculations:

E. J. McGuire *Phys. Rev. A*, **3**, 267 (1971)



BELI fitting curves for single ionization of Ne by electron impact

Fitting coefficients (10^{-16} eV^2 cm^2):

Belfast 82: $A = 2192, B_1 = -447, B_2 = -7006, B_3 = 5927$

Refitted BELI: $A = 2768, B_1 = -2197, B_2 = -3124, B_3 = 1839$

New BELI-3: $A = 2854, B_1 = -2772, B_2 = -1544, B_3 = 422$

New BELI-5: $A = 1732, B_1 = -1721, B_2 = -104.5, B_3 = 1441, B_4 = -8429, B_5 = 9106$

Exponential fitting formula for ionization cross sections

New analytical expression for the cross sections of single ionization by electron impact:

$$\sigma(E) = \frac{A}{IE} \ln\left(\frac{E}{I}\right) \exp\left[\sum_{k=1}^{N} b_k \left(1 - \frac{I}{E}\right)^k\right]$$

Asymptotic behavior:

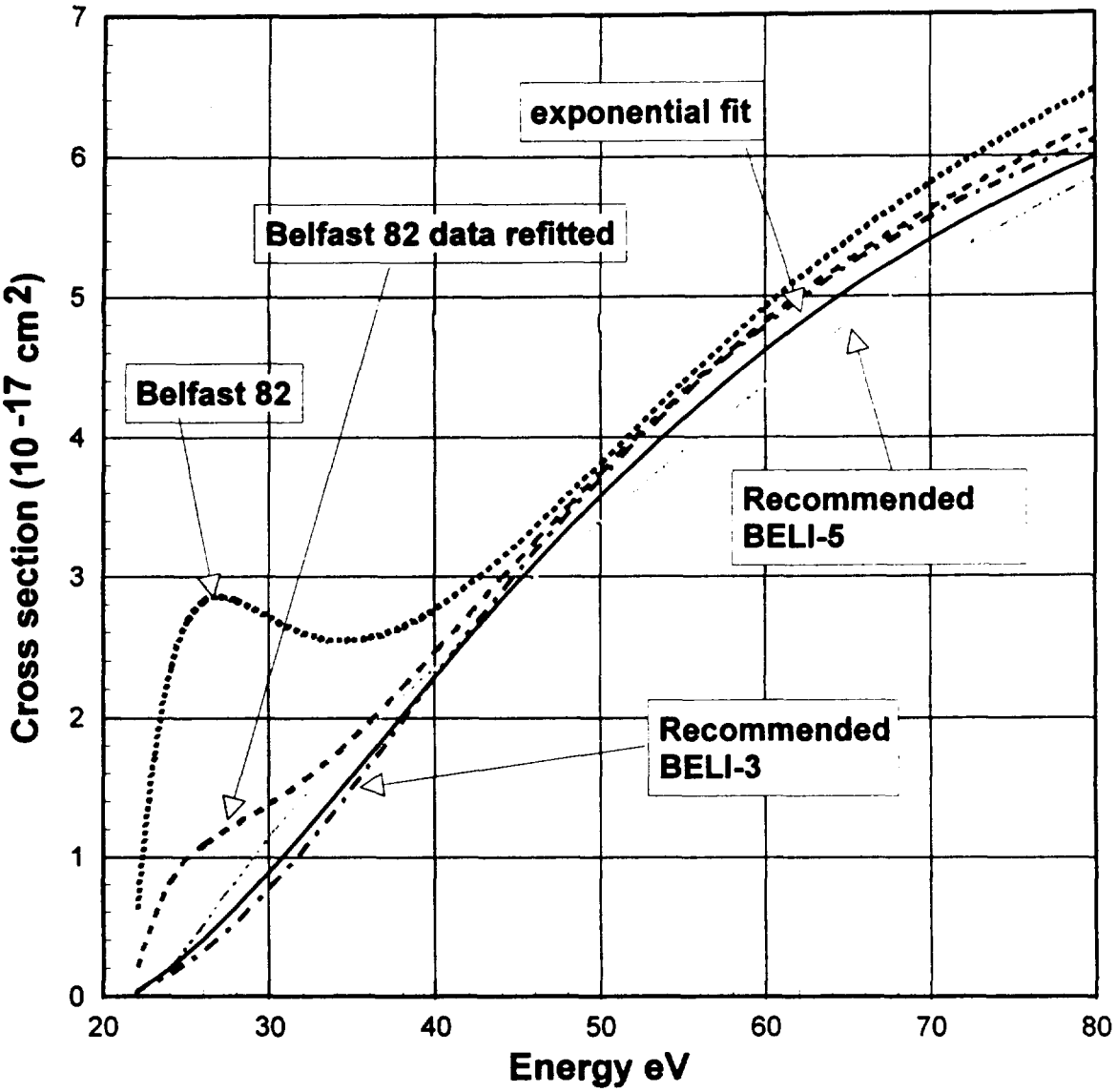
$$\sigma(E) \sim \frac{A}{IE} \ln\left(\frac{E}{I}\right) \text{ at } E \to I, \quad \sigma(E) \sim \frac{A'}{IE} \ln\left(\frac{E}{I}\right) \text{ at } E \to \infty$$

Possible advantages

1. The formula is as simple as BELI.
2. Less parameters required for the same accuracy of approximation.
3. Simpler behavior of the fitting curves.

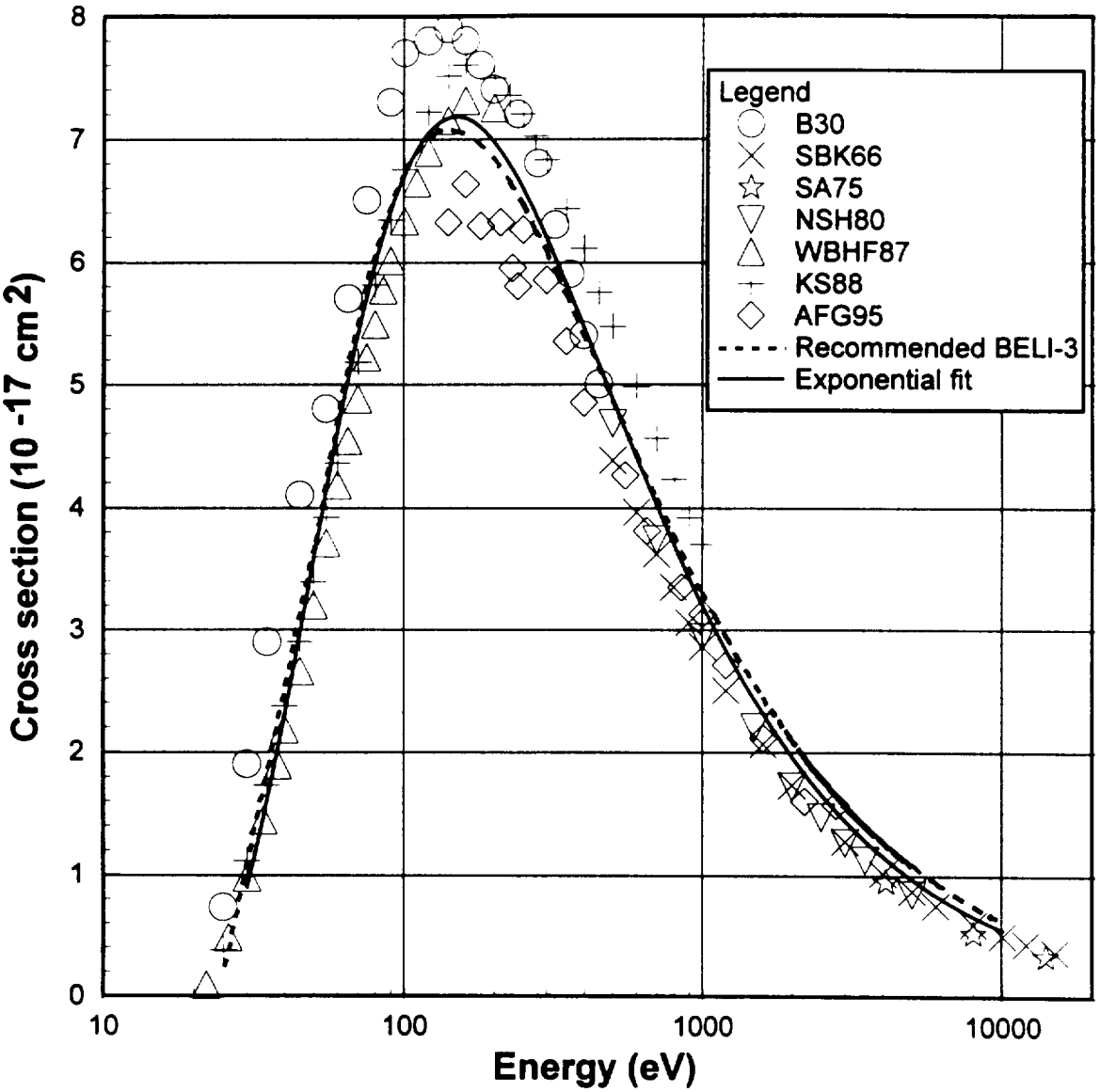
Possible disadvantages

1. Different asymptotic behavior at infinity.
2. Less transparent interpretation of the formula (generalized vapor pressure model).
3. The formula cannot be analytically integrated with to produce the corresponding fitting for reaction rates.

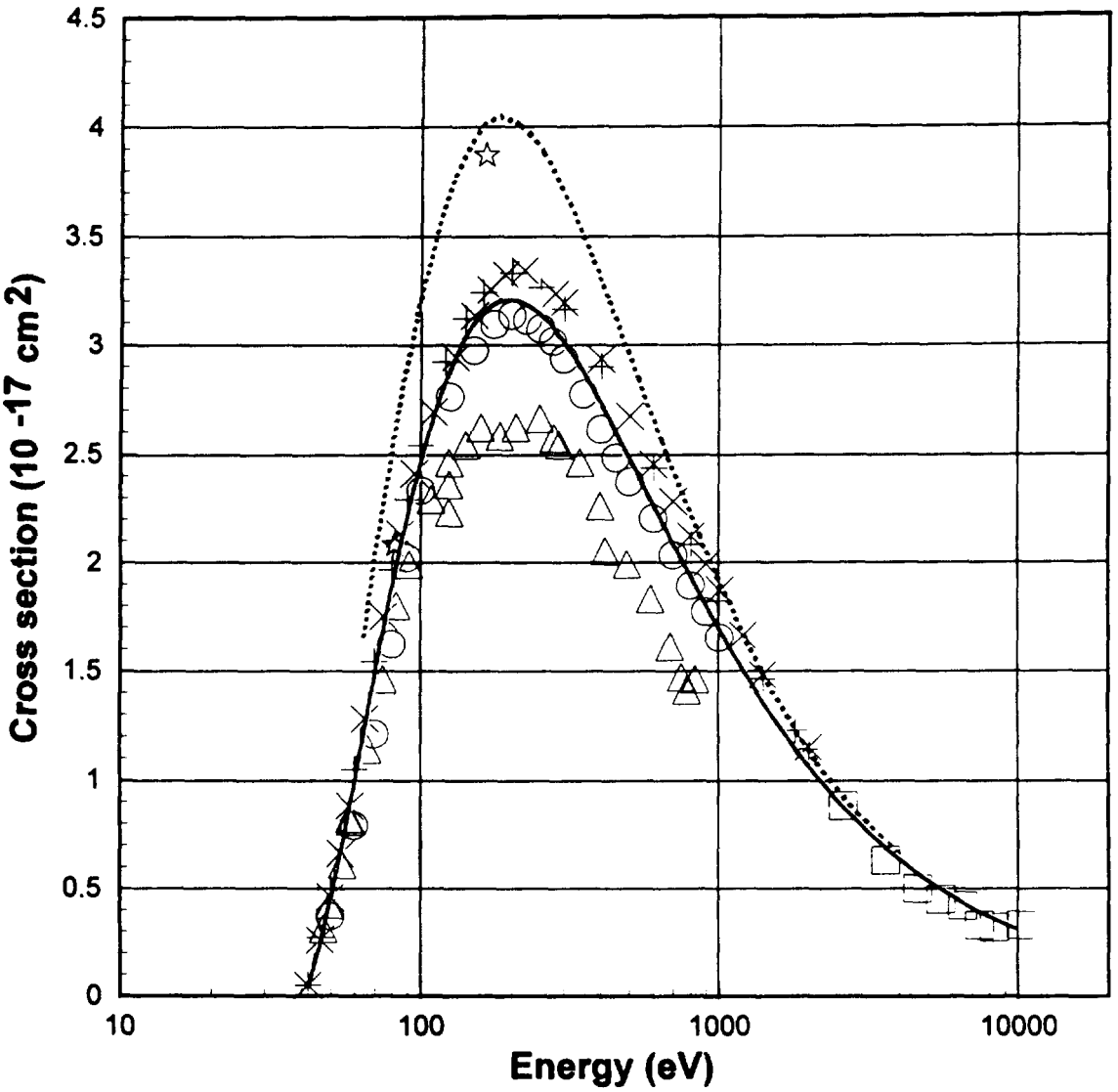


Threshold behavior of analytic fits

Coefficients of the exponential fit: $A = 69.15 \cdot 10^{-16}$ eV^{2}cm^2, $b_1 = 3.342$, $b_2 = -0.009245$



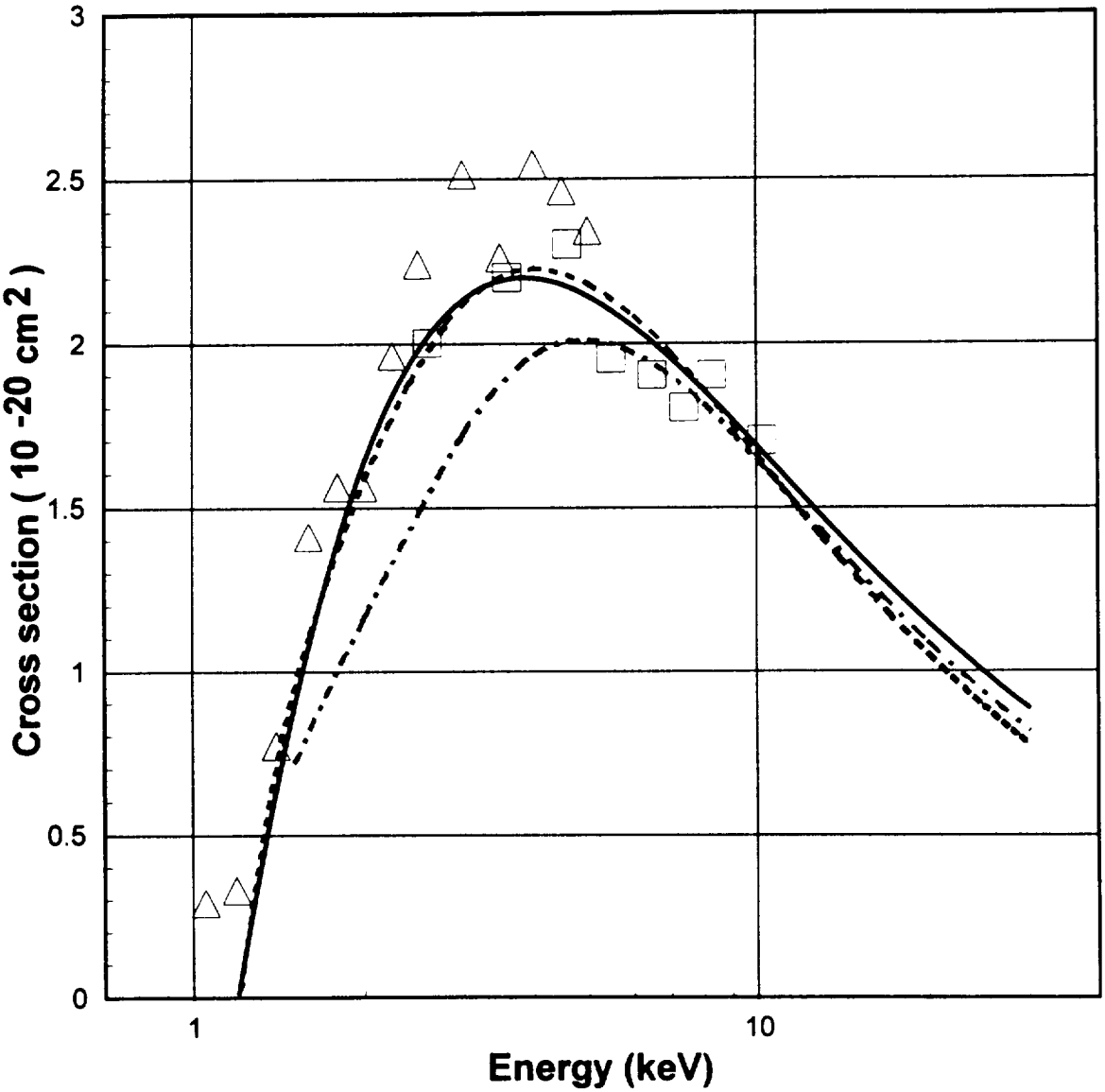
Recommended fits for single ionization of Ne by electron impact



Single ionization of Ne II by electron impact

Legend
- Dolder, Harrison & Thonemann 1963, experiment
- Moores 1972, Coulomb-Born
- Blaha & Davis 1980, distorted wave
- Mueller et al. 1980, experiment
- Diserens, Harrison & Smith 1984, experiment
- Man, Smith & Harrison 1987, experiment
- Donets & Ovsyannikov 1981, experiment

BELI-3
- Exponential fit



Single ionization of Ne IX by electron impact

Legend
- Chandra & Narain 1975, semiempirical
- Donets & Ovsyannikov 1981, experiment
- Duponchelle, Khouilid, Oualim, Zhang & Defrance 1997, experiment
- BELI-3
- Exponential fit

Assessment of the BELI fits

1. The published recommended coefficients contain apparent misprints; refitted data of Belfast (1982) still produce wrong inflection near the threshold.
2. The BELI formulas may produce extraneous inflections due to the polynomial character of the approximation.
3. The quality of approximation generally improves with more parameters, but the fitting curve may experience unphysical oscillations.
4. The BELI expansion cannot be considered as a convergent series, but rather as an asymptotic expansion.

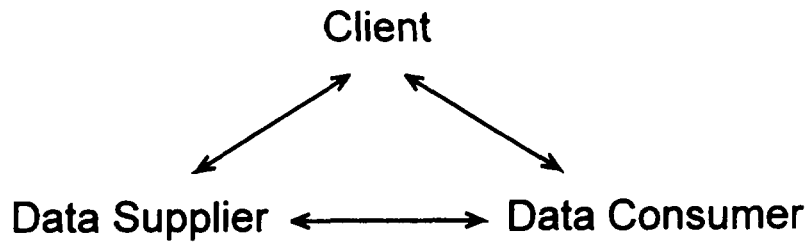
Single ionization of Ne^{q+} by electron impact

Summary

1. The available experimental and theoretical data on single ionization of Ne by electron impact allow to recommend analytic fits presumable accurate within 10%.
2. BELI approximation with N = 3 is preferable for low energies, while the N = 5 formula is better for energies above 1 keV.
3. An alternative exponential approximation ensures good accuracy for all energies, with less parameters. It could be recommended as an alternative standard fit for ionization cross sections.
4. Experimental data on neon ions are insufficient to insure the accuracy of recommended data within 10%.
5. More experiments on Ne^{4+}, Ne^{5+} and Ne^{7+} are desirable.
6. There are too few theoretical calculations on Ne ions
7. The accuracy of available calculations is not enough and more sophisticated physical models are required
8. The recommended analytic fits provide statistical uncertainties within 10%, but the insufficiency of original data would not permit that reliable recommendations
9. Exponential fitting formula leads to the curves rather close to those of the standard BELI format, while fewer parameters are required in the exponential fit.

A+M Data Technology

General scheme of data circulation:



Multilevel Database Scheme:

Client:	Complexes of requirements representing specific tasks
Data Consumer:	Hierarchical data packages for specific complexes
Data Supplier:	Collections of unified software for mass calculations

Promotion:

1. Formation of a world-wide A+M Data Center Network
   - ⇨ Regular international meetings on A+M data
   - ⇨ Mutually linked Internet sites
   - ⇨ Software and data exchange
2. Standardization and common data exchange protocols
   - ⇨ Data representation
   - ⇨ Request forms
   - ⇨ HTML interface
3. Centralized client-side interface
   - ⇨ A+M data central on the WWW
   - ⇨ Professionals to seek for and compile all the data needed for a particular task
   - ⇨ Newsgroups and virtual journals

Current state and perspectives

Achievements

- ◊ Vast experience in A+M data production, compilation, and evaluation
- ◊ Tendency to the development of unified requirements to A+M databases and common priorities

Problems

- ◊ Low level of integrity and compatibility
- ◊ Insufficient rate of software and data exchange
- ◊ Difficulties in culling up all the necessary data for a specific physical problem

Promising directions

- ◊ Rapid development of online databases on the Internet
- ◊ The individual WWW pages becoming an integral network
- ◊ Unification of formats due to the influence of hypertext-based communication technologies

Urgent necessities

- ◊ Joining all the A+M data related WWW sites into a special network with a central homepage where all the links should be maintained
- ◊ Data and software networks merged together
- ◊ Specialists in A+M data management able to find the necessary data on the Internet, or the provide reliable estimates where the data are absent
- ◊ Mailing list or newsgroup for rapid communications

Cross sections for excitation of autoionizing states

Scattering experiments do not distinguish the outcome of target excitation/relaxation from the results of direct scattering. Therefore, the probability of the populating an autoionizing state is not immediately related to the integral intensity of resonance line.

General problem

Can the characteristics of target excitation into an autoionizing state be extracted from experimental data in the presence of strong interference between direct and resonant ionization?

Theoretical consideration

The cross sections of target excitation into an autoionizing state are not directly measurable but can be extracted from the properly parametrized experimental data when the dynamic Stark effect due to the interaction with the scattered projectile is strong enough.

Practical implementation

Joint activity of Troitsk Atomic Data Group and Laboratoiré Collisions, Agrégats, Reactivité, Université Paul Sabatier, Toulouse, France.

Experimental data on the cross section of two-electron excitation of the autoionizing $(2s^2)^1S$, $(2s2p)^1P$ and $(2p^2)^1D$ states of helium in collisions with 100 keV protons have been obtained for the first time despite the fact that these states are embedded into ionization continuum.

Table 1. Experimental and theoretical cross sections (in units 10^{-20} cm^2) and sublevel population for double excitation of the autoionizing $(2s^2)^1S$, $(2s2p)^1P$ and $(2p^2)^1D$ states of helium excited by 100 keV proton impact.

	sublevel population			σ_{exc}
	M=0	M=±1	M=±2	
$(2s^2)^1S$ exp.	1.00			3.40
theory.	1.00			5.97
$(2s2p)^1P$ exp.	0.51	0.49		8.80
theory.	0.55	0.45		11.8
$(2p^2)^1D$ exp.	0.32	0.57	0.11	9.00
theory.	0.51	0.41	0.08	3.51

Data Collection at IPP-Garching(1997)

W.Eckstein
Max-Planck-Institut für Plasmaphysik, Garching, FRG
EURATOM-Association

Sputtering and Reflection

Plasma edge codes for fusion plasmas ask for a complete set of sputtering yields dependent on incident energy and angle and different bombarding species. Especially for new divertor designs not only the sputtering by hydrogen isotopes and selfsputtering but also by noble gas species is of importance.

Computer simulation with the binary collision program TRIM.SP (version TRVMC-MOM) is applied to create sputtering yield and sputtering efficiency (sputtered energy) data as well as particle and energy reflection coefficients for the elements Be, C, and W considered for ITER. The data are given in the form of matrices (fixed energies in lines, fixed angles of incidence in columns) for easy interpolation of data retrieval for plasma edge codes. The data are calculated for 9 angles of incidence: 0, 15, 30, 45, 55, 65, 75, 80, 85 degrees. The lowest incident energy is chosen so that the lowest yields given are about 10^{-5}, values lower than $5 \cdot 10^{-6}$ are put to zero. The highest energy is usually 1 keV, but for He bombardment values for up to the 10 keV range are given. Matrices for H, D, T, N, Ne, Ar and selfbombardment have been produced. The matrices are stored at /afs/ipp/u/wge/trim.data/sputter.data and refl.data and can be retrieved from there if access to afs is possible.

As examples, plots of matrices for the sputtering yields of Be, C, W by D and plots of the matrices for W selfsputtering yields and particle reflection coefficients are given.

For the calculations the krypton-carbon interaction potential [1] and an equipartition of the Lindhard-Scharff [2] and the Oen-Robinson [3] inelastic energy loss models are applied. The data apply for a nearly flat surface. A new method for rough surfaces based on the use of a distribution of local angles of incidence determined from STM measurements

has been developed.

Further tables for the mean depth of implanted atoms can be produced.

References

1 W.D.Wilson, L.G.Haggmark, J.P.Biersack: Phys. Rev. B **15**, 2458 (1977)

2 J.Lindhard, M.Scharff: Phys. Rev. **124**, 128 (1961)

3 O.S.Oen, M.T.Robinson: Nucl. Instrum. Methods **132**, 647 (1976)

Figure Captions.

Fig. 1. Sputtering yield of D on Be, C, W

Fig. 2. Sputtering yield of W on W

Fig. 3. Particle reflection coefficient of W on W

Fig. 4. Sum of sputter yield and particle reflection coefficient for W on W

[redacted]

AMODS

in

Korea Atomic Energy Research Institute

Yongjoo Rhee

[redacted]

presented in Vienna (July 21, 1997)

OBJECTIVES

AMO Data Management and Technical Support

- Atomic spectroscopy for trace analysis
- Fusion research
- Atom optics and high precision measurements
- Particle accelaration
- Laser beam propagation and non-linear effects
- Material processing

Establishment of AMO database system

- Availability : int'l data centers
- Connectivity : heavy network traffic
- Necessity : University, Institute, Industry

Current Status

Hardware Implementation

1. External Open Network

   AMODS : Alphastation 600 model 5/333 ----- **Database**
   DISK ARRAY : 24 GB (raid level 6) ------- **Archive**
   Modem Server : Dedicated 3 Phone Lines

2. Internal Network (Firewall'd)

   SPIS : Alphastation 3000 model 400 ------ **AMODS system mgnt**
   PRINTER : Tektronics PHASER550

Software Implementation

1. **WWW server :**

   apache 1.2 beta 7
   CGI program : C / Sh / PERL

2. AMO Database :

   Bibliographic database : Transition Probabilities, Energy Levels
   Flat data : TP, EL, TL

SCOPES

R&D direction and Acitivites

AMO data production and evaluation

- Energy levels, Life time, Transition probabilities,
- Laser propagation and non–linear phenomena,
- Reaction cross sections, Collisional cross sections,
- Electron impact ionization, etc.

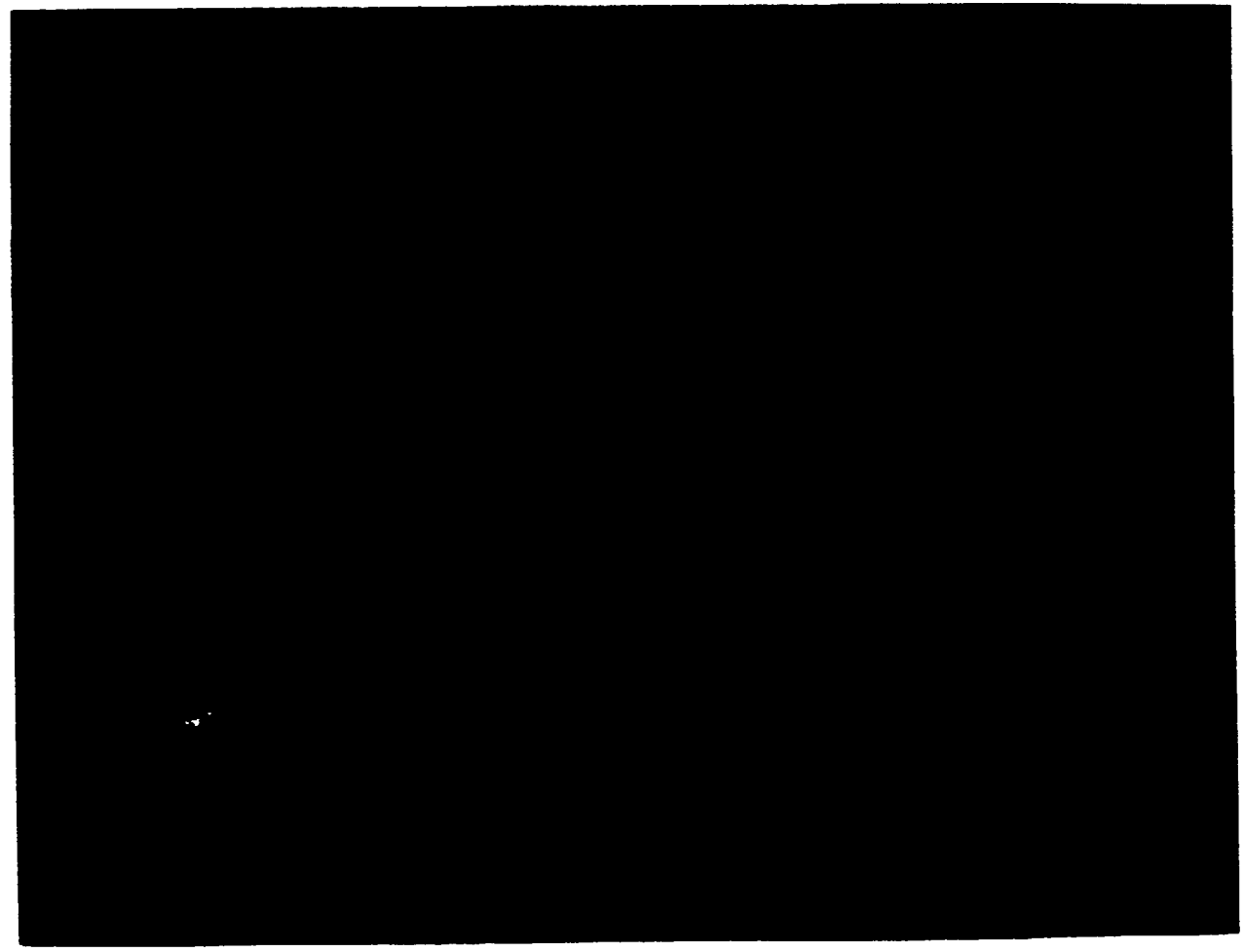
AMO database establishment

- Data Center in KAERI
- WWW server

Efficient methods for data manipulation

- High speed retrieval technology
- Real–time calculation
- Construction of Data Network

Computers and Junks



[redacted]

Korea Atomic Energy Research Institute

[redacted]

Informations on the atomic and molecular structures, transition lines and probabilities, laser propagation characteristics, collisional cross sections, fundamental constants, and bibliographic data on transition probabilities, energy levels and spectra, and references for databases are being compiled in this site.

[redacted]

[redacted] for Scandium (Z = 21) through Ni (Z = 28) for about 16,300 spectral lines are compiled here. The bibliographic database of atomic transition probabilities presently contains over [redacted] references, including those in the NBS Special Publication 305, (1970) and Supplement 1, ([redacted]), as well as more recent references through 1993.

[redacted]

[redacted] energy levels of 28 elements including Lanthanide elements are currently compiled with appropriate bibliographic status. The bibliographic database presently contains approximately 1400 references.

[redacted]

[redacted] are compiled in this database at this time.

[redacted]

[redacted] the reference data sources for the data center.

[redacted]

This document gives the values of the fundamental constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as published by the CODATA Task Group on Fundamental Constants and as recommended for international use by CODATA.

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

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FAX: +82-42-861-8292

AMODS [redacted]

Atomic Transition Probabilities

To get the bibliographic database of atomic transition probabilities click here

H																He
Li	Be										B	C	N	O	F	Ne
Na	Mg										Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

AMODS: Atomic Transition Probabilities for Sc

Choose one of the ionization states from the following list:

● Sc I	Sc VI	○ Sc XI	○ Sc XVI
Sc II	Sc VII	○ Sc XII	○ Sc XVII
Sc III	Sc VIII	○ Sc XIII	○ Sc XVIII
Sc IV	Sc IX	○ Sc XIV	○ Sc XIX
Sc V	Sc X	○ Sc XV	○ Sc XX

Submit Query | Reset Form

[redacted]

Atomic Transition Probabilities of Sc(01)

For the meaning of the symbols click here

--Type--	------Lo_c,t,E------			------Up_c,t,E--------			WaveLen-	gi	gk	-Aki--	-fik--	--S--	log_gf	Ac	Ref
A	1	3d.4s2	2D	101.0	4s2.4p	2P*	18808	5344.1	10	6	0.0053	0.0014	0.24	-1.87	C	1
A	1	3d.4s2	2D	168.3	4s2.4p	2P*	18856	5349.73	6	4	0.0040	0.0012	0.12	-2.16	C	1
A	1	3d.4s2	2D	0.0	4s2.4p	2P*	18711	5342.99	4	2	0.0051	0.0011	0.077	-2.36	C	1
A	1	3d.4s2	2D	0.0	4s2.4p	2P*	18856	5302.98	4	4	0.0013	5.6E-4	0.039	-2.65	C	1
A	2	3d2.(3F).4s	4F	11677	3d2.(3F).4p	4D*	32782	4743.82	10	8	1.8	0.48	75	0.68	E	1
A	2	3d2.(3F).4s	4F	11610	3d2.(3F).4p	4D*	32697	4741.02	8	6	1.7	0.42	53	0.53	E	1
A	2	3d2.(3F).4s	4F	11558	3d2.(3F).4p	4D*	32659	4737.65	6	4	2.0	0.46	43	0.44	E	1
A	3	3d.4s2	2D	168.3	3d2.(3F).4p	4D*	32782	3068.19	6	8	0.0056	0.0011	0.064	-2.20	C	1
A	3	3d.4s2	2D	168.3	3d2.(3F).4p	4D*	32697	3073.34	6	6	0.0074	0.0011	0.064	-2.20	C	1
A	3	3d.4s2	2D	0.0	3d2.(3F).4p	4D*	32659	3061.03	4	4	0.0067	0.0012	0.049	-2.31	C	1
A	4	3d.4s2	2D	168.3	3d2.(3F).4p	2D*	32856	3039.78	6	8	0.0063	9.8E-4	0.059	-2.23	C	1
A	5	3d.4s2	2D	101.0	3d2.(3F).4p	2D*	33238	3018.1	10	14	0.79	0.15	15	0.18	C	1
A	5	3d.4s2	2D	168.3	3d2.(3F).4p	2D*	33278	3019.35	6	8	0.82	0.15	8.9	-0.05	C	1
A	5	3d.4s2	2D	0.0	3d2.(3F).4p	2D*	33184	3015.37	4	6	0.66	0.13	5.3	-0.27	C	1
A	5	3d.4s2	2D	168.3	3d2.(3F).4p	2D*	33184	3030.76	6	6	0.092	0.013	0.76	-1.12	C	1
A	6	3d.4s2	2D	101.0	3d2.(2F).4p	2D*	33670	2978.1	10	10	0.51	0.068	6.7	-0.17	C	1
A	6	3d.4s2	2D	168.3	3d2.(3P).4p	2D*	33707	2980.76	6	6	0.44	0.059	3.5	-0.45	C	1
A	6	3d.4s2	2D	0.0	3d2.(3P).4p	2D*	33615	2974.01	4	4	0.45	0.060	2.3	-0.62	C	1
A	6	3d.4s2	2D	168.3	3d2.(2F).4p	2D*	33615	2980.97	6	4	0.068	0.0061	0.36	-1.44	C	1
A	6	3d.4s2	2D	0.0	3d2.(2F).4p	2D*	33707	2965.86	4	6	0.071	0.014	0.55	-1.25	C	1
A	7	3d.4s2	2D	168.3	3d2.(3P).4p	4D*	36860	2724.60	6	6	0.016	0.0017	0.094	-1.98	C	1
A	7	3d.4s2	2D	0.0	3d2.(3P).4p	4D*	36784	2717.05	4	4	0.036	0.0040	0.14	-1.80	C	1
A	8	3d.4s2	2D	101.0	3d2.(2P).4p	2D*	41159	2434.8	10	10	0.27	0.024	1.9	-0.63	C	1
A	8	3d.4s2	2D	168.3	3d2.(3P).4p	2D*	41163	2438.63	6	6	0.21	0.019	0.90	-0.95	C	1
A	8	3d.4s2	2D	0.0	3d2.(3P).4p	2D*	41183	2429.19	4	4	0.28	0.025	0.80	-1.00	C	1
A	8	3d.4s2	2D	168.3	3d2.(3P).4p	2D*	41183	2439.17	6	4	0.022	0.0013	0.062	-2.11	C	1

AMODS [redacted]

Atomic Energy Levels

To get the bibliographic database of atomic energy levels click here

																	He
H												B	C	N	O	F	Ne
Li	Be											Al	Si	P	S	Cl	Ar
Na	Mg																
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

AMODS: Atomic Energy Levels for Cu

Choose one of the ionization states from the following list:

- ◉ Cu I
- ○ Cu II
- ○ Cu III
- ○ Cu IV
- ○ Cu V
- ○ Cu VI
- ○ Cu VII
- ○ Cu VIII
- ○ Cu IX
- ○ Cu X
- ○ Cu XI
- ○ Cu XII
- ○ Cu XIII
- ○ Cu XIV
- ○ Cu XV
- ○ Cu XVI
- ○ Cu XVII
- ○ Cu XVIII
- ○ Cu XIX
- ○ Cu XX
- ○ Cu XXI
- ○ Cu XXII
- ○ Cu XXIII
- ○ Cu XXIV
- ○ Cu XXV
- ○ Cu XXVI
- ○ Cu XXVII
- ○ Cu XXVIII
- ○ Cu XXIX

Is leading percentage information needed?

- ○ No (default)
- ◉ Yes

Submit Query | Reset Form

Atomic Energy Levels of Cu(01)

For the meaning of the symbols click here

CONFIG	TERM	J	P	LEVEL	g	LEADING PERCENTAGES
3d10.(1S).4s	2S	1/2	E	0.000	2.00	
3d9.4s2	2D	5/2	E	11202.565	1.23	
3d9.4s2	2D	3/2	E	13245.423	0.80	
3d10.(1S).4p	2P*	1/2	O	30535.302	0.68	96 3d10.(1S).4p 2P* 4 3d9.(2
3d10.(1S).4p	2P*	3/2	O	30783.686	1.33	96 3d10.(1S).4p 2P* 4 3d9.(2
3d9.(2D).4s.4p.(3P*)	4P*	5/2	O	39018.652	1.600	98 3d9.(2D).4s.4p.(3P*) 4P*
3d9.(2D).4s.4p.(3P*)	4P*	3/2	O	40113.99	1.75	96 3d9.(2D).4s.4p.(3P*) 4P*
3d9.(2D).4s.4p.(3P*)	4P*	1/2	O	40943.73	2.62	97 3d9.(2D).4s.4p.(3P*) 4P*
3d9.(2D).4s.4p.(3P*)	4F*	9/2	O	40909.138	1.3340	100 3d9.(2D).4s.4p.(3P*) 4F*
3d9.(2D).4s.4p.(3P*)	4F*	7/2	O	41153.433	1.26	89 3d9.(2D).4s.4p.(3P*) 4F* 8 3d9.(2
3d9.(2D).4s.4p.(3P*)	4F*	5/2	O	41562.895		81 3d9.(2D).4s.4p.(3P*) 4F* 16 3d9.(2
3d9.(2D).4s.4p.(3P*)	4F*	3/2	O	42302.47	0.44	95 3d9.(2D).4s.4p.(3P*) 4F*
3d10.(1S).5s	2S	1/2	E	43137.209		
3d9.(2D).4s.4p.(3P*)	4D*	7/2	O	43513.95	1.45	87 3d9.(2D).4s.4p.(3P*) 4D* 11 3d9.(2
3d9.(2D).4s.4p.(3P*)	4D*	5/2	O	44406.268	1.43	43 3d9.(2D).4s.4p.(3P*) 4D* 33 3d9.(2
3d9.(2D).4s.4p.(3P*)	4D*	3/2	O	44544.153	1.09	65 3d9.(2D).4s.4p.(3P*) 4D* 26 3d9.(2
3d9.(2D).4s.4p.(3P*)	4D*	1/2	O	44915.61	0.00	64 3d9.(2D).4s.4p.(3P*) 4D* 33 3d9.(2
3d9.(2D).4s.4p.(3P*)	2F*	5/2	O	43726.191		51 3d9.(2D).4s.4p.(3P*) 2F* 38 3d9.(2
3d9.(2D).4s.4p.(3P*)	2F*	7/2	O	44963.223	1.22	78 3d9.(2D).4s.4p.(3P*) 2F* 11 3d9.(2
3d9.(2D).4s.4p.(3P*)	2P*	1/2	O	45821.00		65 3d9.(2D).4s.4p.(3P*) 2P* 33 3d9.(2
3d9.(2D).4s.4p.(3P*)	2P*	3/2	O	45879.311	1.22	55 3d9.(2D).4s.4p.(3P*) 2P* 35 3d9.(2
3d9.(2D).4s.4p.(3P*)		3/2	O	46172.842	0.69	40 3d9.(2D).4s.4p.(3P*) 2P* 36 3d9.(2
3d9.(2D).4s.4p.(3P*)	2D*	5/2	O	46598.34	1.22	83 3d9.(2D).4s.4p.(3P*) 2D* 15 3d9.(2
3d10.(1S).5p	2P*	3/2	O	49382.95		
3d10.(1S).5p	2P*	1/2	O	49383.26		
3d10.(1S).4d	2D	3/2	E	49935.200	0.82	

AMODS [redacted]

Atomic Transition Lines

H																He
Li	Be										B	C	N	O	F	Ne
Na	Mg										Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

AMODS: Atomic Transition Lines of Al

Choose one of the ionization states from the following list:

- (•) Al I
- ( ) Al II
- ( ) Al III
- ( ) Al IV
- ( ) Al V
- ( ) Al VI
- ( ) Al VII
- ( ) Al VIII
- ( ) Al IX
- ( ) Al X
- ( ) Al XI
- ( ) Al XII
- ( ) Al XIII

Submit Query | Reset Form

Atomic Transition Lines of Al(01)

For the meaning of the symbols click here

Relative Intensity	Observed WL or WN(k)		Calculated WL or WN(k)	Lower Level Energy	Upper Level Energy	Lower Config. Term, J		Upper Config. Term, J	
3a	145.88								
3a	146.26								
2a	150.40								
3a	150.94								
5a	151.84								
3a	152.32								
6a	152.72								
3a	152.85								
2a	153.06								
2a	153.25	=(	153.23	0.000	652600.	2p6.3s2.3p	2P° 1/2	2p5.3s2.3p.(1S).4s	2S
2a	153.25	(	153.26	112.061	652600.	2p6.3s2.3p	2P° 3/2	2p5.3s2.3p.(1S).4s	2S
2a	153.62								
4a	153.88								
1a	154.26								
1a	154.45								
5a	154.84								
2a	154.99								
2a	155.10								
20a	155.45								
10a	155.83								
9a	156.05								
7a	156.25								
2a	156.65	=(	156.64	0.000	638400.	2p6.3s2.3p	2P° 1/2	2p5.3s2.3p.(3D).4s	4D
2a	156.65	(	156.67	112.061	638400.	2p6.3s2.3p	2P° 3/2	2p5.3s2.3p.(3D).4s	4D
2a	156.72		156.72	112.061	638080.	2p6.3s2.3p	2P° 3/2	2p5.3s2.3p.(3D).4s	4D

AMODS [redacted]

Reference data sources for the AMO database

To retrieve a list of references to critical compilations, databases, reviews, and bibliographies produced by the NIST Atomic Data Centers:

- Choose the categories from the following list by selecting on one or more box(es):

  - ☐ Energy level and wavelength data
  - ☐ Transition probability and oscillator strength data
  - ☐ Line shape and shift data

  Select [Submit Query] to list the references.

To make your search more specific by specifying one or more elements:

- Choose one or more elements from either of the following lists (use the *Ctrl* key to make multiple selections or to toggle an element on/off):

ORDER BY ATOMIC NUMBER	ORDER BY ELEMENT NAME
1 Hydrogen H	89 Actinium Ac
2 Helium He	13 Aluminum Al
3 Lithium Li	95 Americium Am
4 Beryllium Be	51 Antimony Sb
5 Boron B	18 Argon Ar
6 Carbon C	33 Arsenic As
7 Nitrogen N	85 Astatine At
8 Oxygen O	56 Barium Ba
9 Fluorine F	97 Berkelium Bk

[Submit Query] [Clear Entries]

AMODS [redacted]

Korea Atomic Energy Research Institute

The 1986 CODATA Recommended Values of the Fundamental Physical Constants

Journal of Research of the National Bureau of Standards, 92, 85 (1987).

This document gives the values of the basic constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as published by the CODATA Task Group on Fundamental Constants and as recommended for international use by CODATA.

Fundamental Physical Constants

Catalogues and files available at CDS

Catalogues and files available at CDS

Version of 12-Jul-1997

- I. Astrometric Data (178 catalogues)
- II. Photometric Data (159 catalogues)
- III. Spectroscopic Data (130 catalogues)
- IV. Cross-Identifications (15 catalogues)
- V. Combined data (66 catalogues)
- VI. Miscellaneous (56 catalogues)
- VII. Non-stellar Objects (129 catalogues)
- VIII. Radio and Far-IR data (40 catalogues)
- IX. High-Energy data (4 catalogues)
- Tables from *Astronomy and Astrophysics* (298 catalogues)
- Tables from *Astronomy and Astrophysics Supplement Series* (666 catalogues)
- Tables from *Astronomical Journal* (307 catalogues)
- Tables from *Astronomicheskii Zhurnal (Russian)* (17 catalogues)
- Tables from *Astrophysical Journal* (98 catalogues)
- Tables from *Astrophysical Journal Supplement Series* (221 catalogues)
- Tables from *Monthly Notices of the Royal Astronomical Society* (100 catalogues)
- Tables from *Publications of the Astronomical Society of the Pacific* (43 catalogues)
- Tables from *Pis'ma v Astronomicheskii Zhurnal (Astronomy Letters)* (3 catalogues)
- Tables from *publications from other journals* (30 catalogues)
- Catalogues ordered by their *Usual Name* (292 catalogues)

Collaborations

International Collaboration

1. Experimental Flat Data
   - AMO DATA : ready to cowork with the world
   - COLLISIONAL DATA : ADAS consortium
2. WWW server program
   - PERL/C/SH /UNIX program
   - ALADDIN

Domestic Cooperation

1. Service and Data provider
   - POSTECH : accelarator
   - KBSI, KAERI : fusion research
   - SNU, CNU, KAIST : spectroscopic data
   - Nuclear Power Plant : welding, cutting, etc
2. Program development
   - Server program : HTTP 1.1 protocol
   - Graphics program : X window

Experimental Plan

Doppler-free Spectroscopy

Absorption, Polarization, Optogalvanic, Fluorescence

energy level, HFS, IS,

LIF spectroscopy

life time

Multistep Photoionization/Polarization Spectroscopy

energy level, life time, angular momentum, IS, HFS

Autler-Townes Measurement

angular momentum, dipole moment

Rabi Frequency Measurement

dipole moment

CW RIMS

IS, HFS

Quantum Beat Spectroscopy

HFS

Further Consideration

Network Security

- WWW, OS, Flat data

Network Traffic

- high speed browser
- new HTTP protocol

DB and Graphics

- graphic display and transfer speed
- "10 second rule"

Conclusion

KAERI has launched an AMO Data Center

- Transition Probability and Bibliography
- Atomic Energy Levels and Bibliography
- Atomic Transition Lines
- References for database and data center
- CODATA 86

Atomic Data Activities at the Plasma Laboratory of the Weizmann Institute of Science

(Israel)

Yu.V.Ralchenko

IAEA, Vienna, 1997

Principal project: ***Studies of highly transient (non-Maxwellian) plasmas by means of spectroscopic diagnostics***

> **no special program/contract related to atomic data** <

- Development of collisional-radiative time-dependent plasma kinetics code for non-Maxwellian plasmas **NOMAD**

- Large-scale production of atomic data for plasma diagnostics needs (collisional cross sections, photoionization cross sections, oscillator strengths, etc.; most not published)

- Intercombination transitions in Be-like ions (*Phys.Rev. A*, v. **52**, 2449, 1995)

- Semi-empirical formula for **multiple ionization** cross sections (*J. Phys. B*, v. **28**, 3027, 1995) -- independent of Shevelko & Tawara

- Modified Gaunt factors for the Van Regemorter formula for **atoms** (*Phys.Rev. A*, v. **53**, 2425, 1996)

- Fitting formulae for electron impact excitation cross sections for **H-like** (*Phys.Rev. A*, v. **55**, 329, 1997) and **Li-like** (submitted to *Phys.Rev. A*) ions

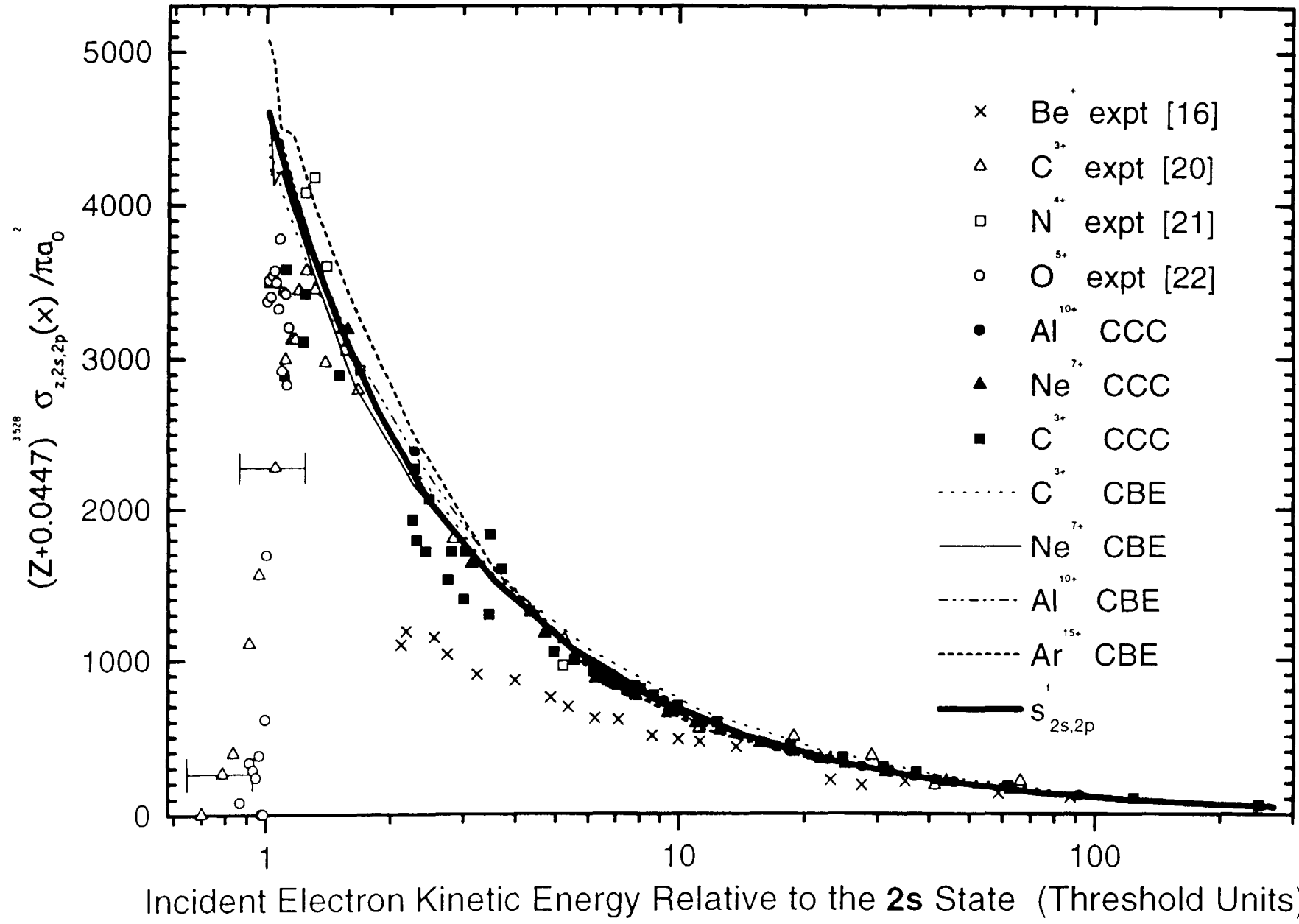

5000
4000
3000
2000
1000
0
1
10
100
$(Z+0.0447)^{3.528}\ \sigma_{2,2s,2p}(x)\ /\pi a_0^2$
Incident Electron Kinetic Energy Relative to the **2s** State (Threshold Units)
Be+ expt [16]
C3+ expt [20]
N4+ expt [21]
O5+ expt [22]
Al10+ CCC
Ne7+ CCC
C3+ CCC
C3+ CBE
Ne7+ CBE
Al10+ CBE
Ar15+ CBE
$S^f_{2s,2p}$

Fig. 4

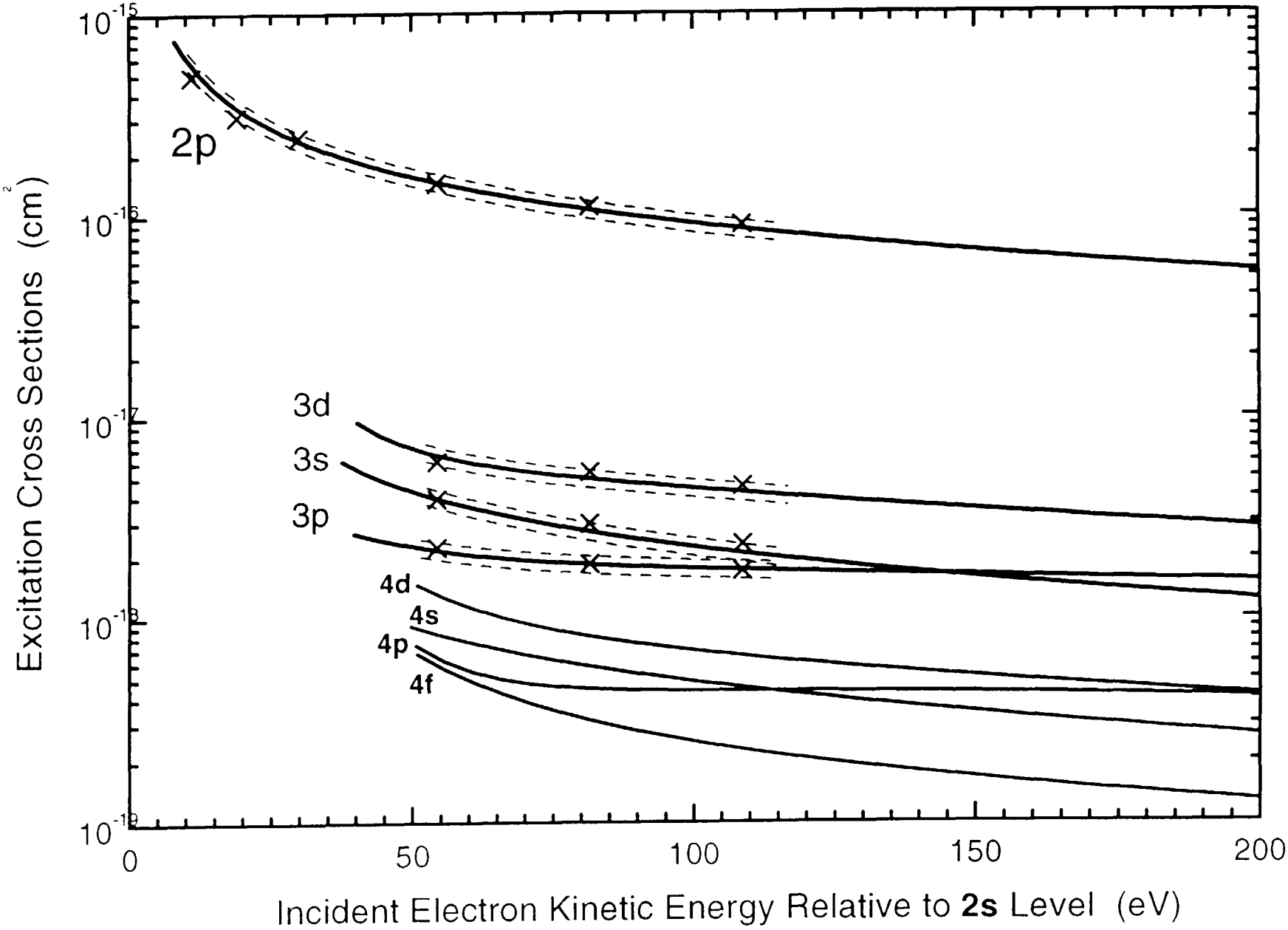

Excitation Cross Sections (cm²)
10⁻¹⁵
10⁻¹⁶
10⁻¹⁷
10⁻¹⁸
10⁻¹⁹
2p
3d
3s
3p
4d
4s
4p
4f
0
50
100
150
200
Incident Electron Kinetic Energy Relative to 2s Level (eV)

Fig. 2

Database of Atomic/Plasma Activities on the Internet

URL http://plasma-gate.weizmann.ac.il/

***Available lists*:**

- **Atomic Physics on the Internet (2586):** servers (**~150**) sorted by country, links to analogous lists, atomic publications
- **Conferences (536):** links to related WWW pages
- **Free software (779):** **>20** entries
- **Jobs (1081):** **~3-5** announcements
- **Plasma on the Internet (2923):** servers (**~220**) sorted by country, links to analogous lists, plasma related newsgroups, plasma publications
- **Who's Who (592):** **~600** entries; self-supported info (addresses, emails, keywords)
- **Databases (1098): ~30 atomic DBs and 6 plasma DBs**

number of hits in June 1997 are given in parentheses

Convergent Close-Coupling (CCC) Database

URL http://yin.ph.flinders.edu.au:8000/CCC-WWW/

Calculational method developed by Igor Bray and collaborators (The Flinders University of South Australia, Adelaide, Australia)

- accurate **excitation** and **ionization cross sections** and/or **asymmetries** for quasi-one- and two-electron systems
- currently, data are available for **H I**, **He I**, **He II**, and **Be I**; more data to come soon
- *'classical'* click-and-get WWW database
- on-line production of both tables and plots with various data units and scales
- was built from a distance of 13072 km (8124 miles)

- **future plans: scattering amplitudes instead of cross sections to allow a user to *generate* the needed cross sections on-line**

Be I: Excitation

Lower state			Upper state		
Conf	Term		Conf	Term	
$2s^2$	^1S	○	$2p^2$	^1S	○
2s2p	^3P	◉	$2p^2$	^3P	○
2s2p	^1P	○	$2p^2$	^1D	○
			2s2p	^1P	○
			2s2p	^3P	○
			2s3s	^1S	○
			2s3s	^3S	○
			2s3p	^1P	○
			2s3p	^3P	○
			2p3d	^1D	○
			2s3d	^1D	○
			2s3d	^3D	○
			2s4s	^1S	◉
			2s4s	^3S	○
			2s4p	^1P	○
			2s4p	^3P	○
			2s4d	^1D	○
			2s4d	^3D	○
			2s4f	^1F	○
			2s4f	^3F	○
			TOTAL		○

Data type:

◉ Cross section — in units of: πa_0^2 ○ | a_0^2 ○ | cm^2 ◉

○ Asymmetry

Make a plot: ☑

X log scale: ☑

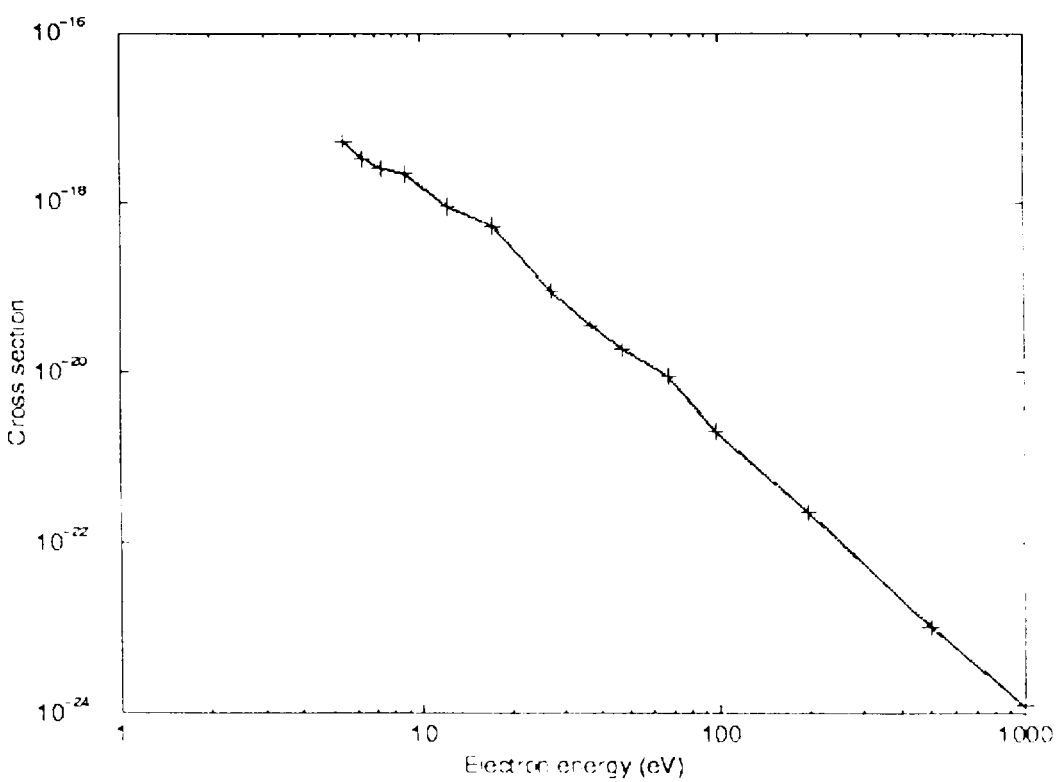
Y log scale: ☑

Go! Clear

Be I: Excitation

Cross section for transition $2s2p\ ^3P \rightarrow 2s4s\ ^1S$

Energy (eV)	Cross section
5.49	5.211e-18
6.35	3.278e-18
7.29	2.518e-18
8.79	2.168e-18
12.29	8.808e-19
17.29	5.238e-19
27.29	8.888e-20
37.29	3.562e-20
47.29	1.862e-20
67.29	8.878e-21
97.29	1.993e-21
197.29	2.276e-22
497.29	1.067e-23
997.29	1.205e-24



WWW Interface for the Hartree-Fock code RCN

URL http://plasma-gate.weizmann.ac.il/~fnralch/rcn.html

Code author: Robert D.Cowan (Los Alamos National Laboratory)

- use first part of the **RCN/RCN2/RCG/RCE** package
- produces **wave functions** and their plots
- elements: **H - Ne**
- ions: **I - X**
- Calculation time for **Ne I** $2p^3 3s 3p 3d$: **55 sec** (with plots for all wavefunctions) on a 100-MHz Pentium
- ~ **5** runs/day

WWW Interface for the Coulomb-Born-exchange code ATOM

URL http://plasmagun.weizmann.ac.il/~fnralch/ATOM/

Code author: Leonid A. Vainshtein (Lebedev Physical Institute, Moscow, Russia)

Current version calculates ***electron-impact excitation cross sections in LS-coupling*** *(full version of **ATOM** calculates ionization, photoionization, dielectronic recombination, excitation and ionization by heavy particles, Maxwellian averaged rates, etc. for various types of coupling)*; includes an on-line help

Input parameters:

mandatory

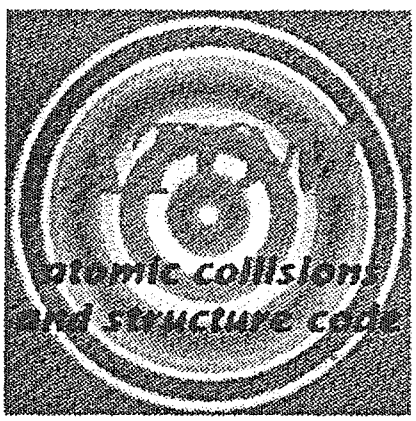
- **configuration and term of lower and upper states and term of the parent ion**
- **transition type**

optional (for better accuracy)

- ionization energies of lower and upper states
- energy difference between lower and upper states
- oscillator strength for dipole-allowed transition

Calculation time on a 100-MHz Pentium (11 energy points): < 25 sec w/o plots; < 50 sec with plots

Disclaimer | Cowan's Code | 2691-symbol calculator | XMgr



The code ***ATOM*** was written and is maintained by Prof. L.A.Vainshtein (Lebedev Physical Institute, Moscow, Russia). This version of the WWW Gateway calculates only **electron-impact excitation cross sections** in the *Coulomb-Born-exchange* approximation. The full version of ***ATOM*** calculates also electron-impact ionization cross sections, photoionization cross sections, heavy particle impact cross sections, autoionization probabilities, Maxwellian-averaged rates, etc. The details of calculations as well as more ***ATOM*** related information can be found in the book 'Atomic Physics for Hot Plasmas' by **V.Shevelko** and **L.A.Vainshtein** (IOP Publishing, Bristol, 1993, ISBN 0 7503 0231 3).
Your comments would be highly appreciated!

Yuri Ralchenko

Calculation time depends on angular momenta of the optical electron. For the worst cases (including plotting), it rarely exceeds **one minute** for 11 energy points. By the way, this computer is a slow 100-MHz Pentium®.
You may want to open a full list of avalable states in a new window (first two columns are the spectroscopic charge and nuclear charge respectively). This would facilitate the selection of states. However, if the parent ion state is not the ground state, you should enter the energy shift = energy difference between the parent state for your particular transition and the ground state.
If the state(s) you want to work with is not present in the full list, it is sufficient to enter the *correct* ionization energies for the ***ATOM*** to work properly. Moreover, without the ionization energies ***ATOM*** will operate too but with lower accuracy. For better results, *check the* ***calculated energy difference*** *in the output and, if it is not very accurate, correct it in the corresponding input field.*

Select element [10. Ne] and ion [VIII] OR Enter element [ ] and ion [ ]

(MUST be correct):

$1^n \rightarrow 1^{n-1}1'$ ◉ (Includes cases like 1s 2p -> 1s 3d etc.)

$1^{N}1', n \rightarrow 1^{N-1}1'_{(n+1)}$ ○ (Here N=4l+2, i.e., a filled shell)

$1^n \rightarrow 1^n$ ○ (Transition within a group of equivalent electrons)

Input Parameters

	Lower state	Upper state	Examples:
Configuration:	2p	4s	2s2 2p3 (note the space between the shell
Term:	2P	2S	1S; 3D; 2P
Parent term:	1S		1S; 3D; 2P
Energy shift:	0.00e+00		Energy units: eV ◉ | cm^{-1} ○ | Ry ○

Optional Parameters

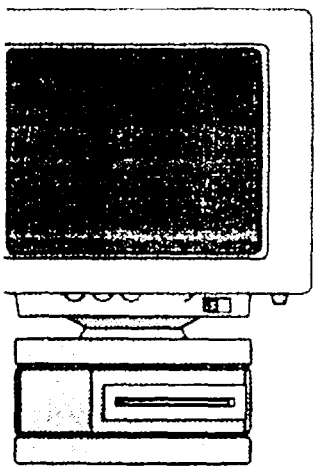
Ionization energies:		
Energy difference between lower and upper states:		
Oscillator strength:		
Cross section units:	cm^2 ◉	$pi*a_0^2$ ○
Energy scale:	Z_{eff}^2Ry ◉	deltaE ○

| Make a plot: ☑ | X log scale: ☑ | Y log scale: ☐ |

Run ATOM Clear

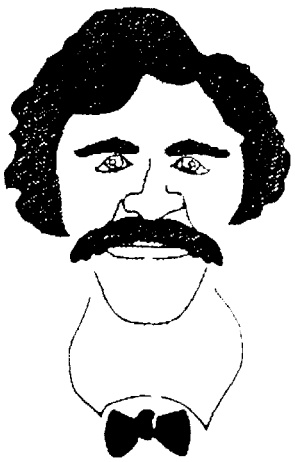
Thanks button

: No one takes any responsibility for the data produced with this software. You have been warned!!!



good code

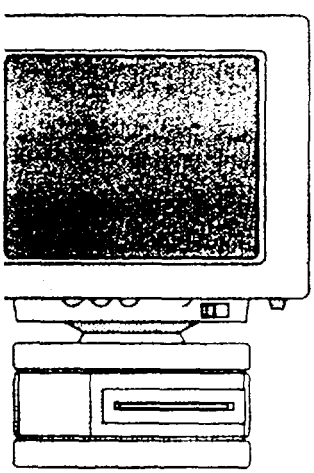
+



good
physicist

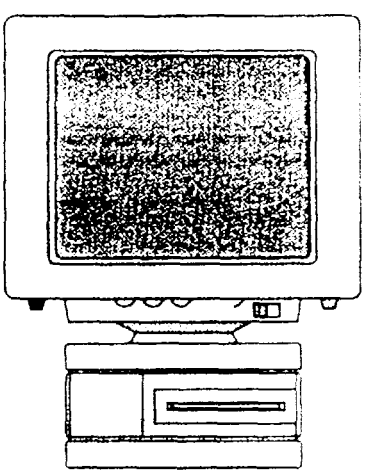
=

reliable
results
(few)



good code

+



good
interface

=

many
results
(reliable?)

Atomic SOFTbase

Activities of the A+M Data at CRAAMD 1995,10--1997,6

Sun Y. S.

We have done the following affairs since the last meeting :

1 Completed one research project entitled " Generation and Evaluation of Ne - Ions Data ", the contract No. 8840/RB. The working period is Dec. 15, 1995 - Dec.15, 1996.

In this job , electron-impact excitation data for neon and neon ions published up to mid-1996 had been collected exhaustively and stored with ALADDIN formatted data files.

2 Collection and Calculation of Electron-impact ionization data for neon and its ions.

(1) Data collection

Following Lotz [1- 3] , Tawara and Kato[4] electron-impact ionization data for neon and its ions published from mid-1986 up to the early of 1997 have been collected and stored with ALADDIN format.

(2) Data calculation

In order to evaluate and check the cross - sections for single ionization of neon ions from the ground state , I asked Prof. Wang * to calculate these data systematically in the distorted-wave Born exchange approximation.

---

* Prof. Y. S. Wang's group at Fudan University in Shanghai is a menber of CRAAMD.

In this mothed, several results have been published recently[5, 6].

All cross-sections for single ionization are fitted with Younger formula

$$UI^2Q = A(1-\frac{1}{U}) + B(1-\frac{1}{U})^2 + C\ln U + D\frac{\ln U}{U} \qquad (1)$$

were $U = \frac{E}{I}$, I is the ionization potential of electrons in a subshell, E is the electron impact energy, UI^2Q is reduced cross section, Q denotes the normal cross section; A,B,C,D are the fit parameters.

Calculated Results:

i) Ionization Potential

The ionization potential I_0 for electron in the outermost shell and I_i for electron in the sub-outermost shell are given in Table 1 for Ne ions.

Table 1.

q^+	I_0(eV)	I_i(eV)
9	1361.4	—
8	1195.7	—
7	239.6	1146.7
6	204.7	1100.2
5	158.8	173.1
4	125.0	143.9
3	94.23	116.8
2	66.52	92.14
1	41.96	69.92

ii) Fit Parameters of Cross Sections

The fit parameters of cross sections for the outermost shell and the sub-outermost shell of Ne^{q+} ions are given in Table 2 and Table 3 respectively.

Table 2 . The fit parameters of the outermost shell for Ne^{q+} ions

q^+	A	B	C	D	Δ(%)
9	14.728	-6.6001	0.0703	-12.217	0.63
8	29.497	-11.532	0.2673	-24.864	0.61
7	8.0824	-2.9527	0.6033	-5.9680	0.63
6	16.414	-5.9598	1.1508	-12.427	0.49
5	15.088	-5.8183	0.0255	-12.018	0.58
4	32.633	-13.261	0.1897	-27.027	0.65
3	47.788	-20.348	1.3130	-41.524	0.47
2	50.106	-22.453	5.1612	-48.565	0.76
1	54.877	-31.767	10.714	-62.956	0.996

Table 3 The fit parameters of the sub- outermost shell for Ne^{q+} ions

q^+	A	B	C	D	Δ(%)
7	27.962	-11.140	0.7113	-23.927	0.63
6	28.649	-11.659	0.7846	-24.822	0.62
5	12.382	-4.4353	1.9784	-9.5495	0.12
4	24.144	-9.5112	0.2593	-19.800	0.70
3	20.482	-7.8330	0.9092	-17.404	0.30
2	17.698	-6.2321	1.3822	-16.267	0.39
1	15.572	-5.0911	1.7423	-16.416	0.28

Δ(%) means the relative deviation of the fit values from the original data.

iii) Rate Coefficients

$$S = \langle Q\, v \rangle = \int_0^\infty vQ(v)f(v)dv \qquad (2)$$

f (v) is the Maxwellian distribution of electrons. Or, using the reduced cross section,

$$S(kT) = \frac{1.090\times10^{-6}}{(kT)^{3/2}} \int_1^\infty e^{-UI/(kT)} \cdot UI^2 Q dU, (cm^3 \cdot s^{-1}) \qquad (3)$$

where kT and I are in eV units, UI^2Q **in** $\pi a_0^2 Ry^2$ **unit.**
Eq.(1) is substituted into Eq.(2),

$$S(kT) = \frac{1.090\times10^{-6}}{(kT)^{3/2}} \frac{e^{-x}}{x} \times$$

$$\times \begin{array}{l} \{A[1-xf_1(x)] + B[1+x-x(x+2)f_1(x)] + \\ \quad + Cf_1(x) + Dxf_2(x)\} \end{array} \qquad (4)$$

where $x = I / (kT)$

$$f_1(x) = e^x \int_1^\infty \frac{e^{-Ux}}{U} dU$$

$$f_2(x) = e^x \int_1^\infty \frac{\ln U \cdot e^{-Ux}}{U} dU$$

$f_1(x)$ **and** $f_2(x)$ **can be calculated by the following fit formulae:**

a) For x < 1.0

$$f_1(x) = e^x(-0.57722 - \ln x + x - \frac{x^2}{4} + \frac{x^3}{18} - \frac{x^4}{96} + \frac{x^5}{600}) \qquad (5)$$

b) For $1.0 < x < \infty$

$$f_1(x) = \frac{1}{x} \frac{x^4 + a_1 x^3 + a_2 x^2 + a_3 x + a_4}{x^4 + b_1 x^3 + b_2 x^2 + b_3 x + b_4} \qquad (6)$$

where a_i , b_i are the fit parameters given by Table 4.

Table 4

i	a_i	b_i
1	8.5733	9.5733
2	18.059	25.633
3	8.6347	21.100
4	0.26777	3.9585

c)

$$f_2(x) = \frac{1}{x^2} \frac{x^3 + a_1 x^2 + a_2 x + a_3}{x^3 + a_4 x^2 + a_5 x + a_6} \qquad (7)$$

in which, the fit parameters a_i are given in Table 5 with three regions

Table 5

a_i	x=1--0.2	x=0.2--1	x=1--∞
1	0.30492(+6)	0.60050(+6)	0.68406(+6)
2	0.10672(+4)	0.16560(+4)	0.45186(+4)
3	-0.86781(0)	-0.89271(0)	-0.46548(+1)
4	-0.32275(+6)	0.63419(+6)	0.68665(+6)
5	0.97598(+6)	0.15300(+7)	0.19197(+7)
6	0.35238(+5)	0.98814(+5)	-0.37030(+5)

The ionization cross sections for Ne^{q+} ions (q=1, 2, ...9) are shown in Fig. 1---Fig.9 separately. The curves in these figures are calculated by Eq.(1) . The rate coefficients for Ne^{q+}(q=1,2,....9) are shown in Fig. 10. The curves in Fig. 10 are obtained by Eq.(4). The points in Fig.10 are given by Voronov [7] (see Appendix). Our results and Voronov's one are close to each other.

Appendix

Dr. Voronov gave the following fit formula [7] for atom and ions from H to Ni recommended by the Belfast group,

$$< \sigma V >= A\frac{(1+PU^{1/2})}{(X+U)}U^{K}e^{-U}, \quad (cm^3 \cdot s^{-1})$$

where, $U=\frac{dE}{T_e}$, dE is threshold energy, T_e is electron temperature; A, X, K, P are adjustable parameters. For Ne atom and its ions they are given in Table 6.

Table 6

ion	dE(eV)	P	$A_{(cm^3 \cdot s^{-1})}$	X	K	T_{min}(eV)	T_{max}(keV)
Ne	21.6	1	0.150(-7)	0.0329	0.43	1	20
Ne^{1+}	41.0	0	0.198(-7)	0.295	0.20	3	20
Ne^{2+}	63.5	1	0.703(-8)	0.0677	0.39	3	20
Ne^{3+}	97.1	1	0.424(-8)	0.0482	0.58	5	20
Ne^{4+}	126.2	1	0.279(-8)	0.305	0.25	7	20
Ne^{5+}	157.9	0	0.345(-8)	0.581	0.28	7	20
Ne^{6+}	207.3	1	0.956(-9)	0.749	0.14	10	20
Ne^{7+}	239.1	1	0.473(-9)	0.992	0.04	10	20
Ne^{8+}	1196.0	1	0.392(-10)	0.262	0.20	50	100
Ne^{9+}	1360.6	1	0.277(-10)	0.661	0.13	70	100

3 The cross sections for charge transfer in Ar^{q+} collisions with atomic hydrogen were calculated in classical trajectory Monte Carlo (CTMC) method. The main results have been published already (See Dr. Qiu Y. B. et ai., J. Phys. B 30, 1955-1960).

Refrences

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[18] Wang, Y. S. et al.
Phys. Rev. A (to be publishted, 1997)

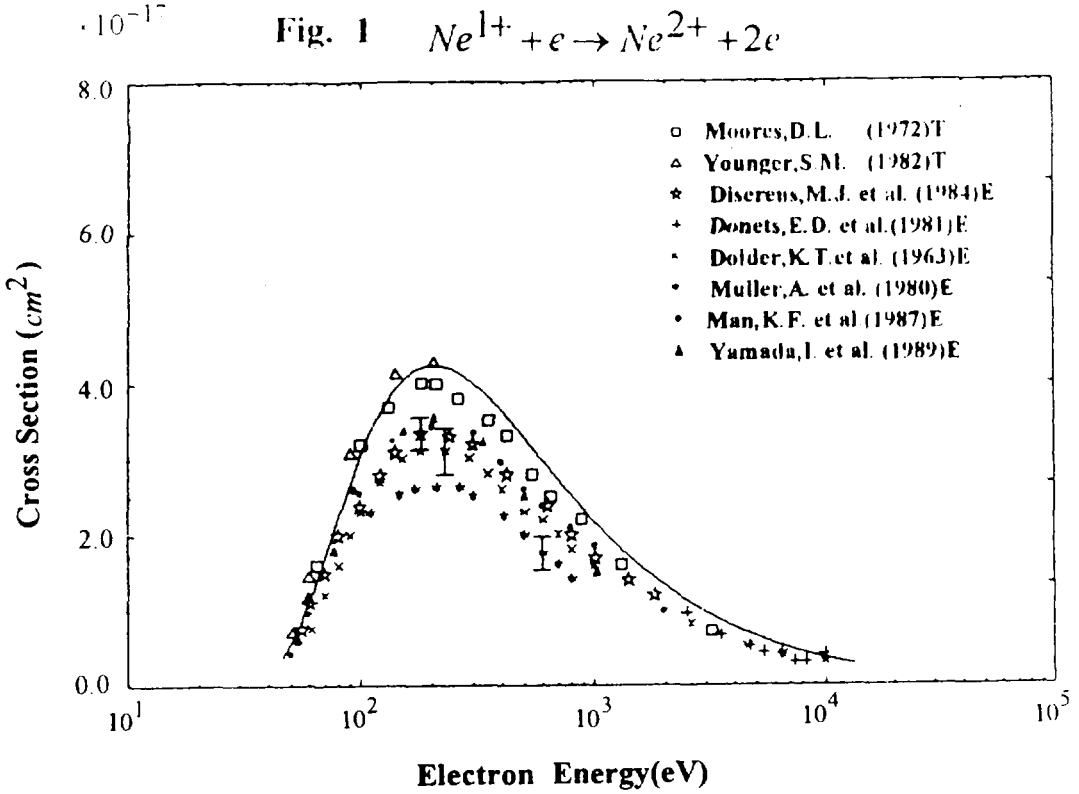


Fig. 1 $Ne^{1+} + e \rightarrow Ne^{2+} + 2e$

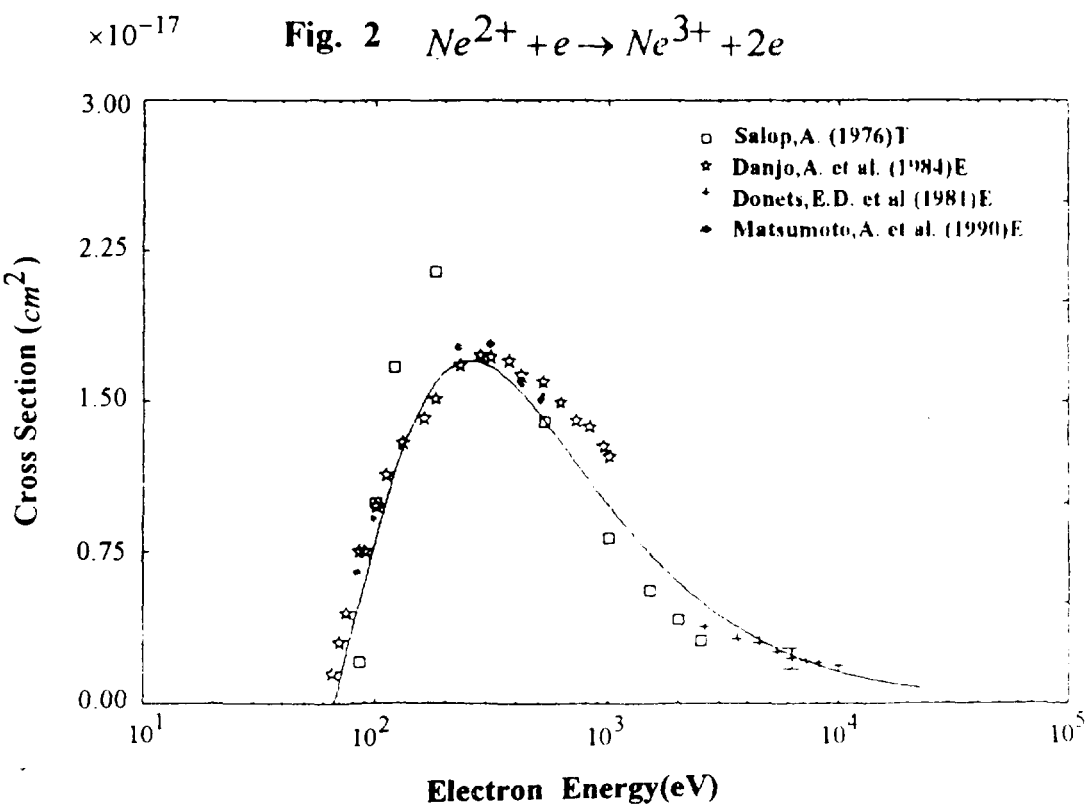


Fig. 2 $Ne^{2+} + e \rightarrow Ne^{3+} + 2e$

Fig. 3 $Ne^{3+} + e \rightarrow Ne^{4+} + 2e$

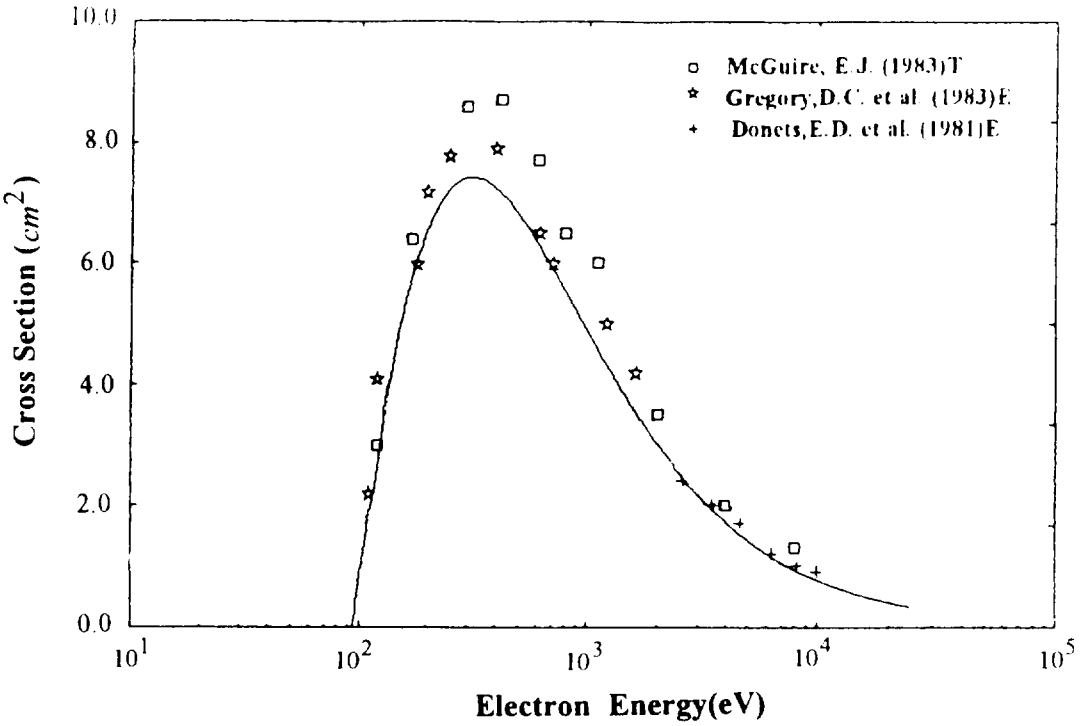


Fig. 4 $Ne^{4+} + e \rightarrow Ne^{5+} + 2e$

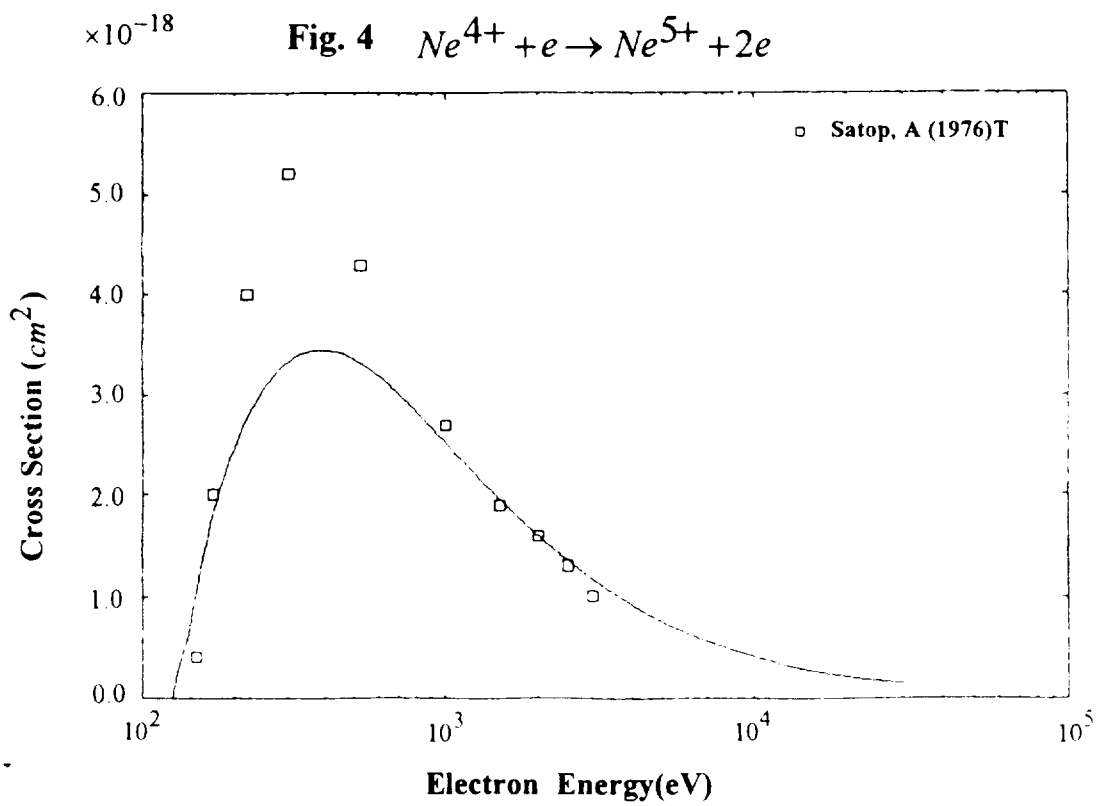


Fig. 5 $Ne^{5+} + e \rightarrow Ne^{6+} + 2e$

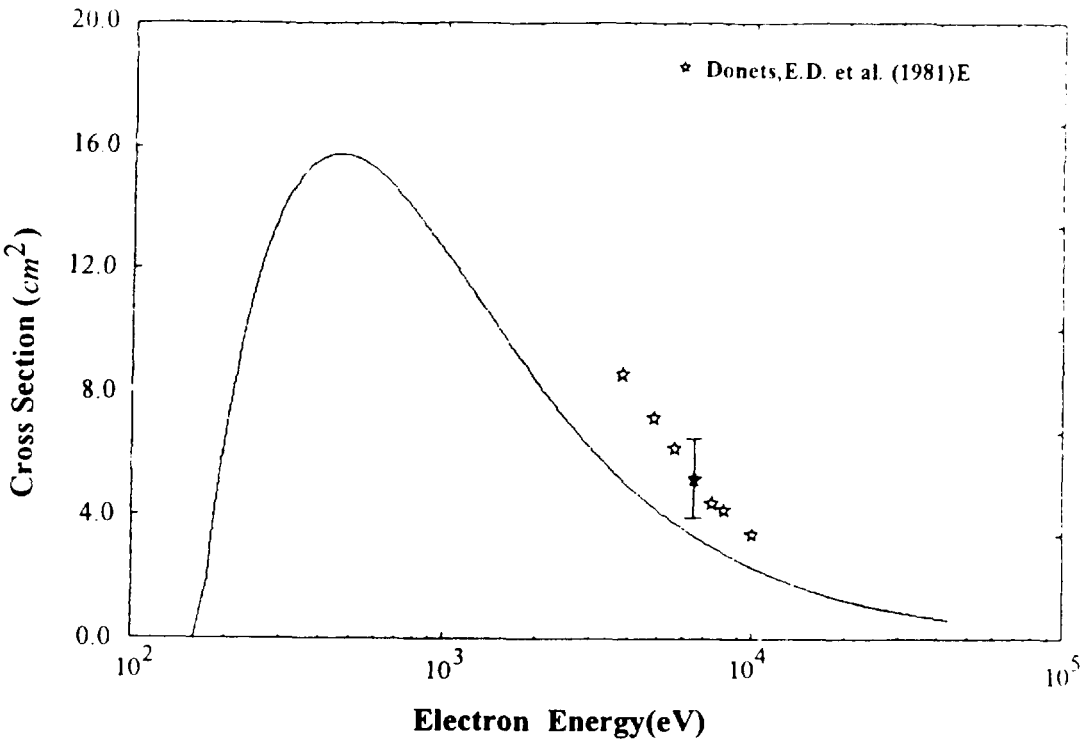


Fig. 6 $Ne^{6+} + e \rightarrow Ne^{7+} + 2e$

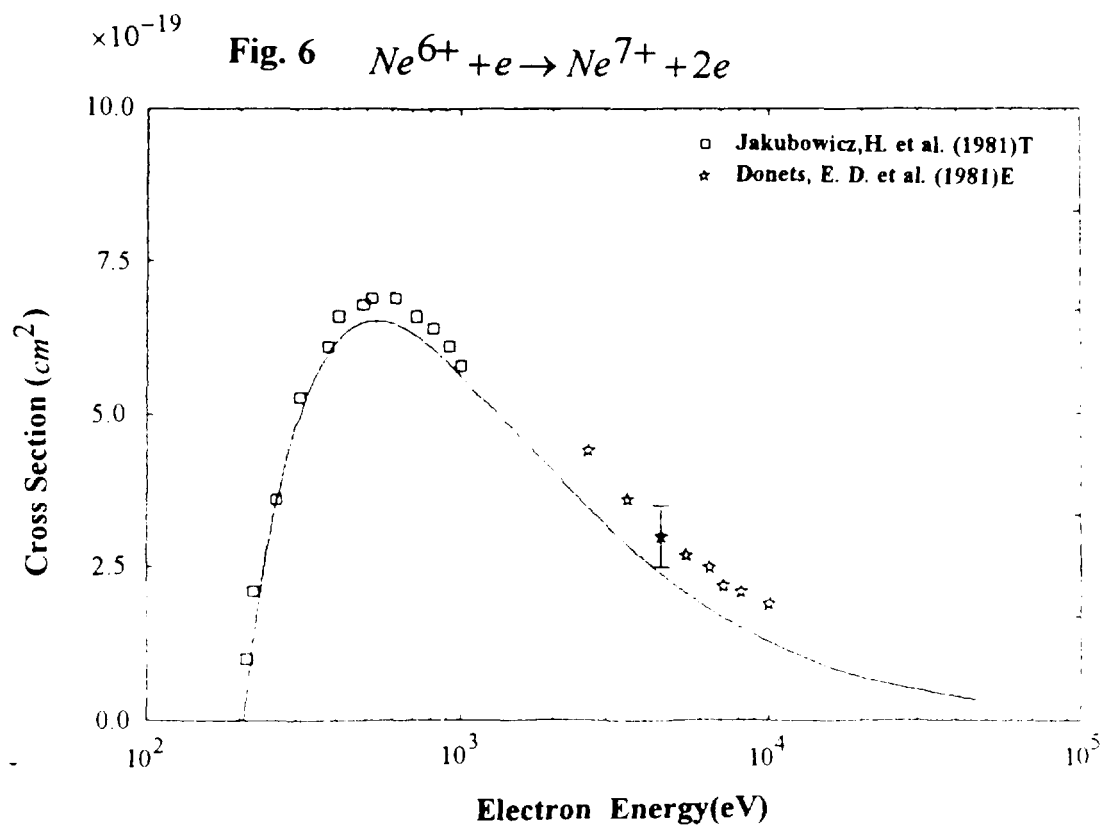


Fig. 7 $Ne^{7+} + e \rightarrow Ne^{8+} + 2e$

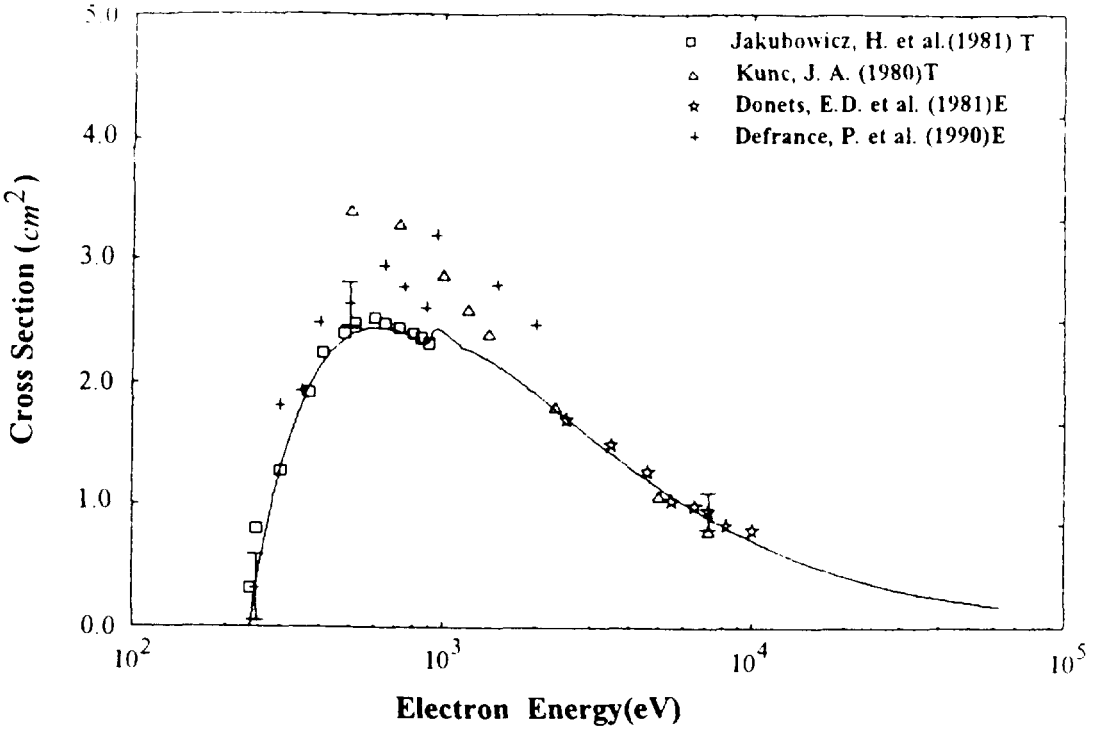


Fig. 8 $Ne^{8+} + e \rightarrow Ne^{9+} + 2e$

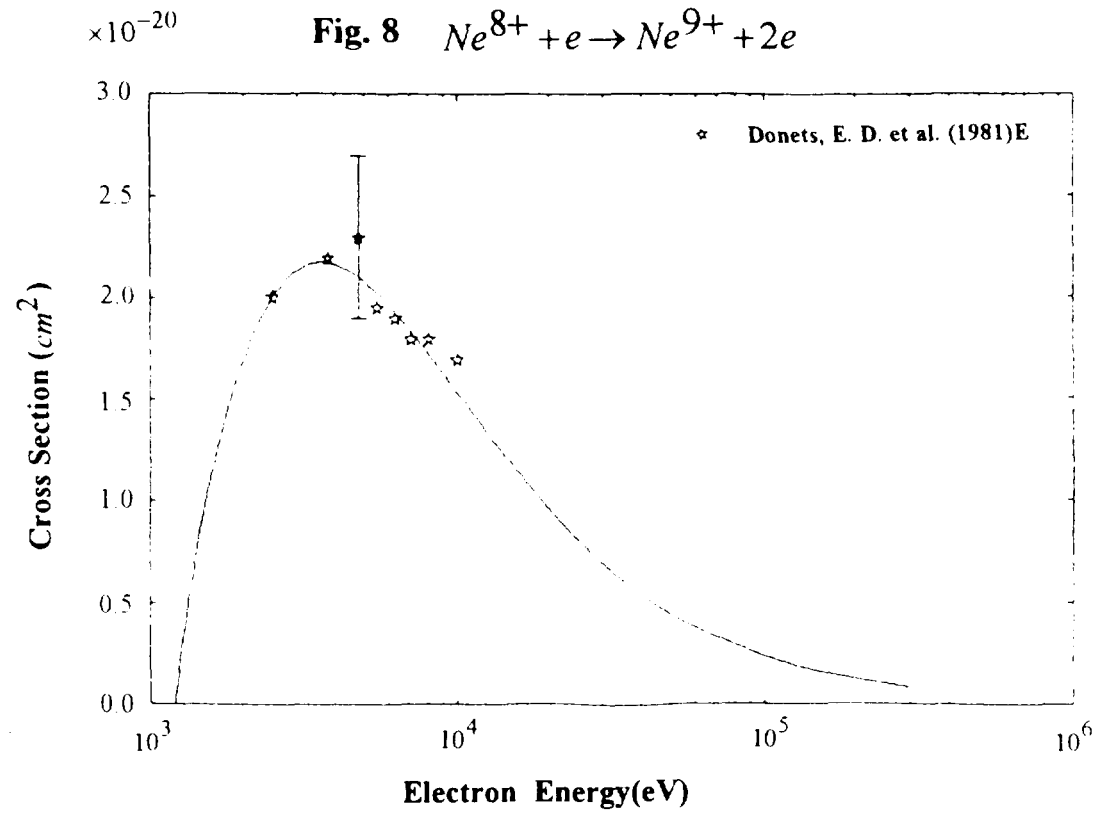


Fig. 9 $Ne^{9+} + e \rightarrow Ne^{10+} + 2e$

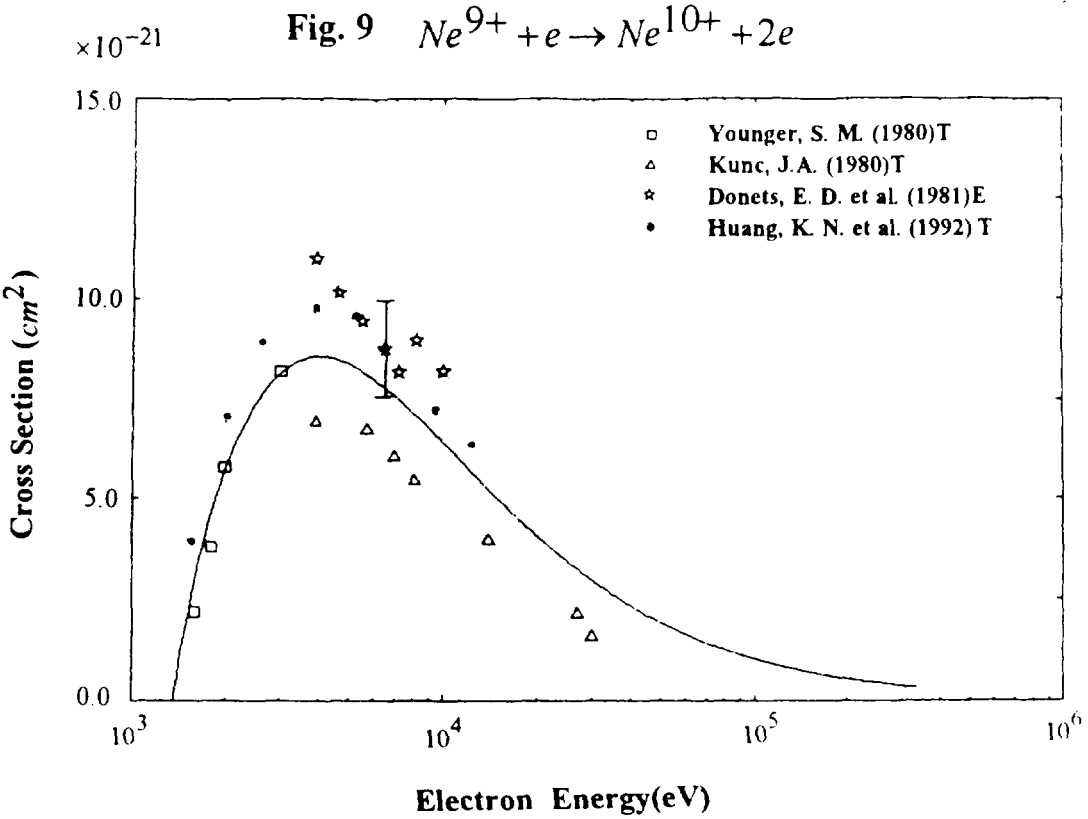
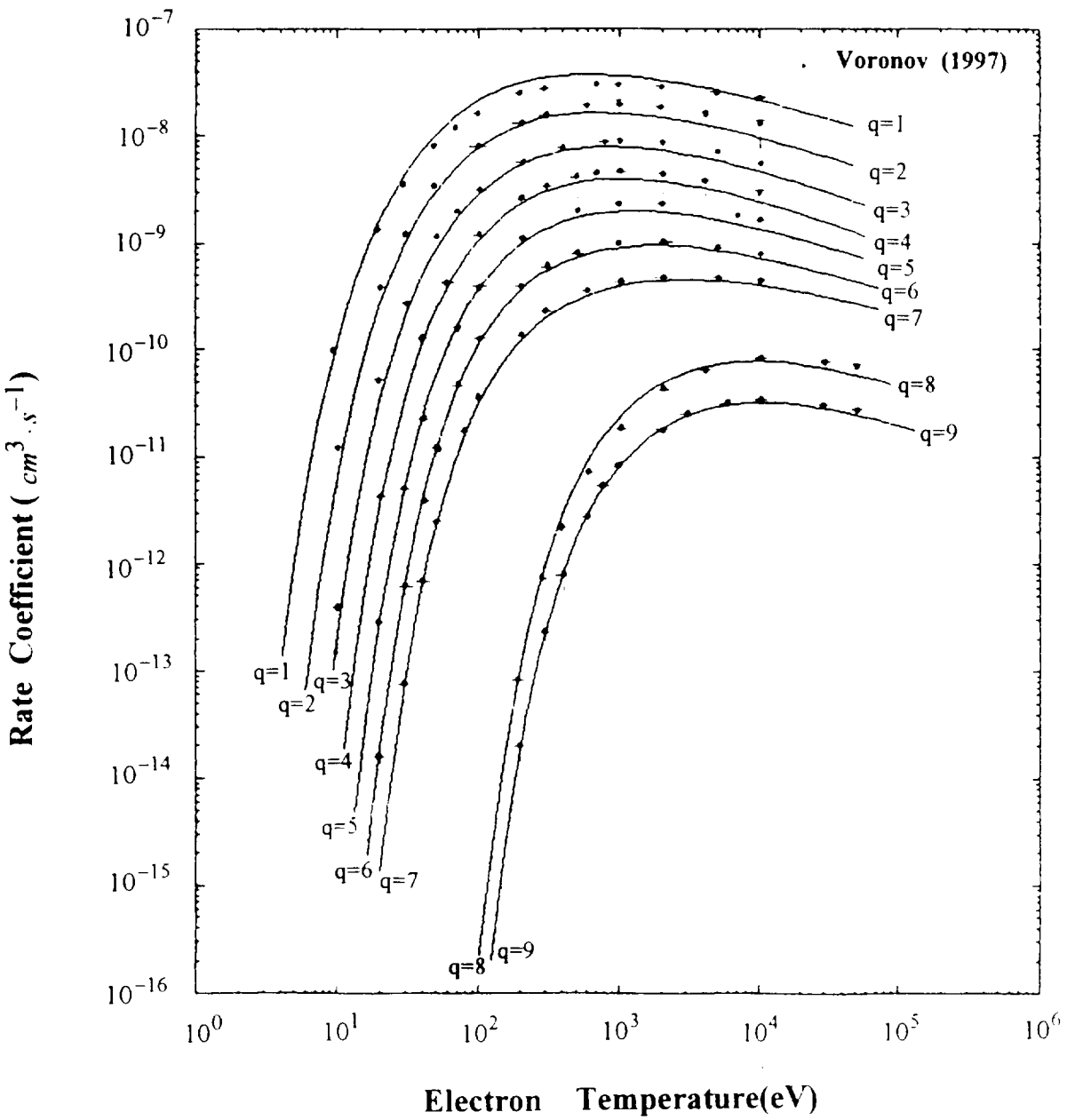


Fig. 10 Rate Coefficients for Neon Ions (Ne^{q+})



INTERNATIONAL ATOMIC ENERGY AGENCY

Atomic and Molecular Data Unit

Nuclear Data Section

Report of Activities: June/1996 to July/1997

Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (14th Meeting of the A+M Data Centres and ALADDIN Network)

Prepared by: J.A. Stephens
July 17, 1997

STAFF AND EQUIPMENT

- Staff
  - 2 Physicists
  - 1 Documentation Clerk and Support
  - Short-term Consultants
- Equipment
  - IBM RS6000/340 Workstation
    - 128 MB of RAM
    - 2 GB of Hard Disc Storage
    - Operating System: UNIX/AIX 3.2 (to be upgraded to 4.2)
  - IBM RS6000/E30 Workstation
    - 384 MB of RAM
    - 9 GB of Hard Disc Storage
    - Operating System: UNIX/AIX 4.2
  - IBM RS6000/PowerPC 40P
    - 32 MB of RAM
    - 1 GB of Hard Disc Storage
    - Operating System: UNIX/AIX 4.1

- Two IBM X-station/140 terminals
- 2 IBM PCs
  * 8 Mbytes RAM
  * 40-80 MB Hard Disc
  * Operating System: MS/DOS, MS/Windows

- Communications
  - INTERNET
    * Anonymous ftp account: user "anonymous" or "ftp"
    * AMDIS on-line service: user "aladdin"
    * WWW page: new version to be released soon.
    * IP Address: ripcrs01.iaea.or.at

AREAS OF INTEREST

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

PROJECTS

- Status of AMDIS Interface and Usage
- Data Evaluation and Recommendation
- Coordinated Research Projects and Research Contracts

Status of AMDIS Interface and Usage

Atomic and Molecular Data Information System (AMDIS):

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

A+M Bibliographic Data System (AMBDAS):

-AMBDAS of the A+M Data Unit contains bibliographic entries with information relevant to fusion research and development.

-Online system gives access to this bibliographic database with a menu-driven, user-friendly environment.

ALADDIN Interface and Database:

-Online database system, menu-driven and user-friendly environment. Within a database a search-tree of hierarchical labels is built to do the search, with selected Boolean labels.

-Both Fortran ("old" version of ALADDIN) and C-versions used. Some bugs have been corrected in menu-interface.

-Most improvements discussed at 13th DCN Meeting still need to be implemented.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Ju -95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

SELECTION CRITERIA

Author
Process
Reactants
Reference
Year of Pub ication
Energy/Te p.
Method (Th/E|p)
RETRIEVAL

HELP: Choose selection criteria.

INTERNATIONAL ATOMIC ENERGY AGENCY 07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

BIBLIOGRAPHIC RETRIEVAL SYSTEM

PROCESS

Code (?)

Category

SELECT PROCESS

Category	Process
Structure an	B Line Shapes and Shifts
Structure an	GS Structure, Spectra
Structure an	I Interatomic Potentials
Structure an	P Polarizabilities, Electric mom
Structure an	S Energy Leves, Wavelengths
Structure an	T Transition probabil., Oscill.
Photon colli	GP Photon Collisions
Photon colli	PA Total Absor., Scat.

HELP: Select process that you want.

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INTERNATIONAL ATOMIC ENERGY AGENCY                          07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

                              ALADDIN

 HIERARCHICAL LABEL
 ?????????????????????????????????????????????????????????????????????????????
 ?  ASDET: Associative detachment:A + B[-] -> AB + e                            ?
 ?  ASION: Associative Ionization:A + B ->  AB[+] + e                           ?
 ?  BEM: Spectral band emission:A + BC -> \lambda \lambda'                      ?
 ?  CHEMION: Chem. ionization = Penning + associative + other ionization        ?
 ?  CX: Charge Exchange (Single), Total:A[+q] + B -> A[+(q-1)] + B[+]            ?
 ?  CX2: Double Charge Exchange Total:A[+q] + B -> A[+(q-2)] + B[+2]             ?
 ?  CXSS: State Selec. Elec. Capture, Single:A[+q] + B -> A[+(q-1)] + B[+]      ?
 ?  DEST: Destruction of Projectile or Target                                   ?
 ?  DEXC: Collisional De-Excitation (of target):A + B (*) -> A + B              ?
 ?  DEXC+STRIP: Projec. De-Excit. by Stripping:A(*) + B -> A[+](*) + B + C      ?
 ?  DIS: Direct (Impact) Dissociation:A + BC  -> A + B + C                      ?
 ?  DISCX: Dissociative Charge Exch.:A[+q] + BC -> A[+(q-1)] + B + C[+]         ?
 ?????????????????????????????????????????????????????????????????????????????
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INTERNATIONAL ATOMIC ENERGY AGENCY                          07-Jul-95
ATOMIC AND MOLECULAR DATA INFORMATION SYSTEM

                              ALADDIN

 HIERARCHICAL LABEL
 CX C [+1] H

                          ????????
  ASD| *C  | *[+1| *H  ?  [+0] ?A + B[-] -> AB + e
  ASI|  Fe |  [+2|  H(2?????????A + B ->  AB[+] + e
  BEM|  H  |  [+3|_______|ion:A + BC -> \lambda \lambda'
  CHE|  He |  [+4| |ization = Penning + associative + other ionization
 *CX:|  H(2|  [+5| |e (Single), Total:A[+q] + B -> A[+(q-1)] + B[+]
  CX2|  O  |  [+6| | Exchange Total:A[+q] + B -> A[+(q-2)] + B[+2]
  CXS|_____|_____| | Elec. Capture, Single:A[+q] + B -> A[+(q-1)] + B[+]
  DEST: Destruction of Projectile or Target
  DEXC: Collisional De-Excitation (of target):A + B (*) -> A + B
  DEXC+STRIP: Projec. De-Excit. by Stripping:A(*) + B -> A[+](*) + B + C
  DIS: Direct (Impact) Dissociation:A + BC  -> A + B + C
  DISCX: Dissociative Charge Exch.:A[+q] + BC -> A[+(q-1)] + B + C[+]
```

New ALADDIN formatted data added to AMDIS collisional database:

-Collisional database for Lithium-beam interaction with fusion plasmas. (Published as "Cross sections for collision processes of Li atoms interacting with electrons, protons, multiply-charged ions and hydrogen molecules", by D. Wutte, R.K. Janev, F. Aumayr, M. Schneider, J. Schweinzer, J.J. Smith and HP. Winter, At. Data Nucl. Data Tables **65**, 155 (1997).)

New ALADDIN formatted data (stored on disk only):

-Collisional database for electron-impact excitation of Neon. (From Institute of Applied Physics and Computational Mathematics-China).

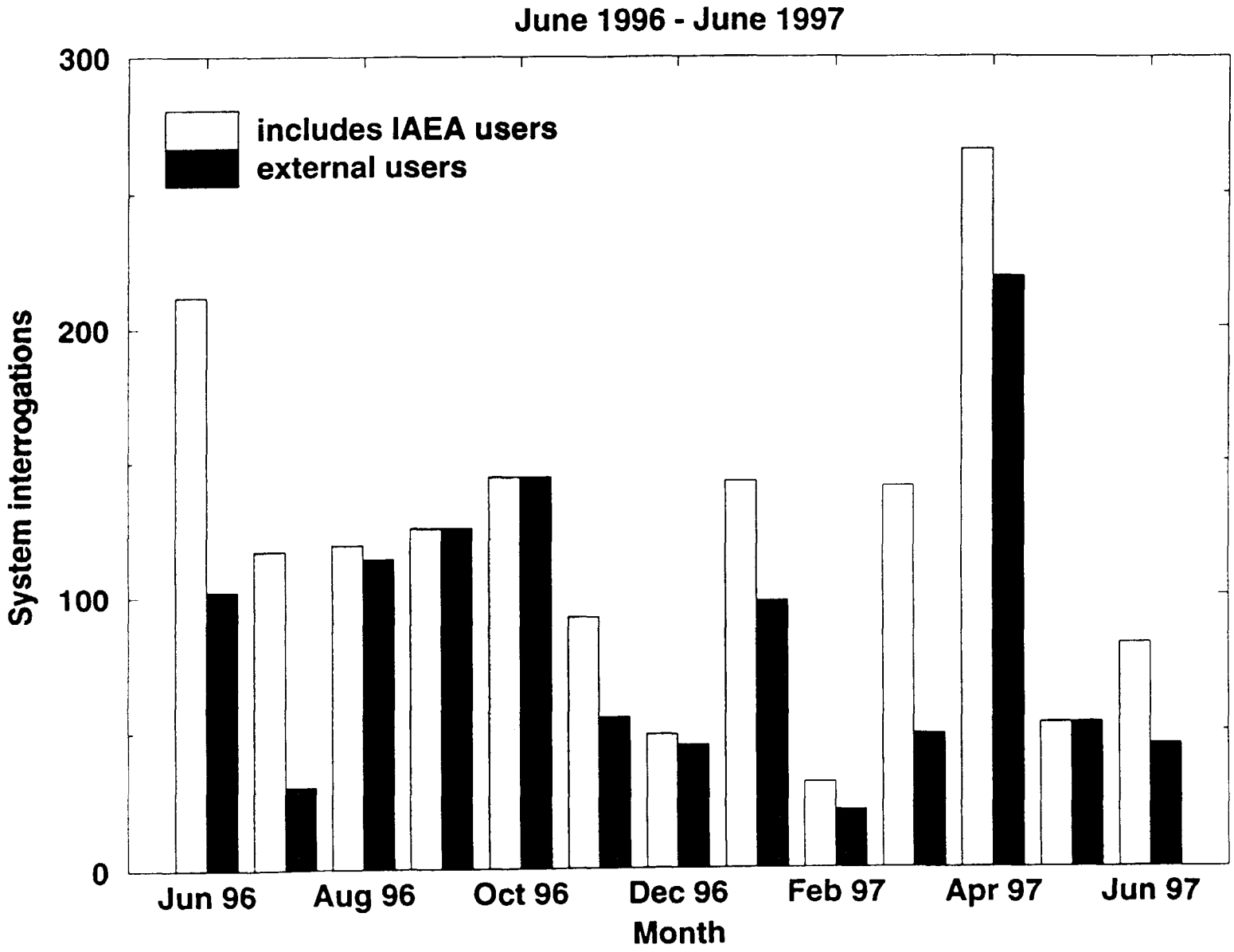
Maintenance of the IAEA Bibliographic Database:

~34600 entries, dating from 1950 to present. Includes *International Bulletin on Atomic and Molecular Data for Fusion* (published semiannually) through Vols.1-52 (Vol. 52 in preparation).

Contributors:

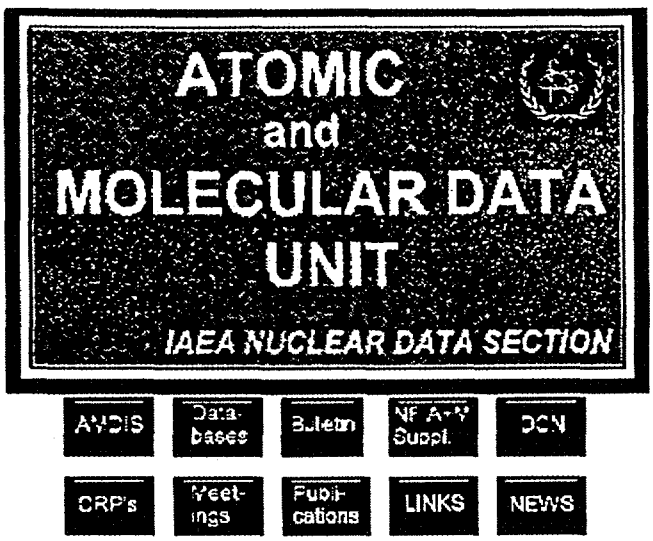
ORNL (USA)
NIST (USA)
Kurchatov Institute (Russian Federation)
NIFS (Japan)

AMDIS Usage Statistics



World Wide Web Homepage-

- Provide new or potential users informative background of A+M Data Unit function and services, and Telnet/FTP access to database server.
- Provide experienced ALADDIN users or other experts easy and user-friendly access to A+M Data Unit services.
- Direct access to existing databases in block data form (if desired), direct downloading of databases from Web page.
- Information on current and upcoming activities, meetings, publications, etc.
- Links to DCN laboratories, major fusion laboratories.



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

The primary objective of Atomic and Molecular Data Unit is to establish and maintain internationally recommended numerical databases on atomic and molecular collision and radiative processes, atomic and molecular structure characteristics, particle-solid surface interaction processes and physico-chemical and thermo-mechanical material properties for use in fusion energy research and other plasma science and technology applications.

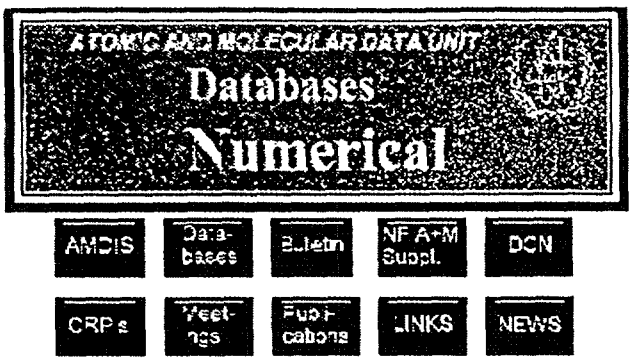
The IAEA Atomic and Molecular Data Unit achieves this objective by coordinating the activities of the International Atomic and Molecular Data Center Network (DCN), initiation and conducting international Coordinated Research Programmes (CRP's), organization of various types of Expert's Meetings, and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

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

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

The IAEA Atomic and Molecular Data Unit links with national A+M and PMI data centers and with the major fusion research laboratories.

The activity of the IAEA Atomic and Molecular Data Unit is supervised and biennially reviewed by the



A = ALADDIN formatted database

R = Recommended database

EV = Evaluated database

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1. Spectroscopic Databases

There are presently no entries in the IAEA database in this category. The interested data searchers are directed to the US NIST Atomic Data Centre.

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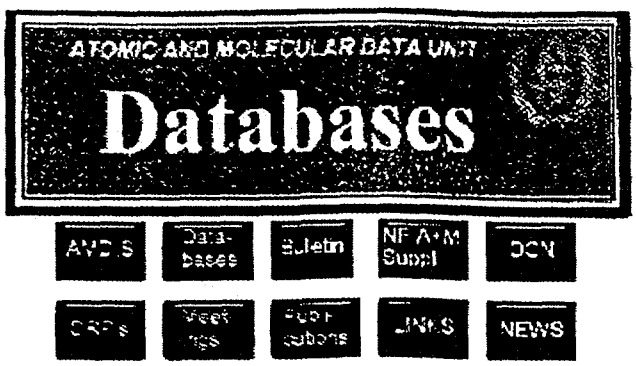
2. Collisional Databases

2.1 Electron-Atom/Ion/Molecule Collisions

- **(A,R) 1. "Atomic and Molecular Data for Fusion, Part I - Recommended Cross Sections and Rates for Electron Ionization of Light Atoms and Ions", by K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, F.J. Smith.**
  J. Phys. Chem. Ref. Data 12, 891 (1983).
  (This database has been updated and attached to database #4 below.)
- **(A,R) 2. "Recommended Data on Excitation of Carbon and Oxygen Ions by Electron Collisions", by Y. Itikawa, S. Hara, T. Kato, S. Nakazaki, M.S. Pindzola, D.H. Crandall.**
  At. Data Nucl. Data Tables (ADNDT) 33, 149 (1985)
  (This database has been updated in the database 2.3#1 below.)
- **(A,R) 3. "Recommended Data on Atomic Collision Processes Involving Iron and its Ions", by C. Bottcher, D.C. Griffin, H.T. Hunter, R.K. Janev, A.E. Kingston, M.A. Lennon, R. A. Phaneuf, M.S. Pindzola, S.M. Younger.**



The IAEA Atomic and Molecular Data Unit stores and maintains recommended and critically assessed (evaluated) numerical databases of atomic and molecular (A+M) collisional and radiative properties (cross sections, spectroscopic data), particle-surface interactions (PSI) processes (such as physical sputtering, erosion, etc.) and bulk material properties (e.g. thermomechanical properties, particle diffusion, retention, etc.). The ALADDIN formatted numerical databases (called also ALADDIN database) and the entire Bibliographic Database (AMBDAS) constitute the factual content of AMDIS.

The attribute "recommended" means that the data information contained in the respective database has been considered as the best available at the moment of its recommendation for use in fusion research (and for other applications). The recommendation is usually made by a group of experts, by the A+M Data Center Network and by the IFRC A+M Subcommittee.

Evaluated databases are collections of data critically assessed by individual experts or group of experts, but have not passed the more stringent procedure of "recommendation" by a broader expert body.

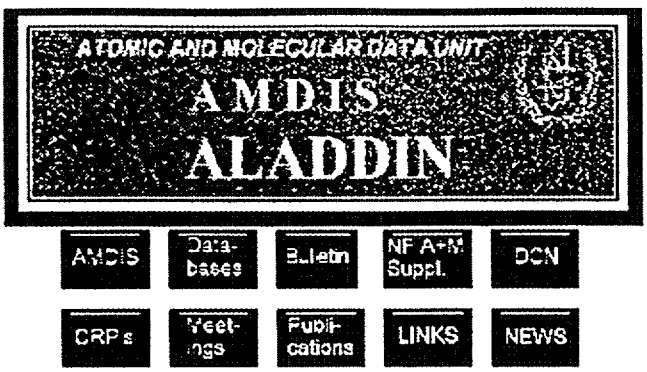
Categories of available databases:

• Numerical Databases:

1. Spectroscopic Databases
2. Collisional Databases
3. Particle-Surface Interaction Databases
4. Material Properties Databases
5. Special Purpose Databases

• Bibliographic Database (AMBDAS)

• Main Page



What is ALADDIN?

ALADDIN Data Storage and Retrieval Principles

General Description of ALADDIN Data Files

ALADDIN Dictionaries

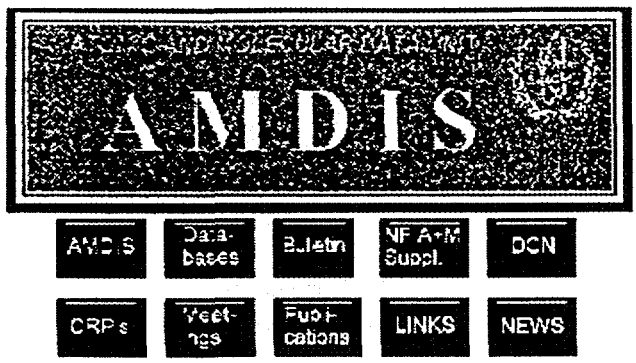
Dictionary files contain documentation which describes the particular labels forming data entries. These files support a simple label based search structure for accessing the documentation and can be used with the interactive system.

- 1. Dictionary for atomic and molecular (spectroscopic and collisional) data.
- 2. Dictionary for particle-surface interaction data.
- 3. Dictionary for material properties data.
- 4. Dictionary of Boolean labels.
- 5. Dictionary of ALADDIN evaluation functions.

• Sample of ALADDIN Files

• ALADDIN Data Files

• INTERACTIVE ACCESS TO



Atomic and Molecular Data Information System (AMDIS)

AMDIS is a database information system consisting of the Atomic and Molecular Bibliographic Data System (AMBDAS) and numerical databases of recommended and evaluated atomic, molecular and plasma-surface interaction data (ALADDIN) for fusion research.

- **Numerical Databases and**
- **ALADDIN**

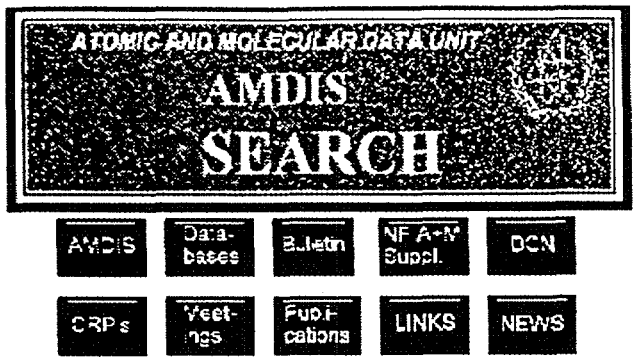
- **Bibliographic Database (AMBDAS)**

• INTERACTIVE ACCESS TO AMDIS

AMDIS DOCUMENTATION

- **PostScript Version of AMDIS User's Manual**
- **Latex Version of AMDIS User's Manual**

- **Brief Instructions for Running AMDIS**



The AMDIS database system contains atomic, molecular, plasma-material interaction and material properties data. Both bibliographic and numeric information is available covering the main processes, species and materials of interest in thermonuclear energy research and development. The data storage and retrieval principles for ALADDIN are described in the AMDIS/ALADDIN Section. A search within AMDIS can be initiated via a telnet session to the A+M Data Unit server either as a guest or registered user.

To use this service as a guest or registered user, choose

• TELNET SESSION

to start a telnet session (username 'ALADDIN', userid 'GUEST' for guest users, or userid 'PASSWD' for registered users).

To register as a user or to obtain more information, send an e-mail to:
PSM@RIPCRS01.IAEA.OR.AT
giving your name, affiliation, and full mailing address.

• Retrieve Data

This opens an FTP session to the database server and provides an opportunity to download the data files that were named and saved in AMDIS.

• Main Page

Data Evaluation, Assessment, and Recommendations:

- Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions. IAEA INDC(NDS)-369. (Bartschat, Berrington, Bray, Stephens, Janev).

- Collisional Database for Excited Hydrogen and He^{+}(n) with Fully Stripped Fusion Plasma Impurities (He^{4+}, Li^{+3}, Be^{+4}, B^{+5+}). INDC(NDS) Report in preparation. (Solov'ev, Janev, Stephens).

- Plasma-Surface Interaction Induced Erosion Database: In progress (Stephens).

CRP: "Plasma-surface interaction induced erosion of fusion reactor materials"

A. Haasz (U. Toronto), W. Eckstein (MPI-Garching),
E. Vietzke (KFA-Jülich), Y. Hirooka (U. San Diego).

Handbook and database for:

- -Chemical Erosion
- -Physical Sputtering
- -Radiation Enhanced Sublimation
- -Erosion Data Derived from Tokamaks

Target materials: mainly Be, C, W, plus some doped graphites, B_4C, TiC, SiC..
Projectiles: H, D, T, He, C, O, Ne, Ar, N.
Parameters: Chemical and sputtering yields as functions of temperature, incident flux, incident energy.

-To be published in "Atomic and Plasma-Material Interaction Data for Fusion" (Nucl. Fusion Suppl.) Vol. 7 (1997), and included in the PSI ALADDIN database.

1.6.1 H^0/H_3^+ + pyrolytic graphite → C_xH_y

Source: J. W. Davis, A. A. Haasz and P. C. Stangeby, J. Nucl. Mater. **155**, 234 (1988).

Accuracy: Yield: ±35%; T: ±25K.

Comments: (1) Steady-state hydrocarbon production.
(2) Specimen: graphite (pyrolytic).
(3) H^+ ions: mass analyzed accelerator; H^0 (sub-eV) is produced via dissociation of H_2 on a hot W ribbon.
(4) Methane measured via QMS-RGA.

Analytic fitting function:

Erosion yield:

$$P = 1.0 \times 10^{-2}[A_1 \exp(-(T - A_2)^2/A_3)T^{A_4} + A_5 \exp(-A_6 T)T^{A_7}] \quad [\text{molecules}/H^0]$$

where T is in Kelvin. The rms deviation of analytic fits for reactions A (*), B (•), C (○) and D (△) are 5.2%, 11.2%, 8.7% and 7.3%, respectively.

Fitting parameters A_1-A_7

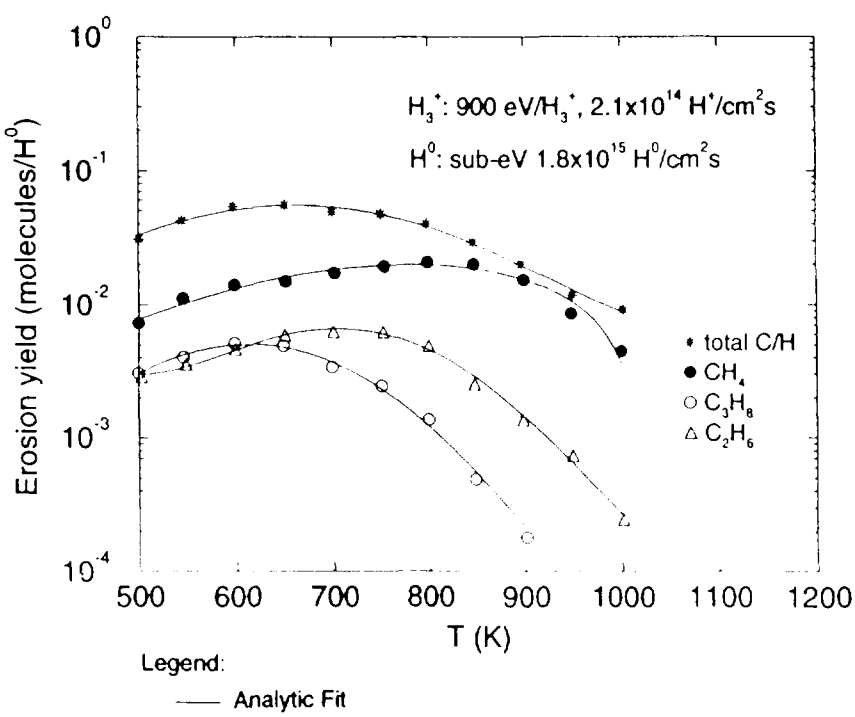
Reaction:

A	2.4666E+00	6.5490E+02	4.9773E+04	1.2144E-01	4.5660E-03	-4.3563E-03
	3.9673E-03					
B	3.1975E+00	8.5960E+02	1.2173E+05	-6.3220E-03	-3.6816E-02	-4.1054E-03
	8.4117E-04					
C	2.0100E-01	6.1025E+02	2.3821E+04	1.4164E-01	2.1990E-02	1.3259E-03
	-9.2740E-05					
D	3.8383E+00	7.1665E+02	2.1767E+04	-2.8401E-01	2.3351E+00	5.6815E-03
	7.8341E-02					

ALADDIN evaluation function for erosion yield: EYIELD7A

ALADDIN hierarchical labelling:

SST H [+0] H [+1] graphite T=HPG OR=basal-plane C
SST H [+0] H [+1] graphite T=HPG OR=basal-plane CH{4}
SST H [+0] H [+1] graphite T=HPG OR=basal-plane C{3}H{8}
SST H [+0] H [+1] graphite T=HPG OR=basal-plane C{2}H{6}



Coordinated Research Projects:

Active in 1997:

- "Radiative cooling rates of fusion plasma impurities" (8 collaborating laboratories). 2nd RCM held on 14-15 October 1996. Completion of CRP in 1997.
- "Atomic and plasma-wall interaction data for fusion reactor divertor modeling" (12 collaborating laboratories and research groups). 2nd RCM scheduled for July 30-31, 1997. Extension of this CRP for additional two years is expected.
- "Collection and evaluation of thermo-mechanical properties data of fusion reactor plasma facing materials" (8 participating laboratories). 2nd RCM held on 25-27 March 1996. Expected completion in 1998.
- "Reference data for tritium retention and release in fusion reactor plasma facing components" (8 participating laboratories). Terminated in 1996.

CRPs to be initiated in 1997:

- "Recommended charge exchange cross section data for fusion plasma studies"
- "Erosion properties data for mixed plasma facing fusion reactor materials"

Short-term consultants-

Dr. J. Botero (Colombia)

Dr. P.S. Krstić (ORNL, USA)

Dr. E.A. Solov'ev (Macedonia)

Dr. I.V. Komarov (Russia)

Dr. D. Wang (IAEA)

Opacity Project

$\gamma + A^{n+}$

A = H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si,
S, Ar, Ca, Fe

J. Phys. B. also OP vol. 1, 2 (IOP)

• • • • •

TOPBASE @ CDS

The P-Cl project

ATOMIC & IONIC P^{q+}

ATOMIC & IONIC Cl^{q+}

The calculation of bound-bound oscillator strengths for all bound states to $n=10$ (cf opacity Project).

- USING R-MATRIX TECHNIQUES WITH MULTI-STATE AND INNER-SHELL EXCITATIONS.
- f's AND PHOTOIONIZATION CROSS SECTIONS.

Cl-like Cl

Term energies relative to $3s^2 3p^4\ ^3P$ ionization threshold for each symmetry

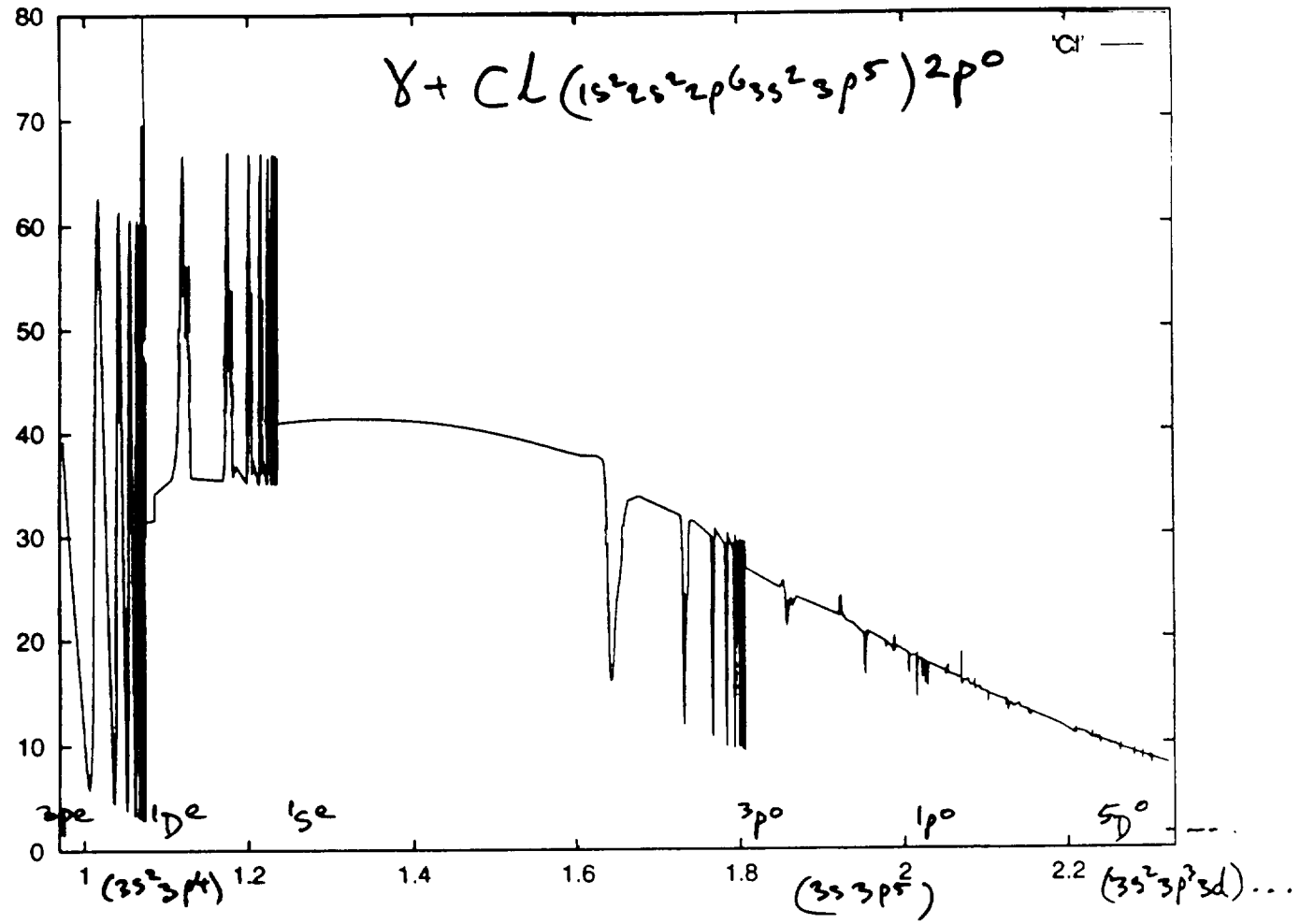
i	E(Ryds)	Description	i	E(Ryds)	Description	i	E(Ryds)	Description	i	E(Ryds)	Description
		$^2P^o$	4	−.03404	$3s^2 3p^4\ ^3P\ 7p$	7	−.04058	$3s^2 3p^4\ ^3P\ 7s$	7	−.01807	$3s^2 3p^4\ ^1D\ 3d$
1	−.97357	$3s^2 3p^5$	5	−.02425	$3s^2 3p^4\ ^3P\ 8p$	8	−.03256	$3s^2 3p^4\ ^3P\ 6d$:	8	−.01474	$3s^2 3p^4\ ^3P\ 8d$:
2	−.17393	$3s^2 3p^4\ ^3P\ 4p$	6	−.01815	$3s^2 3p^4\ ^3P\ 9p$	9	−.02810	$3s^2 3p^4\ ^3P\ 8s$	9	−.01203	$3s^2 3p^4\ ^3P\ 9d$:
3	−.09022	$3s^2 3p^4\ ^3P\ 5p$			$^2S^e$	10	−.02462	$3s^2 3p^4\ ^3P\ 7d$:			
4	−.07186	$3s^2 3p^4\ ^1D\ 4p$	1	−.19084	$3s3p^6$	11	−.02061	$3s^2 3p^4\ ^3P\ 9s$			
5	−.04910	$3s^2 3p^4\ ^3P\ 6p$	2	−.02073	$3s^2 3p^4\ ^1S\ 4s$	12	−.01911	$3s^2 3p^4\ ^3P\ 8d$:			
6	−.03316	$3s^2 3p^4\ ^3P\ 7p$			$^2P^e$			$^2D^e$			
7	−.02379	$3s^2 3p^4\ ^3P\ 8p$	1	−.26945	$3s^2 3p^4\ ^3P\ 4s$	1	−.17226	$3s^2 3p^4\ ^1D\ 4s$			
8	−.01788	$3s^2 3p^4\ ^3P\ 9p$	2	−.11910	$3s^2 3p^4\ ^3P\ 3d$	2	−.11897	$3s^2 3p^4\ ^3P\ 3d$			
		$^2S^o$	3	−.11450	$3s^2 3p^4\ ^3P\ 5s$	3	−.06702	$3s^2 3p^4\ ^3P\ 4d$			
1	−.17481	$3s^2 3p^4\ ^3P\ 4p$	4	−.06930	$3s^2 3p^4\ ^3P\ 4d$	4	−.04303	$3s^2 3p^4\ ^3P\ 5d$			
2	−.08612	$3s^2 3p^4\ ^3P\ 5p$	5	−.06372	$3s^2 3p^4\ ^3P\ 6s$	5	−.03017	$3s^2 3p^4\ ^3P\ 6d$			
3	−.05129	$3s^2 3p^4\ ^3P\ 6p$	6	−.04551	$3s^2 3p^4\ ^3P\ 5d$:	6	−.02269	$3s^2 3p^4\ ^3P\ 7d$:			

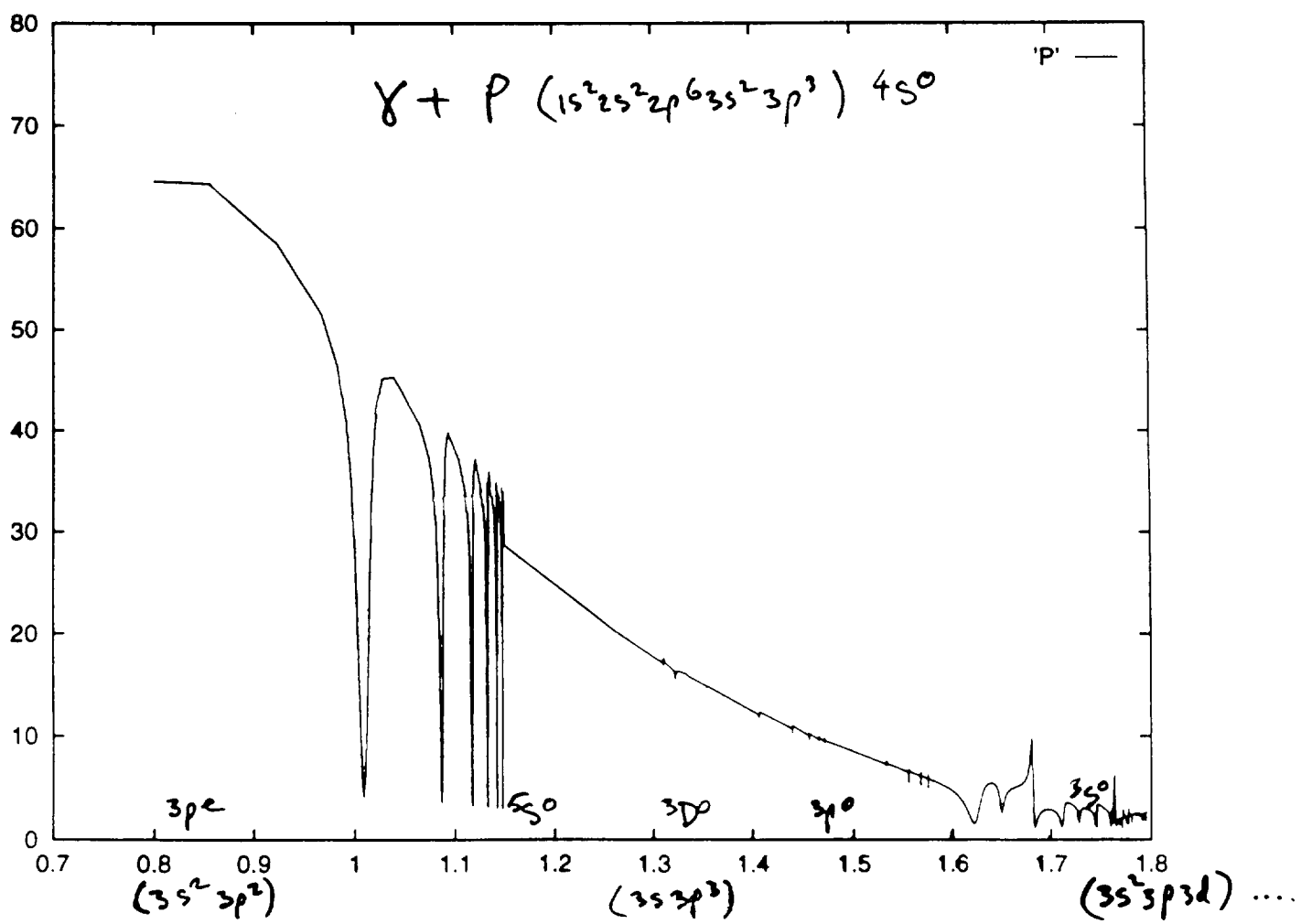
Energies in ascending order from ground state for terms with effective $n \leq 10.0$, $L \leq 2$

Term	i	E(Ryds)	Term	i	E(Ryds)	Term	i	E(Ryds)	Term	i	E(Ryds)	Term	i	E(Ryds)
$^2P^o$	1	0.00000	$^2S^o$	2	0.88745	$^2S^o$	4	0.93953	$^2P^e$	11	0.95297	$^2P^e$	15	0.96113
$^2P^e$	1	0.70412	$^2P^o$	4	0.90171	$^2P^o$	6	0.94041	$^2P^e$	12	0.95446	$^2P^e$	16	0.96145
$^2S^e$	1	0.78273	$^2P^e$	4	0.90427	$^2P^e$	8	0.94101	$^2S^o$	6	0.95543	$^2D^e$	9	0.96154
$^2S^o$	1	0.79877	$^2D^e$	3	0.90655	$^2D^e$	5	0.94340	$^2D^e$	7	0.95550	$^2S^o$	8	0.96231
$^2P^o$	2	0.79964	$^2P^e$	5	0.90985	$^2P^e$	9	0.94547	$^2P^o$	8	0.95569	$^2P^o$	10	0.96243
$^2D^e$	1	0.80131	$^2S^o$	3	0.92228	$^2P^e$	10	0.94896	$^2P^e$	13	0.95781	$^2P^e$	17	0.96350
$^2P^e$	2	0.85447	$^2P^o$	5	0.92447	$^2S^o$	5	0.94933	$^2P^e$	14	0.95848			
$^2D^e$	2	0.85460	$^2P^e$	6	0.92806	$^2P^o$	7	0.94978	$^2D^e$	8	0.95883			
$^2P^e$	3	0.85907	$^2D^e$	4	0.93054	$^2D^e$	6	0.95088	$^2S^o$	7	0.95948			
$^2P^o$	3	0.88335	$^2P^e$	7	0.93299	$^2S^e$	2	0.95284	$^2P^o$	9	0.95965			

gf-values for transitions involving terms with effective $n \leq 99.0$, $L \leq 2$

i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L
					$^2P^o$–$^2P^e$												
1	1	-1.06E−3	1	1	-1.02E+0	2	3	-1.75E+0	3	6	-3.51E−6	4	9	-1.04E−4	5	12	-7.35E−2
1	2	-3.09E−1	1	2	-2.18E−1	2	4	-4.61E−2	3	7	-1.51E−1	4	10	-1.92E−1	5	13	-2.08E−2
2	1	4.87E−4	1	3	-1.08E−1	2	5	-1.17E−1	3	8	-1.06E−4	4	11	-8.46E−6	5	14	-2.14E−2
2	2	-1.87E−2	1	4	-3.87E−2	2	6	-4.13E−2	3	9	-4.77E−2	4	12	-1.07E−1	5	15	-1.15E−2
3	1	2.47E−2	1	5	-4.43E−2	2	7	-3.52E−2	3	10	-6.21E−3	4	13	-1.03E−5	5	16	-6.29E−3
3	2	-8.46E−2	1	6	-9.02E−5	2	8	-1.59E−2	3	11	-2.10E−2	4	14	-5.74E−2	5	17	-7.22E−3
4	1	5.21E−2	1	7	-1.95E−2	2	9	-1.54E−2	3	12	-1.46E−2	4	15	-7.53E−5	6	1	4.87E−3
4	2	-1.24E−1	1	8	-3.22E−2	2	10	-1.58E−3	3	13	-1.06E−2	4	16	-3.27E−2	6	2	3.43E−3
5	1	3.96E−3	1	9	-9.52E−3	2	11	-7.91E−3	3	14	-1.70E−2	4	17	-1.98E−4	6	3	3.73E−2
5	2	-5.53E−3	1	10	-7.80E−2	2	12	-4.93E−4	3	15	-5.66E−3	5	1	1.84E−2	6	4	3.01E−2
6	1	7.91E−4	1	11	-4.84E−3	2	13	-4.41E−3	3	16	-1.58E−2	5	2	8.20E−3	6	5	2.12E−1
6	2	-6.01E−4	1	12	-8.35E−2	2	14	-2.61E−3	3	17	-2.95E−3	5	3	1.75E−1	6	6	1.90E−1
7	1	2.72E−4	1	13	-2.41E−3	2	15	-2.53E−3	4	1	9.46E−2	5	4	1.78E−1	6	7	5.36E+0
7	2	-6.62E−5	1	14	-6.46E−2	2	16	-3.68E−3	4	2	7.96E−3	5	5	4.18E+0	6	8	-1.85E−1
8	1	1.19E−4	1	15	-1.08E−3	2	17	-1.42E−3	4	3	1.05E+0	5	6	-5.49E−1	6	9	-4.84E+0
8	2	3.52E−5	1	16	-4.59E−2	3	1	1.04E−4	4	4	-5.27E−2	5	7	-3.68E+0	6	10	-1.01E+0
9	1	6.00E−5	1	17	-3.48E−4	3	2	2.62E−2	4	5	-9.87E−1	5	8	-6.13E−1	6	11	-2.47E−1
9	2	5.45E−5	2	1	2.22E+0	3	3	2.27E+0	4	6	-5.74E−1	5	9	-1.64E−1	6	12	-1.84E−1
10	1	3.34E−5	2	2	-6.47E−1	3	4	-9.53E−1	4	7	-1.63E−4	5	10	-2.33E−1	6	13	-7.07E−2
						3	5	-1.50E+0	4	8	-3.01E−1	5	11	-4.62E−2	6	14	-3.85E−2


γ + Cl (1s²2s²2p⁶3s²3p⁵) 2p°
'Cl'
80
70
60
50
40
30
20
10
0
3pe
1De
1Se
3p°
1p°
5D°
1
(3s²3p⁴)
1.2
1.4
1.6
1.8
(3s3p⁵)
2.2
(3s²3p³3d)...


γ + P (1s²2s²2p⁶3s²3p³) 4S°
'P'
80
70
60
50
40
30
20
10
0
3pe
5S°
3D°
3p°
3S°
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
(3s²3p²)
(3s3p³)
(3s²3p3d) ....

Iron Project

$e + A^{n+}$

- $A = 2p^x, 3p^x$ I/R transitions
- $A = Fe^{n+}$

TIPBASE

Astron. & Astro. Ss (1993–99)

KEITH BERRINGTON, QUEEN'S UNIVERSITY BELFAST, JULY 97.

— NEW METHODS — EXCITING TIMES —

R-MATRIX

OP (opacity Project)

CONVERGENT METHODS (CCC, IERM, RMPS)

QB (resonances)

INNER-SHELL MODELS

RELATIVISTIC MODELS

- BOUND/CONTINUUM STATES
- COLLISIONAL/RADIATIVE PROPERTIES
- ELECTRON EXCITATION/IONIZATION
- SINGLE/DOUBLE PHOTOIONIZATION
- OUTER/INNER SHELL PROCESSES

— UNIFIED TREATMENT —

AWAY FROM INDEPENDENT-PROCESSES DIVIDE & RULE STRATEGIES FOR PROCESS AND/OR ENERGY RANGE

(eg. CIVS, MCHF / R-MATRIX / CCC, RMPS / DW, BORN ...)

negative E / low E / intermediate E / high E

— QUALITY DATA —

CONVERGENCE CRITERION — INCLUSION OF ALL SIGNIFICANT CHANNELS

J. Phys. B: At. Mol. Opt. Phys. 29 (1996) 4529–4542. Printed in the UK

The QB method: analysing resonances using R-matrix theory. Applications to C^+, He and Li

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Received 10 June 1996, in final form 7 August 1996

Abstract. A procedure for analysing resonances in atomic and molecular collision theory is introduced, which exploits the analytic properties of R-matrix theory to obtain the energy derivative of the reactance (K) matrix, without assuming a pure Coulomb potential at large distances. The QB method defines matrices Q and B in terms of asymptotic solutions, the R-matrix and energy derivatives, such that $dK/dE = B^{-1}Q$, from which eigenphase gradients of the K-matrix can be obtained. Resonance positions are defined at the points of maximum gradient; resonance widths are related to the inverse of the eigenphase gradients. Resonance properties such as identifications are discussed.

The QB method is illustrated for some overlapping resonances in C^+ between the $1s^2 2s2p\ ^3P^o$ and $^1P^o$ ionization thresholds. It is then tested for accuracy against recent experimental measurements of positions and widths for doubly excited states of He between the $n = 2$ and $n = 3$ ionization thresholds, and for positions, widths and profiles of resonances in Li above the first inner-shell threshold.

INDC(NDS)-369

International Atomic Energy Agency

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Consultants' Meeting on "Critical Assessment of Electron-Impact Cross Section Database for Be and B Plasma Impurity Ions"

2-3 September 1996, IAEA Headquarters, Vienna

SUMMARY REPORT

Prepared by
K. Bartschat, K.A. Berrington, I. Bray,
J.A. Stephens and R.K. Janev

April, 1997

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

$e^- + Be\ 1s^2 2s^2$ ground state

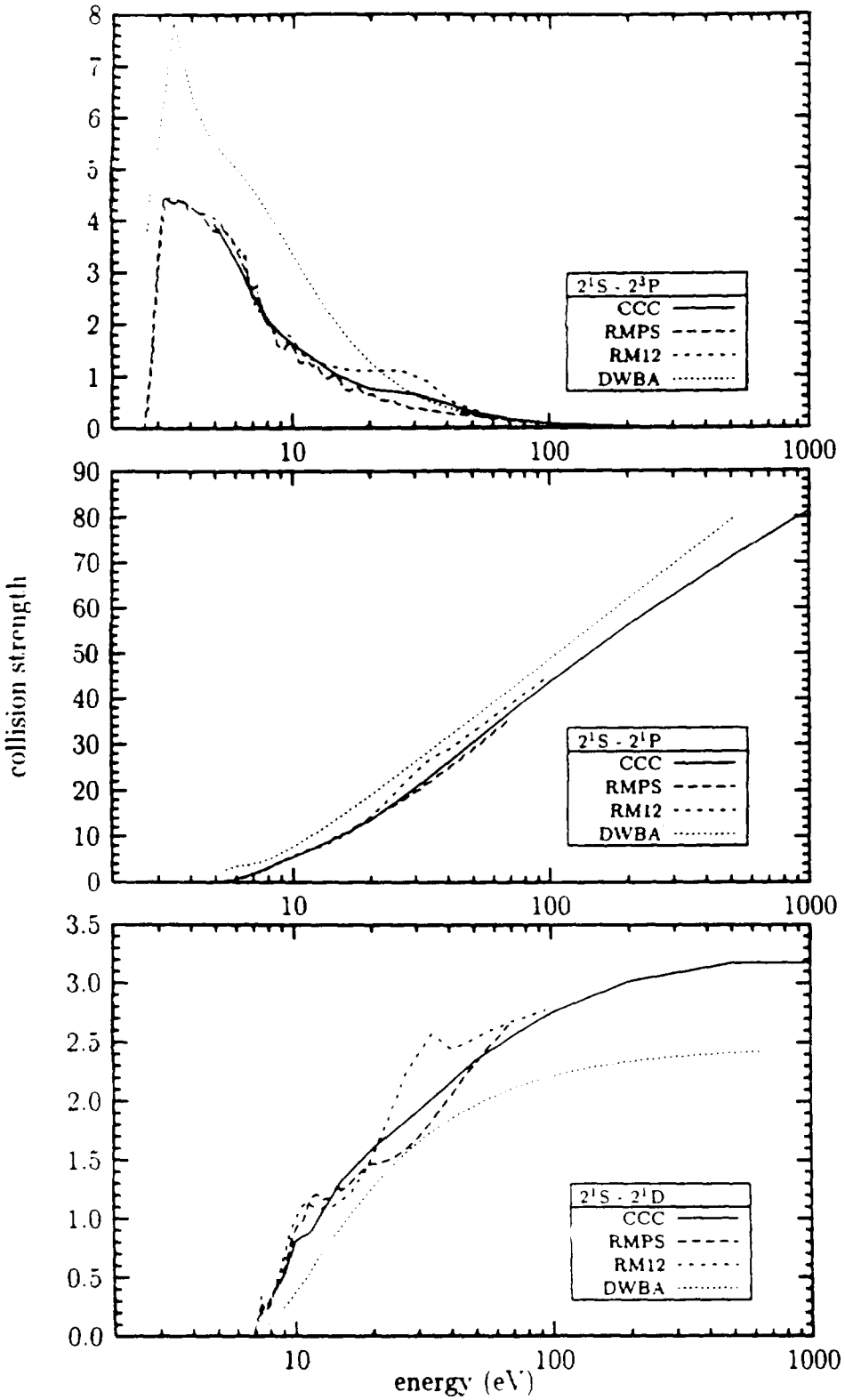

Figure 2: Collision strength for the $(2s^2)^1S - (2s2p)^3P$ (top), $(2s^2)^1S - (2s2p)^1P$ (center), and $(2s^2)^1S - (2p^2)^1D$ (bottom) transitions in Be. The individual curves are: CCC [4], RMPS [2], RM12 [5], and DWBA [5].

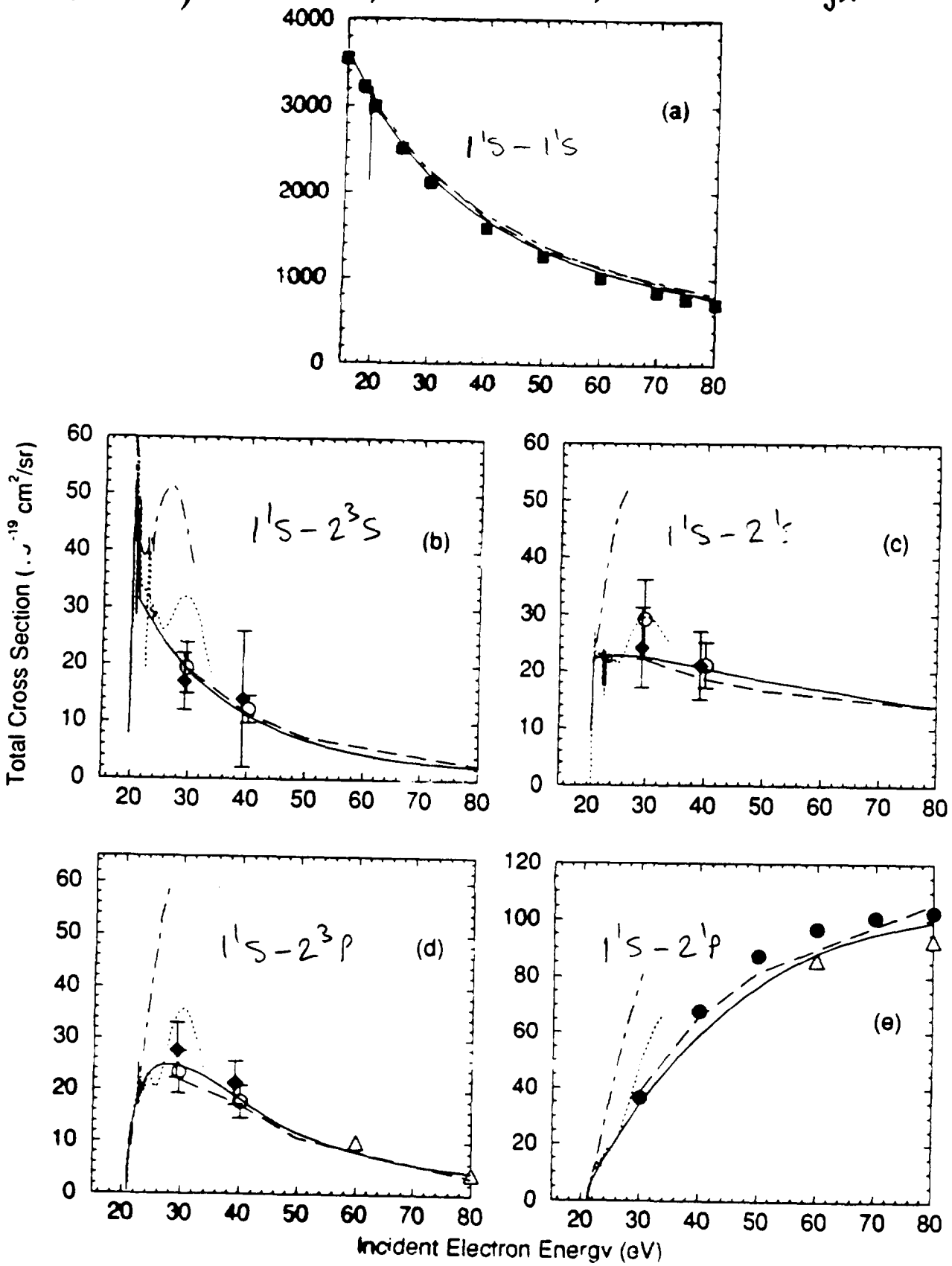

Figure 4. Integrated cross sections for elastic scattering (a) and electron impact excitation of the 2^3S (b), 2^1S (c), 2^3P^o (d) and 2^1P^o (e) states from the ground state 1^1S. The theoretical curves correspond to: ——, RMPS; – – –, CCC of Fursa and Bray (1995); – · – · (a), Two-state R-matrix calculation of Fon *et al* (1981a); – · – · (b–e), five-state R-matrix calculation of Fon *et al* (1981b); · · · · ·, 29-state R-matrix calculation of Sawey and Berrington (1993). The sources for the experimental data are: squares, Register *et al* (1980); open circles, Trajmar (1973); triangles, Chutjian and Srivastava (1975); solid diamonds, Hall *et al* (1973); solid circles, Donaldson *et al*

Hudson, Bartschat, Scott, Burke, Burke: J. Phys. B

Electron impact ionization (He)

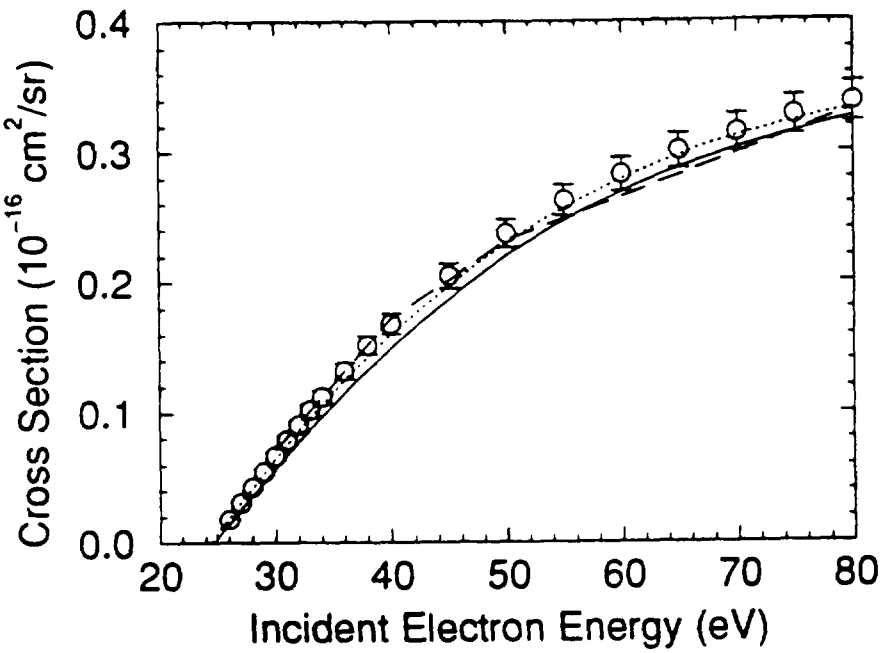

Figure 9. Total cross section for electron impact ionization of the He ground state. The theoretical curves correspond to: ——, RMPS with contribution from the positive-energy pseudo-states only; · · · · ·, RMPS with contributions from the positive-energy pseudo-states and the $3^{1,3}\bar{D}$ states: – – –, CCC (Fursa and Bray 1995). The experimental data (open circles) are taken from Montague *et al* (1984).

FIGURE 9

Hudson et al.

Subm. J. Phys. B 1997

Electron Impact Ionization of Be^+ and Photoionization of Be at the K Edge

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Abstract

We present new R-matrix calculations for ionization processes involving the beryllium K-shell, namely electron impact ionization of Be^+ $1s^22s$ and single and double photoionization of Be. These are modelled near inner-shell thresholds in a unified way, coupling direct and indirect processes, enabling comparison of the respective autoionization features. Below the K edge, we predict that direct double photoionization contributes 4% to the total cross section background for photoionizing Be; the onset of K-shell excitation-autoionization, an indirect mechanism, increases the background by a factor 20. By contrast, we find that EA in e^-+Be^+ ionization increases its background by only 4%; this is less than previous estimates, but in line with experiment. We also study high energy behaviour for photoionizing excited states, eg. Be $1s^22sns$, where we find a background dominated by $2s \rightarrow \epsilon p$ ionization. This process is normally omitted in R-matrix schemes used in opacity and recombination calculations, leading to orders-of-magnitude underestimation at high energies of excited state photoionization, which also exhibits a large $1s \rightarrow 2p$ core resonance above the K edge.

2 The beryllium example

Figure 1 shows some of the states of Be and its ions relevant to the scope of this paper. We investigate the following electron and photon impact processes at a total energy around the threshold for K-shell excitation, where nl indicates the principal and angular momentum quantum numbers of an excited outer electron:

$$\left.\begin{array}{l} e^- + Be^+(1s^2 2s) \\ h\nu + Be(1s^2 2s^2) \\ h\nu + Be(1s^2 2snl) \end{array}\right\} \rightarrow \qquad (1)$$

$$\left\{\begin{array}{lll} Be^+(1s^2 nl) + e^- & & \\ Be^{++}(1s^2) + 2e^- & & \\ Be(1s2s^2 nl) & \rightarrow Be^{++}(1s^2) + 2e^- & \text{READI} \\ Be^+(1s2s2l) + e^- & \rightarrow Be^{++}(1s^2) + 2e^- & \text{EA} \\ Be(1s2s2pnl) & \rightarrow Be^+(1s2s^2) + e^- & \\ & \rightarrow Be^{++}(1s^2) + 2e^- & \text{REDA} \end{array}\right. \qquad (2)$$

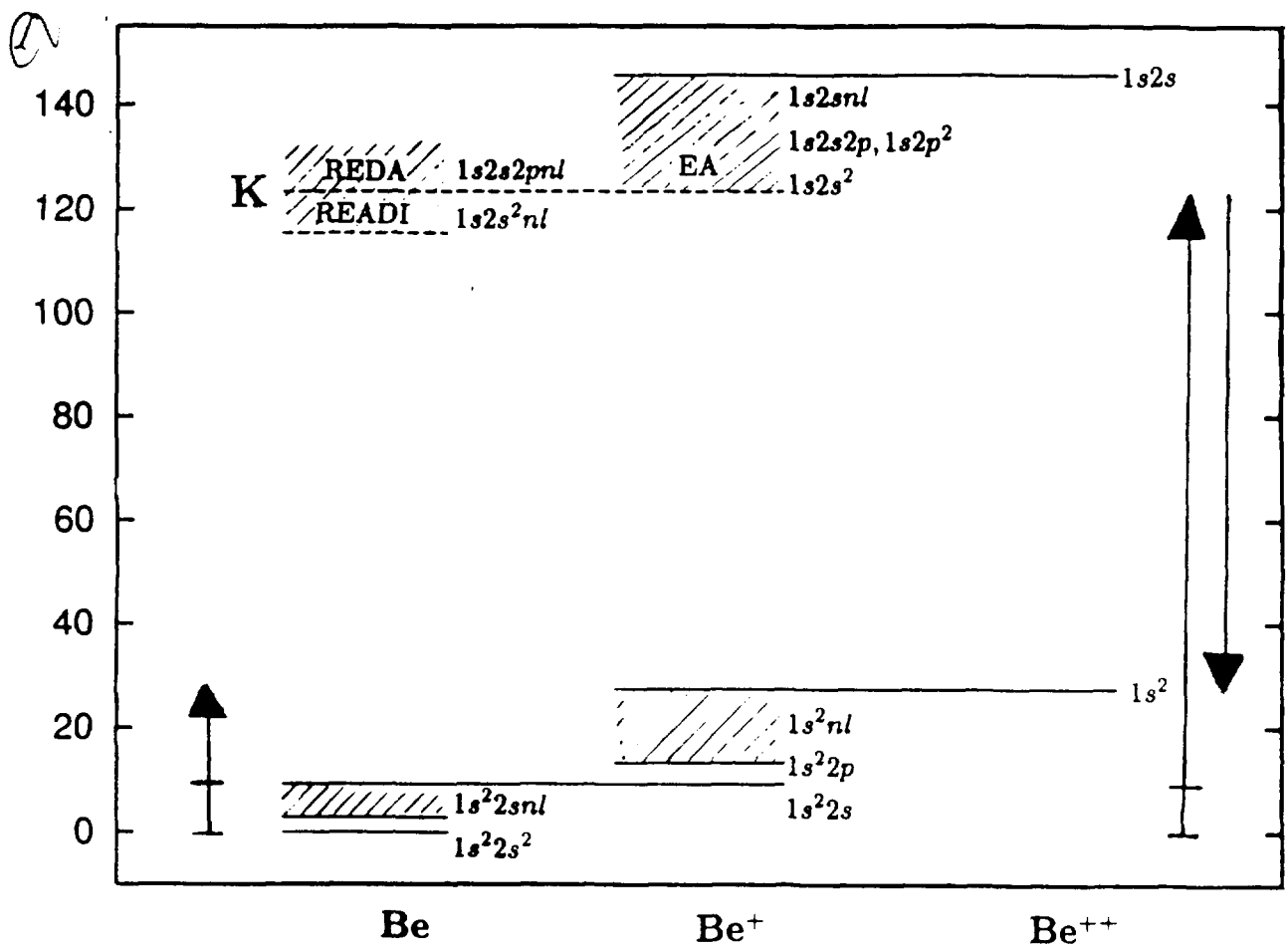

Figure 1: Simplified energy level diagram for Be and its ions, showing some representative bound (—) and autoionizing (- - -) states, the latter being classified READI, EA and REDA as expained in the text. nl indicates an excited outer electron, hatching indicates the $n \rightarrow \infty$ series, 'K' marks the K-shell edge. The vertical arrow on the left side of the figure indicates the direct process, the ones on the right the indirect processes, for electron impact ionization of Be^+ and double photoionization of Be.

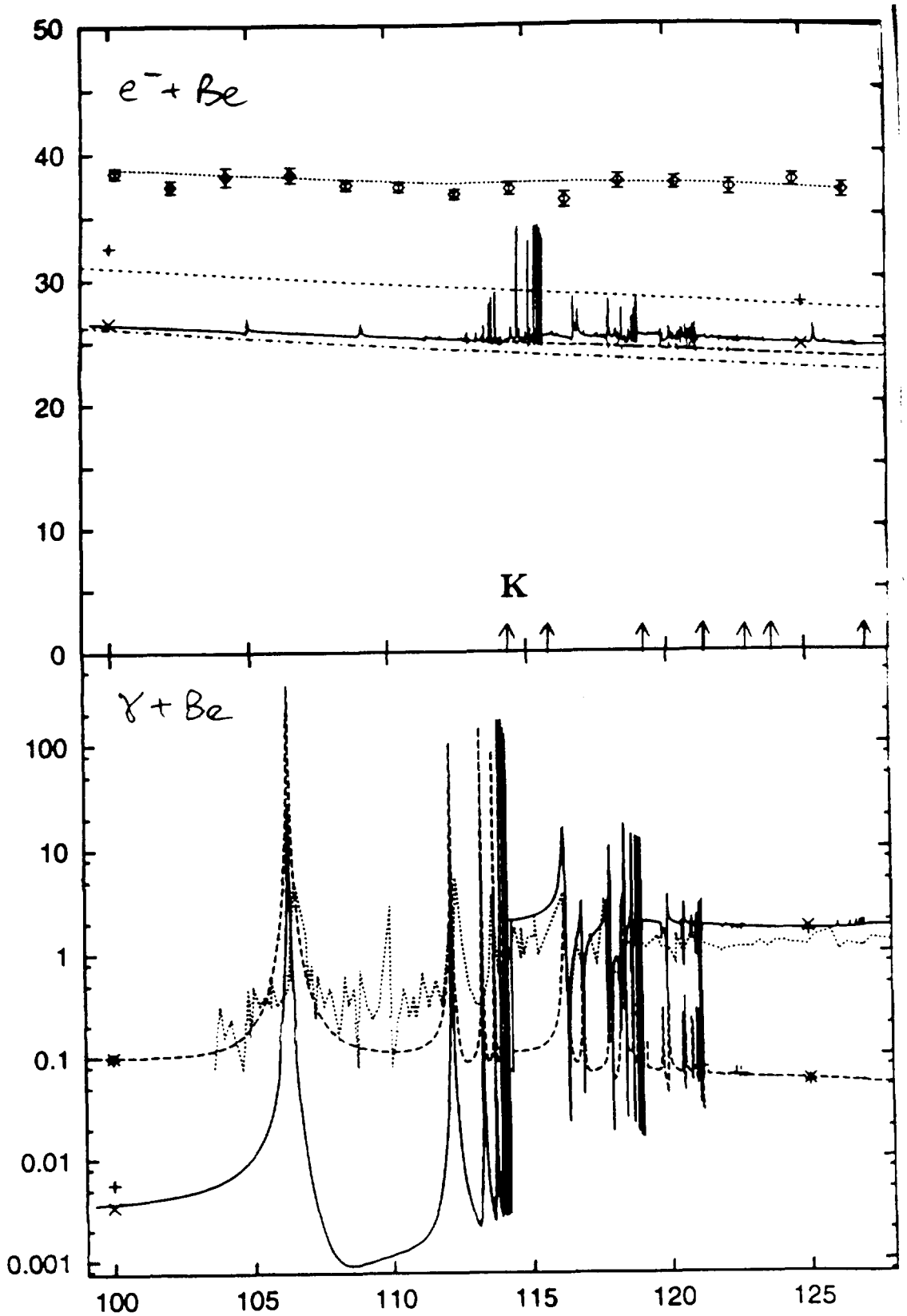

Figure 2: Ionization cross sections in units of 10^{-18}cm^2 across the K edge of Be as a function of electron energy (eV), showing from the left the READI resonances, the EA jump at 'K' and the REDA resonances. Arrows indicate the EA thresholds.

Top panel, electron impact ionization cross section of Be^+ $1s^22s$: —, our total cross section; - - - -, direct contribution background; · · · ·, distorted-wave calculation of Younger (1980); - · - · -, CCC calculation of Bray (1995). The measurements of Falk and Dunn (1983) are shown with error bars: ....., our total cross section with the addition of an arbitrary constant 12.4×10^{-18} cm^2 and convolved over the experimental energy spread of 0.22eV.

Bottom panel, photoionization cross section of Be $1s^22s^2$: —, our double photoionization cross section; - - - - -, single photoionization; ....., total cross section measurements of Jannitti et al (1987) with arbitrary normalization. In both panels, at 100 eV and 125 eV: +, calculation with states $n = 2$ plus pseudo-states, ×, with $n \leq 4$ plus pseudo-states.

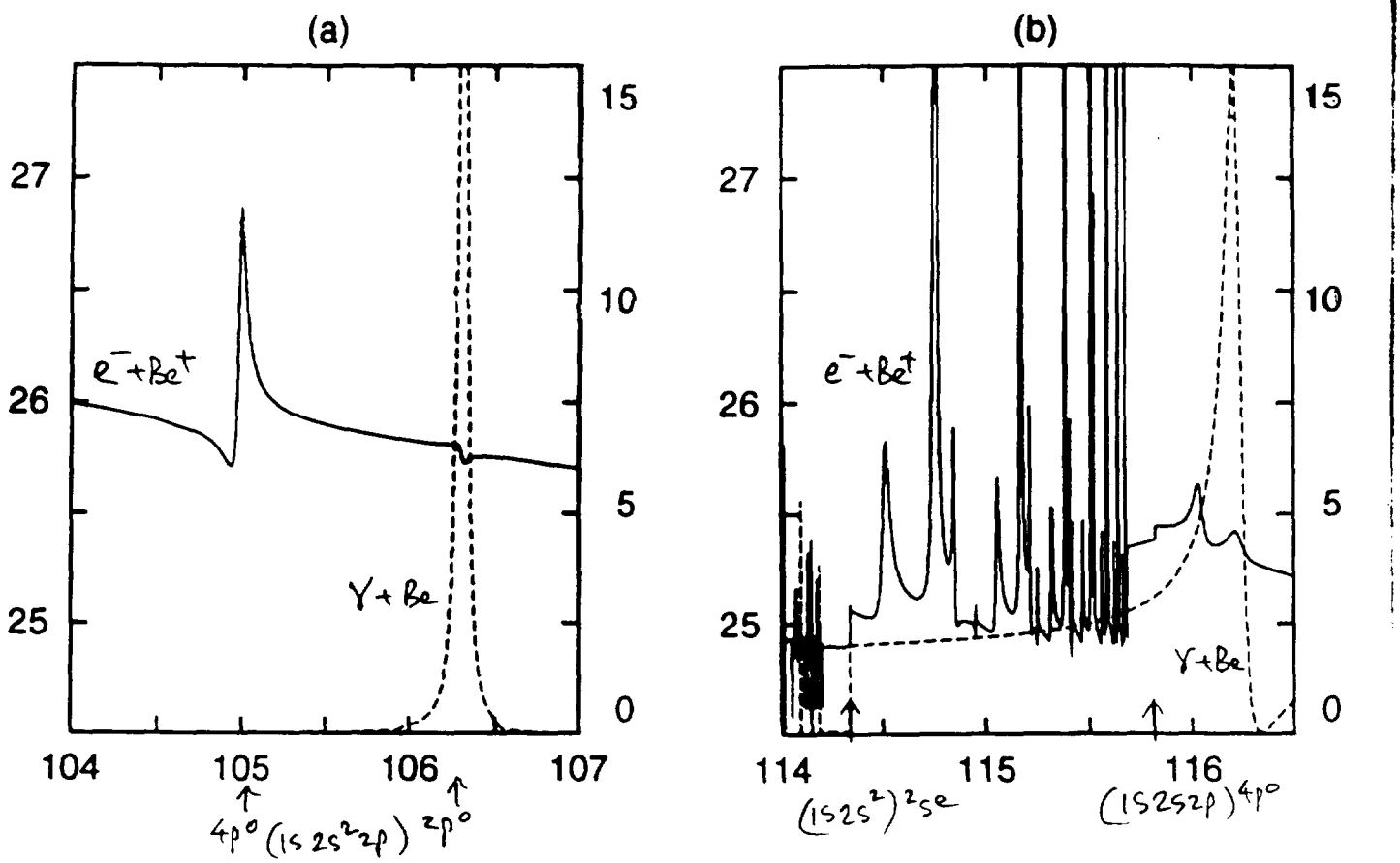

Figure 3: A close-up of the features near the K edge: —, our electron impact ionization cross section of Be^+ $1s^22s$ in units of $10^{-18}cm^2$ (left-hand scale); - - - -, our double photoionization cross section of Be $1s^22s^2$ in units of $10^{-18}cm^2$ (right-hand scale), as a function of electron energy eV. (a) shows the lowest READI resonances, $1s2s^22p\ ^{4,2}P^o$; (b) shows the EA and REDA behavior across the two lowest inner-shell thresholds, $1s2s^2\ ^2S^e$ and $1s2s2p\ ^4P^o$ (marked by arrows). Some of the resonances are elucidated in table 4.5.

PRL 1997.

A Unified Theory of Direct and Indirect Ionization Processes near the Li 'Hollow Atom' Threshold

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Abstract

We propose a unification in the theoretical treatment of different ionization processes occurring in photon and electron impact on atoms and ions, and in so doing uncover some interesting behavior of lithium near its 'hollow-atom' threshold. By introducing a set of 'core base states' for the Li^+ target, and optimising the collisional representation within an R-matrix model, we show for the first time how to combine *ab initio*, outer-shell and inner-shell effects, excitation and ionization channels, direct and indirect ionisation processes, resonant and non-resonant behavior, for photon and electron impact processes. We use the new method to interpret experimental data on electron impact ionization of ground state Li^+ and photoionization of Li, and look at double photoionization. We examine and quantify hollow-atom interference effects and resonances. We also, for the first time, give a reliable prediction for electron impact ionization out of metastable Li^+, and of excitation at the hollow atom threshold.

PACS 32.80.Dz 34.80.Dp 34.80.Kw

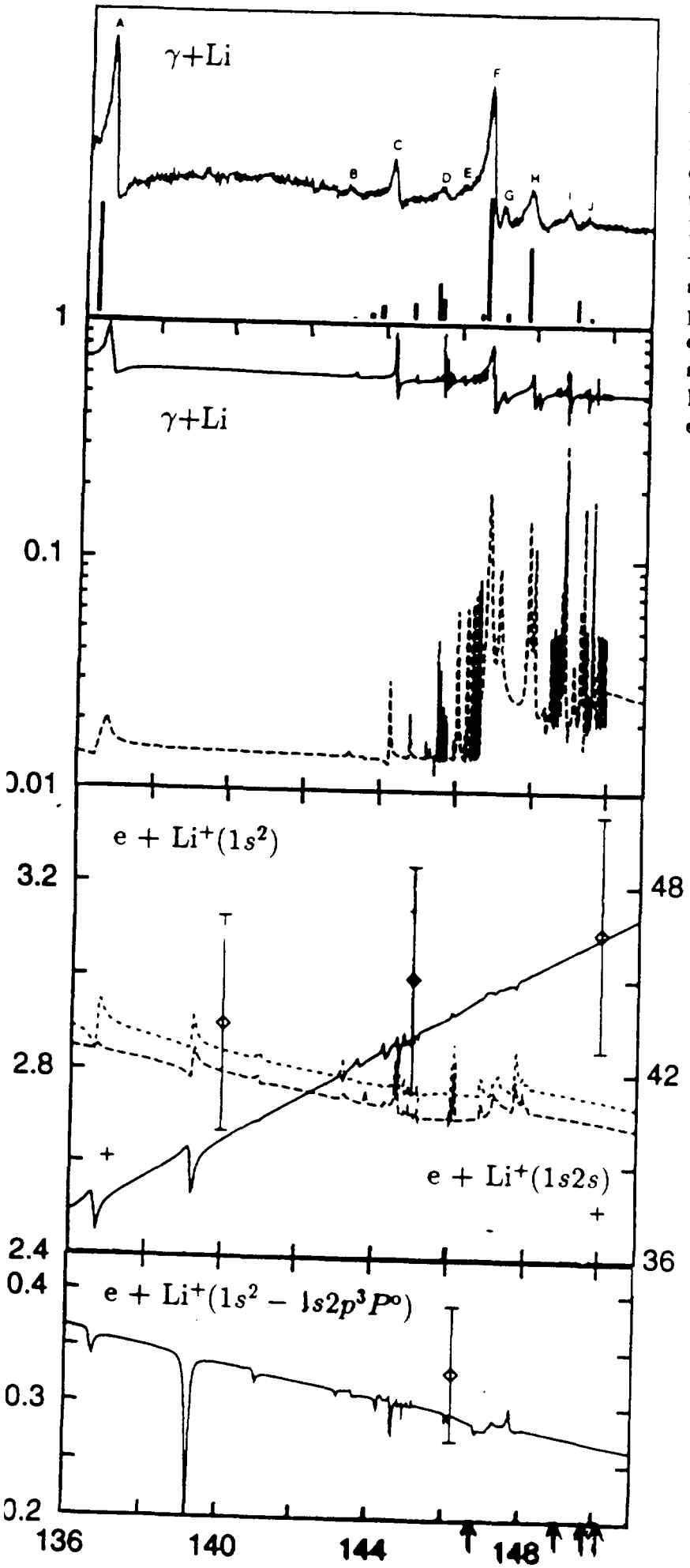

Figure 1: Cross sections (10^{-18}cm^2) across the L hollow-atom thresholds (marked by arrows) as a function of electron energy (eV). Top frame: — photoionization of Li from Azuma et al [4], measurement plotted linearly on a relative scale. Upper middle frame: — single and - - - double photoionization of Li, present calculation plotted on a log scale Lower middle frame: — Li^+1s^2 (left-hand scale), - - - $Li^+1s2s^3S^e$ and - - - - - $Li^+1s2s^1S^e$ (right-hand scale) electron impact ionization calculation. The experiment is for $1s^2$ from Müller et al [6] with 8% error bars. The two crosses are for $1s2s^3S^e$ by Z scaling Moores' formular [26]. Bottom frame: — $Li^+(1s^2 - 1s2p^3P^o)$ electron impact excitation. The experiment is Rogers et al [27] interpolated.

'Core base states'

- Let $x^n y^m$ indicate n inner and m outer electrons in target.
- Assume a common orthonormal set of one-electron orbitals.
- Allow for inner-shell vacancies and outer-shell polarization by introducing a set of:
  - short-range correlation orbitals $\bar{l}$
  - long-range polarized orbital $\bar{2}l$
- Define the **core base states** of the target as the set of one-electron excitations:

  $x^n y^m$, $x^n y^{m-1} \bar{2}l$, $x^n y^{m-1} \bar{l}l$, $(x^{n-1} y^{m+1} + x^{n-1} y^m \bar{l}l)$

  where the brackets indicate that $\bar{l}l$ are to be chosen such as to minimise the energy of the inner-shell excited states $x^{n-1} y^{m+1}$.
  (In practice there might also be further correlation orbitals optimised on outer-shell states $x^n y^m$)
- All states formed from CI wavefunctions by diagonalizing target H.

- The pseudo-states $x^n y^{m-1} \bar{l}l$ are required:
  - for completeness
  - for correlation
  - for continuum channels (ie ionization).

- Connection between $\bar{l}l$ and ionization ...

  At the inner-shell thresholds E_i the two processes of direct and indirect ionization are both energetically accessible:

$$E_i + x^n y^m \longrightarrow \begin{cases} x^n y^{m-1} \epsilon l & \text{direct} \\ x^{n-1} y^{m+1} & \text{EA} \end{cases}$$

  In order to model interference between the 2 final states, continuum electron $^{\epsilon l}$ becomes indistinguishable from an excited inner electron $^{x^{n-1}}$ in interaction region in the vicinity of the open inner-shell : $\Rightarrow$ can chose $\bar{l}l \approx \epsilon l \approx$ min (inner-shell state

Oscillator Strengths

10% → 3%

F.S.
inner-shell cor.

Physica Scripta 1997

An integrated approach to bound and continuum states: application to C III

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Abstract

An integrated approach to atomic structure calculations is described, using recent developments in the pseudo-state/R-matrix method, within the high optimization offered by close-coupling. These include the exploitation of the 'QB' method for systematic resonance analysis, the definition and use of 'core base states' for the target, and the incorporation of relativistive effects via the Breit-Pauli Hamiltonian in the Opacity Project codes. For the first time, a complete set of data is calculated for fine-structure energy levels for bound and continuum states of the form $1s^2 2snl$ and $1s^2 2pnl$ ($J = 0^e$ and $J = 1^o$) up to $n = 10$ for the Be-like ion C III, together with oscillator strengths and photoionization cross sections.

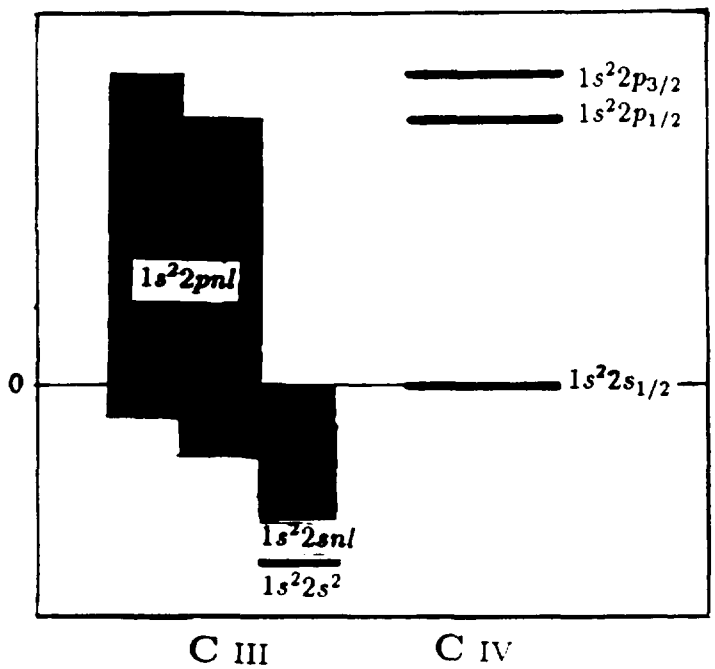

Figure 1: Schematic energy level diagram for C III and C IV; the blocks represent the $1s^2 2lnl'$ bound and resonant states (below and above $1s^2 2s$ respectively).

Table 2: Comparison of gf-values for C III $J = 0^e - 1^o$: OP = Opacity Project [12,13,22]; LScore and Present, see text. The Wiese et al [7] tabulation included Weiss[9], Allard et al [23] and the OP. Others include CIV3 [1,2] and MCDF[3], and experiments [8,10]. Indexing is defined in Tables 1 and 4.

$i - i'$	OP	LScore	Present	Wiese et al	Others
1-1			1.93E-7	[9]1.87E-7	[1]1.89±0.07E-7, [10]2.20±0.13E-7
1-2	0.780	0.760	0.761	[9]0.759	[2,3]0.757, [8]0.754±0.014
1-3	0.232	0.240	0.224	[OP]0.232	
1-4			5.98E-5	[23]3.47E-5	
1-5			3.61E-6		
1-6	4.51E-2	4.25E-2	4.26E-2	[OP]4.52E-2	
1-7			8.50E-9		
1-9	2.84E-2	3.27E-2	3.22E-2	[OP]2.84E-2	
2-1			0.273	[9]0.272	[1]0.273
2-2			2.43E-7	[9]3.24E-7	[1]3.03E-7
3-1			0.76E-7	[9]1.01E-7	[1]1.70E-7
3-2	0.521	0.493	0.493	[9]0.486	[1]0.486
4-1			4.49E-7		
4-2	5.44E-2	6.09E-2	6.61E-2	[9]5.94E-2	

$J = 1^e$

Table 4. Energies of C III bound and continuum states $1s^2 2snl$ and $1s^2 2pnl$ ($n \leq 10$) for $J = 0^e$ (left) and 1^o (right), in cm^{-1} relative to the C IV $1s^2 2s$ ground state. n_{eff} is relative to 1)$1s^2 2s$, 2)$1s^2 2p_{1/2}$ and 3)$1s^2 2p_{3/2}$. A colon (:) indicates uncertainty in the descroption due to strong mixing.

i	Description	n_{eff}	Energy
1	$1s^2 2s^2\ ^1S^e_0$	1)1.5993	-386147
2	$1s^2 2p^2\ ^3P^o_0$	2)1.7748	-248378
3	$1s^2 2p^2\ ^1S^e_0$	2)1.9223	-202090
4	$1s^2 2s3s\ ^1S^e_0$	1)2.6649	-139069
5	$1s^2 2s4s\ ^1S^e_0$	1)3.6411	-74495
6	$1s^2 2p_{1/2}3p\ ^3P^e_0$	2)2.8551	-55982
7	$1s^2 2s5s\ ^1S^e_0$	1)4.5649	-47396
8	$1s^2 2p_{3/2}3p\ ^1S^e_0$	3)3.0557	-40492
9	$1s^2 2s6s\ ^1S^e_0$	1)5.6884	-30523
10	$1s^2 2s7s\ ^1S^e_0$	1)6.6653	-22232
11	$1s^2 2s8s\ ^1S^e_0$	1)7.6557	-16852
12	$1s^2 2s9s\ ^1S^e_0$	1)8.6494	-13203
13	$1s^2 2s10s\ ^1S^e_0$	1)9.6444	-10619
32	$1s^2 2p_{1/2}4p\ ^3P^e_0$	2)3.8584	-1165
1)	$1s^2 2s_{1/2}$		0
a	$1s^2 2p_{3/2}4p\ ^1S^e_0$	3)4.0355	4632
b	$1s^2 2p_{1/2}5p\ ^3P^e_0$	2)4.8609	23376
c	$1s^2 2p_{3/2}5p\ ^1S^e_0$	3)5.0251	26167
d	$1s^2 2p_{1/2}6p\ ^3P^e_0$	2)5.8614	36428
e	$1s^2 2p_{3/2}6p\ ^1S^e_0$	3)6.0185	38013
f	$1s^2 2p_{1/2}7p\ ^3P^e_0$	2)6.8631	44208
g	$1s^2 2p_{3/2}7p\ ^1S^e_0$	3)7.0138	45202
h	$1s^2 2p_{1/2}8p\ ^3P^e_0$	2)7.8658	49213
i	$1s^2 2p_{3/2}8p\ ^1S^e_0$	3)8.0095	49884
j	$1s^2 2p_{1/2}9p\ ^3P^e_0$	2)8.8686	52619
k	$1s^2 2p_{3/2}9p\ ^1S^e_0$	3)9.0052	53100
l	$1s^2 2p_{1/2}10p\ ^3P^e_0$	2)9.8716	55041
m	$1s^2 2p_{3/2}10p\ ^1S^e_0$	3)10.001	55405
2)	$1s^2 2p_{1/2}$		65176
3)	$1s^2 2p_{3/2}$		65279

$J = 0^e$

i	Description	n_{eff}	Energy
1	$1s^2 2s2p\ ^3P^o_1$	1)1.7204	-333688
2	$1s^2 2s2p\ ^1P^o_1$	1)1.8667	-283424
3	$1s^2 2s3p\ ^1P^o_1$	1)2.7863	-127216
4	$1s^2 2s3p\ ^3P^o_1$	1)2.7944	-126473
5	$1s^2 2p_{1/2}3s\ ^3P^o_1$	2)2.6316	-77434
6	$1s^2 2s4p\ ^1P^o_1$:	1)3.6072	-75905
7	$1s^2 2s4p\ ^3P^o_1$	1)3.8005	-68379
8	$1s^2 2p_{3/2}3s\ ^1P^o_1$:	3)2.7693	-63507
9	$1s^2 2p_{1/2}3d\ ^3D^o_1$:	1)2.9548	-47947
10	$1s^2 2p_{3/2}3d\ ^3P^o_1$:	3)2.9858	-45503
11	$1s^2 2s5p\ ^1P^o_1$	1)4.8050	-42781
12	$1s^2 2s5p\ ^3P^o_1$	1)4.8581	-41850
13	$1s^2 2p_{3/2}3d\ ^1P^o_1$:	3)3.0827	-38652
14	$1s^2 2s6p\ ^3P^o_1$	1)5.8175	-29185
15	$1s^2 2s6p\ ^1P^o_1$	1)5.8238	-29122
16	$1s^2 2s7p\ ^1P^o_1$	1)6.8023	-21346
17	$1s^2 2s7p\ ^3P^o_1$	1)6.8138	-21274
18	$1s^2 2s8p\ ^1P^o_1$	1)7.7814	-16313
19	$1s^2 2s8p\ ^3P^o_1$	1)7.8115	-16187
20	$1s^2 2s9p\ ^1P^o_1$	1)8.7526	-12893
21	$1s^2 2s9p\ ^3P^o_1$	1)8.8087	-12728
22	$1s^2 2s10p\ ^1P^o_1$	1)9.7042	-10489
23	$1s^2 2s10p\ ^3P^o_1$	1)9.8005	-10284
24	$1s^2 2p_{1/2}4s\ ^3P^o_1$	2)3.6426	-9258
27	$1s^2 2p_{3/2}4s\ ^1P^o_1$:	3)3.6821	-7566
a	$1s^2 2p_{1/2}4d\ ^3D^o_1$:	2)3.9574	2112
b	$1s^2 2p_{3/2}4d\ ^3P^o_1$	3)3.9834	3036
c	$1s^2 2p_{3/2}4d\ ^1P^o_1$:	3)4.0650	5511
d	$1s^2 2p_{1/2}5s\ ^3P^o_1$	2)4.6470	19440
e	$1s^2 2p_{3/2}5s\ ^1P^o_1$	3)4.6878	20337
f	$1s^2 2p_{1/2}5d\ ^3D^o_1$:	2)4.9609	25045
g	$1s^2 2p_{3/2}5d\ ^3P^o_1$	3)4.9737	25354
h	$1s^2 2p_{3/2}5d\ ^1P^o_1$:	3)5.0554	26635
i	$1s^2 2p_{1/2}6s\ ^3P^o_1$	2)5.6493	34229
j	$1s^2 2p_{3/2}6s\ ^1P^o_1$	3)5.6851	34721
k	$1s^2 2p_{1/2}6d\ ^3D^o_1$:	2)5.9628	37398
l	$1s^2 2p_{3/2}6d\ ^3P^o_1$	3)5.9699	37567
m	$1s^2 2p_{3/2}6d\ ^1P^o_1$:	3)6.0501	38297
n	$1s^2 2p_{1/2}7s\ ^3P^o_1$	2)6.6517	42854
o	$1s^2 2p_{3/2}7s\ ^1P^o_1$	3)6.6830	43166
p	$1s^2 2p_{1/2}7d\ ^3D^o_1$:	2)6.9648	44816
q	$1s^2 2p_{3/2}7d\ ^3P^o_1$	3)6.9679	44937
r	$1s^2 2p_{3/2}7d\ ^1P^o_1$:	3)7.0463	45387
s	$1s^2 2p_{1/2}8s\ ^3P^o_1$	2)7.6541	48317
t	$1s^2 2p_{3/2}8s\ ^1P^o_1$	3)7.6813	48540
u	$1s^2 2p_{1/2}8d\ ^3D^o_1$	2)7.9669	49615
v	$1s^2 2p_{3/2}8d\ ^3P^o_1$	3)7.9667	49718
w	$1s^2 2p_{3/2}8d\ ^1P^o_1$	3)8.0431	50012
x	$1s^2 2p_{1/2}9s\ ^3P^o_1$	2)8.6560	51994
y	$1s^2 2p_{3/2}9s\ ^1P^o_1$	3)8.6795	52169
z	$1s^2 2p_{1/2}9d\ ^3D^o_1$	2)8.9690	52898
a'	$1s^2 2p_{3/2}9d\ ^3P^o_1$	3)8.9659	52993
b'	$1s^2 2p_{3/2}9d\ ^1P^o_1$	3)9.0398	53193
c'	$1s^2 2p_{1/2}10s\ ^3P^o_1$	2)9.6572	54586
d'	$1s^2 2p_{3/2}10s\ ^1P^o_1$	3)9.6782	54735

Table 3: Positions and widths in eV of the lowest lying resonance states of C III $J = 0^e$ and 1^o relative to the $1s^22s$ state of C IV. Indexing is defined in Table 4. Our calculated $E(1s^22s - 1s^22s^2)$=47.874 eV.

0^e	Position (eV)	Width (eV)	1^o	Position (eV)	Width (eV)
a	0.574	0.212	a	0.262	0.146
b	2.898	0.128	b	0.377	0.062
c	3.244	0.121	c	0.683	0.054
d	4.516	0.019	d	2.410	0.005
e	4.713	0.075	e	2.521	0.138
f	5.480	0.006	f	3.105	0.021
g	5.604	0.049	g	3.143	0.032
h	6.101	<0.001	h	3.302	0.029
i	6.184	0.033	i	4.243	0.004
j	6.523	<0.001	j	4.305	0.074
k	6.583	0.024	k	4.636	0.004
l	6.824	<0.001	l	4.657	0.019
m	6.869	0.017	m	4.748	0.018

Table 5. gf-values for C III fine-structure transitions. Indexing is defined in Table 4. Sign is of $(E_i - E_{i'})$.

i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L	i	i'	gf_L
		0^e–1^o	3	4	−4.24E−6	5	8	−8.15E−1	7	12	−6.87E−6	9	16	−2.21E−1	11	20	−3.25E−1
1	1	−1.93E−7	3	5	−2.15E−5	5	9	−1.52E−7	7	13	−7.22E−2	9	17	−6.70E−5	11	21	−8.84E−6
1	2	−7.61E−1	3	6	−1.25E−1	5	10	−6.63E−9	7	14	−2.26E−5	9	18	−7.92E−2	11	22	−1.34E−1
1	3	−2.24E−1	3	7	−1.17E−8	5	11	−1.07E−1	7	15	−4.01E−2	9	19	−5.64E−6	11	23	−7.35E−6
1	4	−5.98E−5	3	8	−5.18E−2	5	12	−3.87E−7	7	16	−3.31E−2	9	20	−3.94E−2	12	1	4.29E−9
1	5	−3.61E−6	3	9	−1.16E−5	5	13	−1.39E−2	7	17	−9.66E−6	9	21	−1.57E−6	12	2	4.33E−4
1	6	−4.26E−2	3	10	−3.14E−7	5	14	−3.99E−5	7	18	−2.57E−2	9	22	−2.25E−2	12	3	3.27E−3
1	7	−8.50E−9	3	11	−8.52E−2	5	15	−7.55E−2	7	19	−1.61E−6	9	23	−1.98E−6	12	4	6.85E−7
1	8	−3.22E−2	3	12	−6.86E−8	5	16	−5.34E−2	7	20	−2.22E−2	10	1	3.36E−9	12	5	5.96E−7
1	9	−7.00E−7	3	13	−8.37E−1	5	17	−1.65E−5	7	21	−6.47E−7	10	2	1.50E−3	12	6	6.46E−3
1	10	−1.63E−7	3	14	−7.14E−6	5	18	−4.55E−2	7	22	−2.18E−2	10	3	7.69E−3	12	7	1.60E−9
1	11	−4.60E−2	3	15	−1.18E−2	5	19	−3.14E−6	7	23	−8.68E−7	10	4	1.57E−6	12	8	6.01E−3
1	12	−1.82E−7	3	16	−9.67E−4	5	20	−4.65E−2	8	1	2.71E−8	10	5	2.07E−6	12	9	1.19E−7
1	13	−2.48E−3	3	17	−2.09E−7	5	21	−1.50E−6	8	2	1.35E−2	10	6	1.92E−2	12	10	0.00E−0
1	14	−9.21E−6	3	18	−5.61E−7	5	22	−5.75E−2	8	3	2.13E−3	10	7	1.10E−9	12	11	2.14E−2
1	15	−1.71E−2	3	19	−2.03E−9	5	23	−2.33E−6	8	4	2.86E−6	10	8	1.78E−2	12	12	1.41E−7
1	16	−1.17E−2	3	20	−4.03E−4	6	1	2.59E−2	8	5	5.52E−5	10	9	2.59E−7	12	13	3.35E−4
1	17	−3.46E−6	3	21	−1.45E−8	6	2	2.90E−7	8	6	2.06E−1	10	10	0.00E+0	12	14	2.48E−5
1	18	−7.93E−3	3	22	−1.70E−3	6	3	7.06E−3	8	7	6.42E−8	10	11	1.00E−1	12	15	5.19E−2
1	19	−5.16E−7	3	23	−1.17E−8	6	4	1.07E−1	8	8	4.85E−3	10	12	7.23E−7	12	16	1.64E−1
1	20	−5.50E−3	4	1	4.49E−7	6	5	2.93E−1	8	9	4.83E−8	10	13	7.21E−3	12	17	5.85E−5
1	21	−1.97E−7	4	2	6.16E−2	6	6	3.77E−5	8	10	3.96E−7	10	14	3.60E−4	12	18	9.78E−1
1	22	−3.74E−3	4	3	−3.14E−1	6	7	1.44E−3	8	11	1.92E−1	10	15	7.63E−1	12	19	1.02E−4
1	23	−3.53E−7	4	4	−7.88E−5	6	8	7.79E−6	8	12	1.22E−6	10	16	−1.31E+0	12	20	−1.27E−0
2	1	2.73E−1	4	5	−8.45E−5	6	9	−1.30E−1	8	13	−1.45E−1	10	17	−4.85E−4	12	21	−1.14E−4
2	2	2.43E−7	4	6	−6.91E−1	6	10	−3.14E−2	8	14	−1.19E−4	10	18	−2.46E−1	12	22	−5.08E−1
2	3	−1.17E−5	4	7	−9.29E−8	6	11	−1.69E−6	8	15	−2.42E−1	10	19	−1.52E−5	12	23	−2.00E−5
2	4	−2.11E−4	4	8	−2.26E−2	6	12	−1.23E−2	8	16	−3.32E−2	10	20	−9.63E−2	13	1	4.83E−9
2	5	−1.30E−1	4	9	−5.08E−7	6	13	−1.51E−7	8	17	−1.18E−5	10	21	−3.25E−6	13	2	2.63E−4
2	6	−2.09E−5	4	10	−9.59E−8	6	14	−5.28E−4	8	18	−6.63E−3	10	22	−5.37E−2	13	3	2.29E−3
2	7	−4.04E−3	4	11	−4.76E−3	6	15	−5.50E−7	8	19	−7.85E−7	10	23	−3.58E−6	13	4	4.81E−7
2	8	−4.82E−7	4	12	−7.62E−8	6	16	−4.98E−8	8	20	−5.93E−4	11	1	3.83E−9	13	5	3.82E−7
2	9	−7.30E−1	4	13	−4.38E−2	6	17	−1.55E−4	8	21	−1.51E−7	11	2	7.62E−4	13	6	4.43E−3
2	10	−1.83E−1	4	14	−9.30E−6	6	18	0.00E+0	8	22	−5.88E−4	11	3	4.88E−3	13	7	4.87E−9
2	11	−8.47E−6	4	15	−1.90E−2	6	19	−3.12E−5	8	23	−1.79E−7	11	4	1.02E−6	13	8	4.08E−3
2	12	−5.12E−2	4	16	−1.09E−2	6	20	−2.30E−7	9	1	3.05E−9	11	5	1.02E−6	13	9	9.71E−8
2	13	−3.51E−6	4	17	−3.81E−6	6	21	−2.02E−5	9	2	3.87E−3	11	6	1.03E−2	13	10	0.00E−0
2	14	−7.77E−4	4	18	−7.10E−3	6	22	−1.06E−5	9	3	1.16E−2	11	7	0.00E+0	13	11	1.29E−2
2	15	−2.56E−7	4	19	−6.64E−7	6	23	−1.96E−3	9	4	2.14E−6	11	8	9.67E−3	13	12	8.38E−8
2	16	−9.48E−8	4	20	−5.01E−3	7	1	8.06E−8	9	5	6.62E−6	11	9	1.62E−7	13	13	8.95E−5
2	17	−1.21E−4	4	21	−2.81E−7	7	2	2.07E−6	9	6	5.09E−2	11	10	0.00E+0	13	14	1.24E−5
2	18	−3.00E−8	4	22	−3.71E−3	7	3	7.03E−2	9	7	1.07E−8	11	11	4.08E−2	13	15	2.60E−2
2	19	−3.58E−5	4	23	−3.93E−7	7	4	2.57E−5	9	8	3.85E−2	11	12	2.77E−7	13	16	6.27E−2
2	20	−7.99E−8	5	1	1.85E−8	7	5	9.15E−6	9	9	5.20E−7	11	13	1.32E−3	13	17	2.23E−5
2	21	−3.18E−5	5	2	8.82E−3	7	6	7.24E−5	9	10	0.00E+0	11	14	6.56E−5	13	18	1.84E−1
2	22	−1.38E−6	5	3	2.71E−1	7	7	0.00E+0	9	11	4.44E−1	11	15	1.37E−1	13	19	1.80E−5
2	23	−2.72E−4	5	4	5.96E−5	7	8	7.34E−1	9	12	3.76E−6	11	16	8.95E−1	13	20	9.76E−1
3	1	7.55E−8	5	5	1.52E−5	7	9	2.68E−7	9	13	1.24E−1	11	17	3.26E−4	13	21	7.04E−5
3	2	4.93E−1	5	6	8.03E−2	7	10	0.00E+0	9	14	−4.97E−4	11	18	−1.38E+0	13	22	−8.04E−1
3	3	−1.61E−2	5	7	−6.87E−8	7	11	−1.07E+0	9	15	−1.07E+0	11	19	−1.56E−4	13	23	−3.13E−4

FINALLY – A PERSONAL VIEW

CLOSE-COUPLING AND R-MATRIX TECHNIQUES COMBINED WITH HIGH PRECISION ATOMIC STRUCTURE METHODS IMPLY THAT THEORETICAL ATOMIC PHYSICS NOW HAS THE CAPABILITY TO CALCULATE AB INTIO ATOMIC PROPERTIES TO HIGH ACCURACY.

BUT THE ACTION AND EXPERTISE IS LARGELY IN ACADEMIA, WHOSE PRIORITIES MAY NOT COINCIDE WITH DATA APPLICATIONS: (for example much of the work is often done as part of research training for students). SO DATA [illegible] MAY BE [illegible] AND PATCHY, [illegible]

ROLE OF IAEA?

- [illegible] ESSENTIAL DATA NEEDS
- COORDINATION OF TASKS/DEADLINES
- USER/PRODUCER COLLABORATIONS

Atomic Data Generation at Lebedev Physical Institute and Other Research Centers

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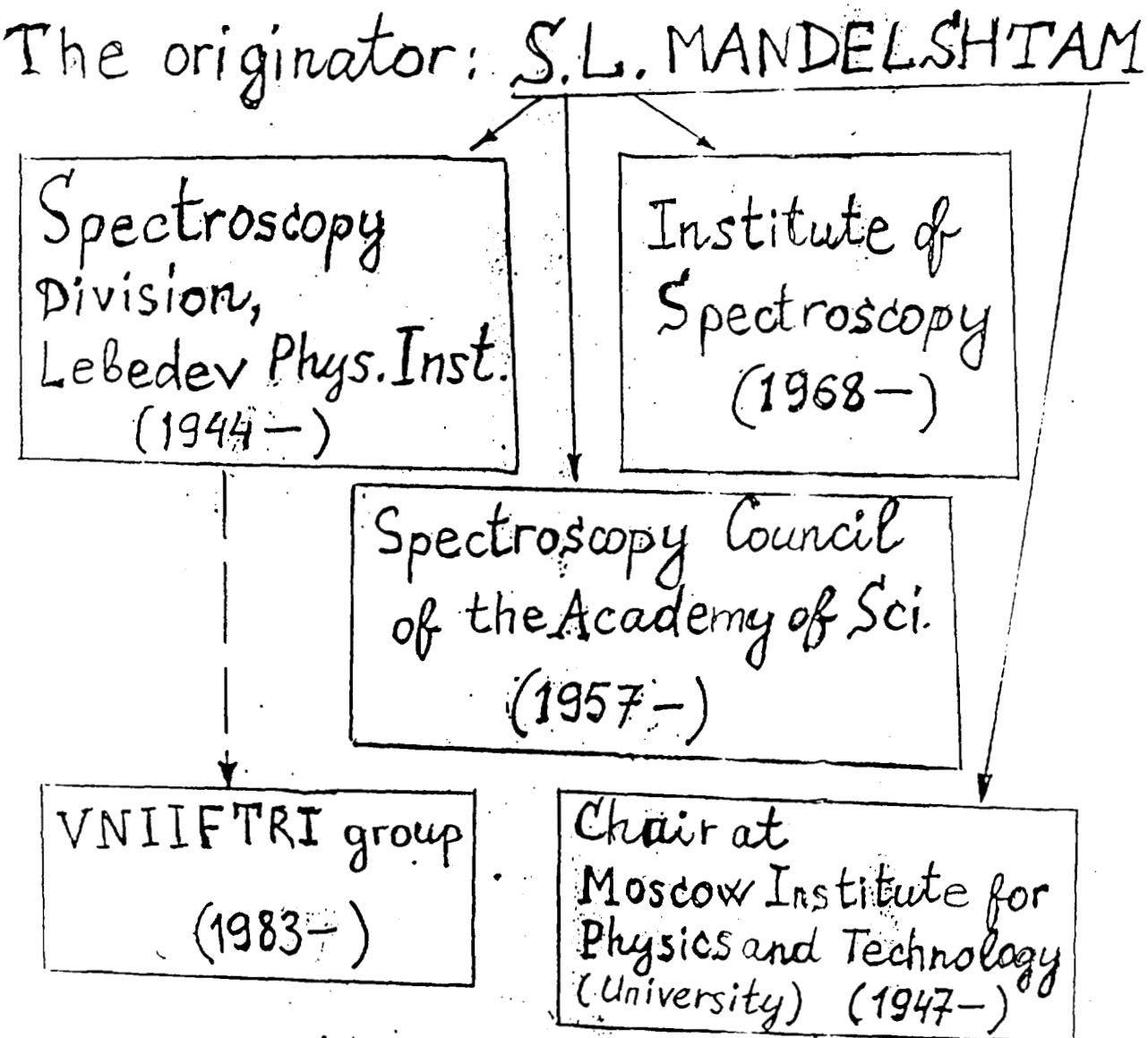
1. Introduction



Fundamental research and Applications for

- Solar EUV- and X-ray astronomy and astrophysics (since 1957);
- Laboratory (laser-produced and other) plasmas: hot core + plasma-wall processes;
- Magnetically confined plasmas.

2. Activities at P.N. Lebedev Physical Institute

Theoretical methods and computer codes for

- atomic and ionic wavefunctions and energy levels;
- oscillator strengths and radiative probabilities;
- autoionization probabilities;
- photoionization cross sections and rates;
- photo- and dielectronic recombination;
- electronic collisions: excitation*, ionization and three-body recombination
- ionic collisions: excitation**, ionization, charge transfer and transfer ionization;
- level populations;
- intensities of spectral lines (both regular and satellite ones);
- EUV and X-ray spectroscopy diagnostics.

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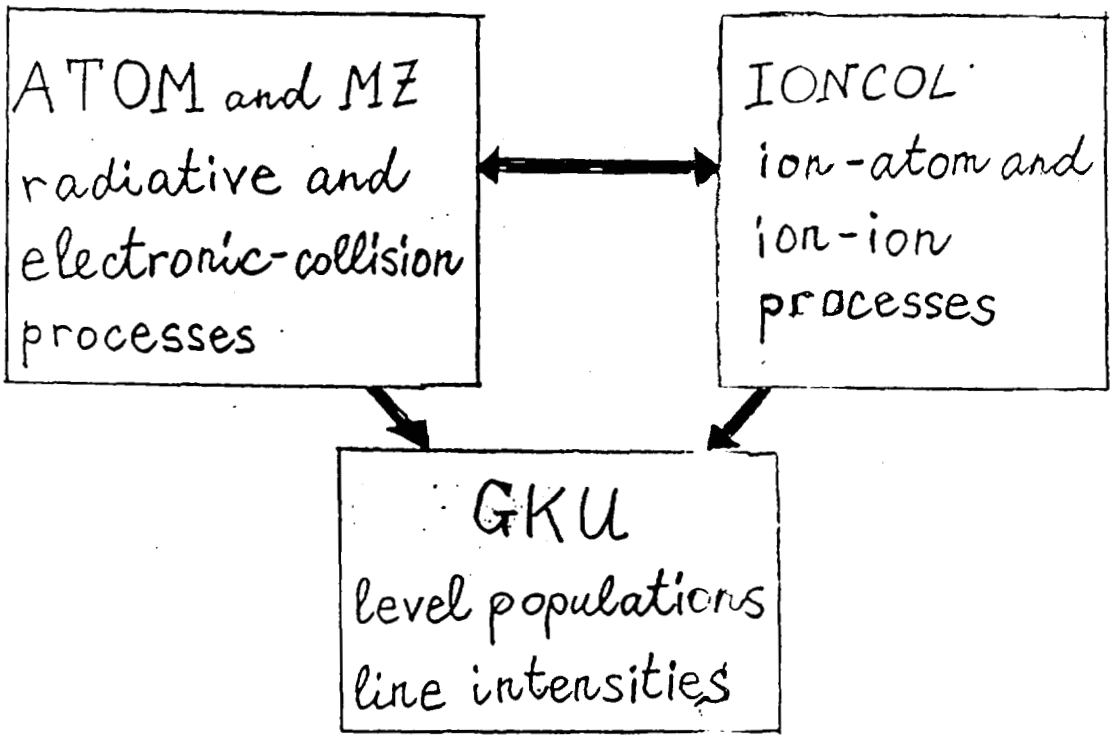
* with resonance excitation

** with transitions between Rydberg states

Main codes for databases



Methods of calculations used in the codes

Wavefunctions	"semi-empirical"	(ATOM)
	expansion over Z^{-1} + QED corrections	(MZ)
Radiation* and autoionization	perturbation theory with intermediate coupling	(ATOM)
		(MZ)
Electron-atom (ion) collisions	normalized BE (atom) CBE (ion) approximation, K-matrix.	(ATOM)

*including photo- and dielectronic recombination

Ion - atom and ion - ion collisions } non-stationary Keldysh - Coulomb method; close coupling + DACC (IONCOL)

Level populations and line intensities in plasmas (both "steady" and transient); ionization stage } kinetic equations for the electron flux (GKU)

Estimated accuracy

ATOM (+MZ): $\frac{\Delta\lambda}{\lambda} \lesssim 10^{-4}$ for $\lambda = 1. \div 100$ A.

$$\frac{\Delta\sigma}{\sigma} \approx \frac{\Delta\langle v\sigma\rangle}{\langle v\sigma\rangle} \lesssim \begin{cases} 0.25 \text{ if } Z = 0 \div 4 \\ 1/Z \text{ if } Z \geq 4 \end{cases}$$

IONCOL: $\frac{\Delta\sigma}{\sigma} \lesssim 0.1$

GKU: $\frac{\Delta I}{I} \lesssim 0.15$

The main idea of our database activities (at Lebedev Phys. Inst.) is to store the methods for calculations and the final formulas instead of storing the numbers. We are two groups:

Astrophysics: L. Vainshtein, I. Beigman, A. Urnov + 1 engineer and 1 student

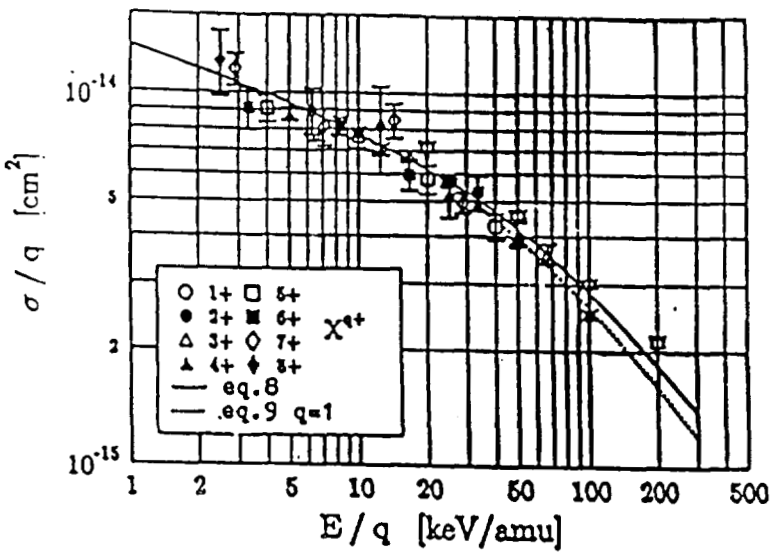
Atomic physics: L. Presnyakov, D. Uskov, V. Shevelko + 2 students

ATOM and MZ have been designed by L. Vainshtein
GKU by I. Beigman
IONCOL by D. Uskov and L. Presnyakov

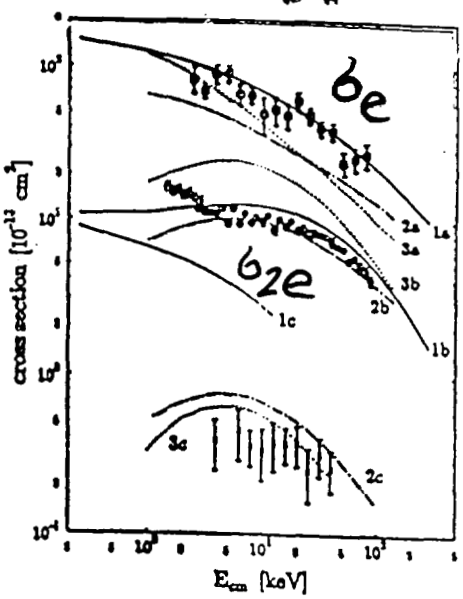
The database work is developed in collaboration with

IAEA (R. Janev), University Giessen (E. Salzborn), NIFS, Japan (H. Tawara), IPP (Julich) and GSI (Darmstadt), and several Russian centers.

$H^- + X^{q+} \rightarrow H^0 + \ldots$



$H^- + H$



$C^{2+} + B^+ \rightarrow C^+ + B^{2+}$

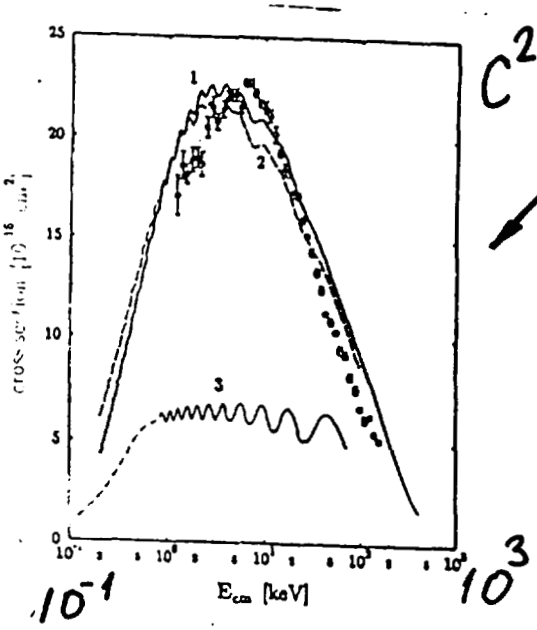
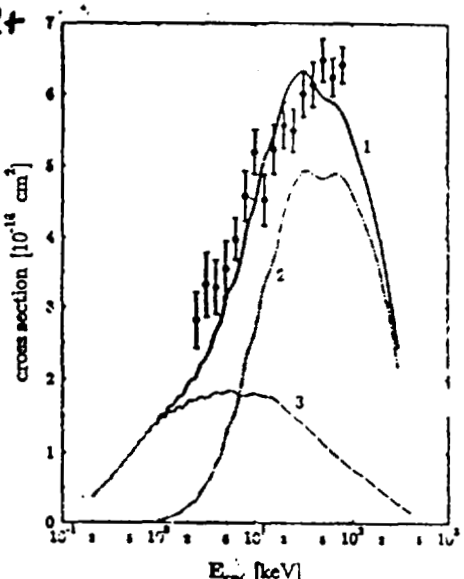


Figure 2. Cross sections for the charge exchange reaction $C^{2+} + B^+ \longrightarrow C^+ + B^{2+}$ as a function of the cm collision energy. Experimental results (•) include a 90% confidence limit on the statistical error. Curve 1: the present theoretical result; curve 2: cross section calculated for the case of 20% concentration of C^{2+} metastable ions in the beam; curve 3: previous theoretical work by Janev and Belic (1982).



$C^+ + B^{2+} \rightarrow C^{2+} + B^+$

Figure 3. Cross sections for the charge-exchange reaction $B^{2+} + C^+ \longrightarrow B^+ + C^{2+}$ as a function of the cm collision energy. Experimental results (•) include 90% confidence limit of statistical error. Curves 1–3 represent our theoretical results: Curve 1: the present theoretical result; curve 2: cross section for electron capture to the $B^+(2s2p^3P)$ state; curve 3: cross section for electron capture into the singlet states of B^+ ion.

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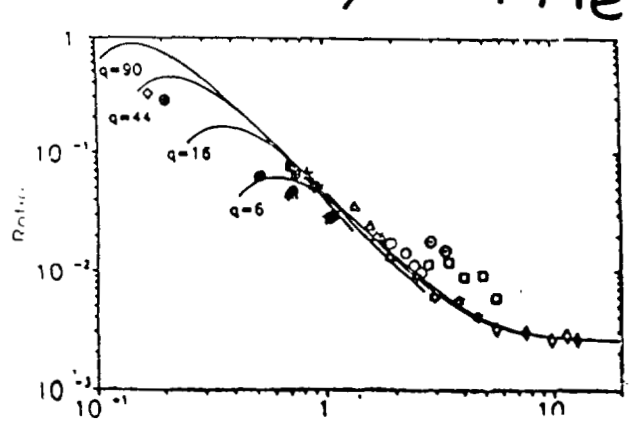
$X^{q+} + He$

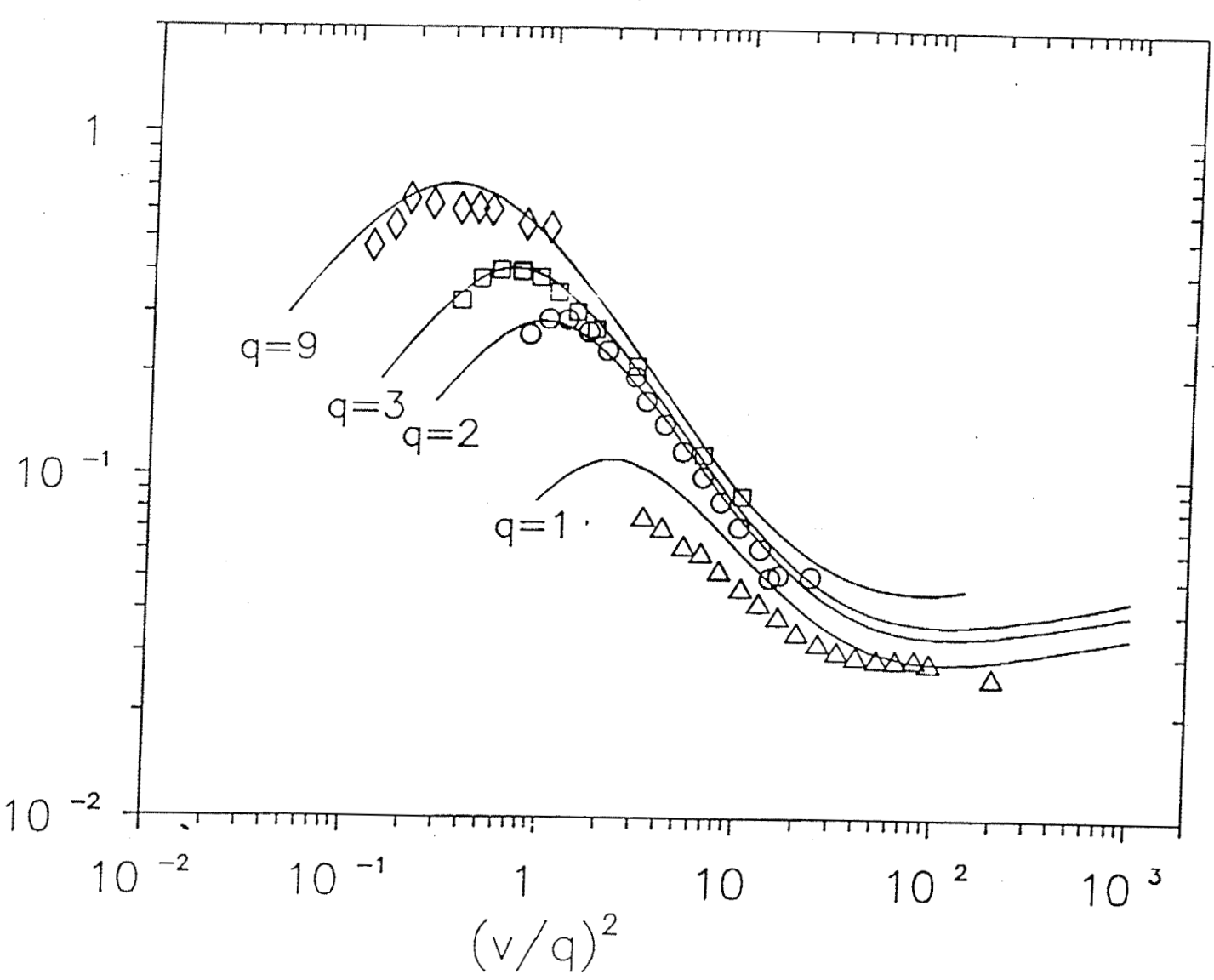


$R = \frac{6_{2e}}{6_e}$

Figure 1. Ratios of doublet-to-single ionization of helium by several ions as a funct v/q (in atomic units). Full curves, theory (the q values are indicated). Experimenta open circle, C^{6+}; open triangle, O^{8+}; open five-pointed star, Si^{14+}; plus within square, (Krishnakumar and Rajgara 199²); open diamond, Ne^{10+}; open six-pointed star, Ni^{21+} (et al 1993); open square, N^{7+} (Herber et al 1990, 1991); circle within circle, Kr^{36+}; star w circle, U^{90+} (Berg et al 1992a, b), plus within circle, Gd^{37+}; open plus, U^{44+} (McGuire 1987).

$R(E) \underset{E \to \infty}{=} R_{SO} = 2.6 \cdot 10^{-3}$

$He + X^{q+} \longrightarrow He^{2+} + \ldots$



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Presnyakov + Uskov
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3. Activities at Institute of Spectroscopy

Research: systematic study of spectra of many-electron ions (wavelengths, energy levels etc)

Experimental setup:
- normal incidence spectrograph ($\lambda = 300 \div 2500$ Å)
- grazing incidence spectrograph ($\lambda = 50 \div 350$ Å)
- bent crystal spectrographs ($\lambda < 50$ Å)
- light sources: laser produced plasmas and low-inductance vacuum spark.

Results:
- H-like ions up to Ga XXXI
- He-like ions up to Mo XLI
- Ne-like ions up to Pr LI
- Cu-, Ni-, Co-, Fe-like ions with 3d-electrons in outer shells from Ga to Mo
- Os III – Os VII and the isoelectronic spectra of Re and Ir

$\gtrsim 250$ ion spectra were studied, $\sim 10^3$ lines were identified in each spectrum

Bibliography on Atomic (and Ionic) Spectra

The databank BIBL contains the bibliography related to experimental and theoretical publications on identification and prediction of ionic structures.

~ 6000 cards are stored in the BIBL system.

The software has been developed for transforming the publications available to the BIBL format

Compilations

Jointly with NIST, the critical compilations of wavelengths, energy levels and life times are performed for the spectra of

Be I — Be II, B I - B III, Fe I — Fe VII and Ne I — Ne VIII.

Laboratory of Atomic Spectroscopy:
A. Ryabtsev, S. Churilov, A. Kramida, V. Azarov, L. Ivereva, R. Kildiyarova, I. Ivanov, E. Ivanova, M. Safronova, K. Koshelev and Yu. Sidelnikov

Collaborators:
NIST, Meudon, Amsterdam Univ.

4. Activities at VNIIFTRI

MISDC of VNIIFTRI and database "SPECTR"

Multicharged Ions Spectra Data Center of VNIIFTRI is a research group working more than years in the field of X-ray spectroscopy of multicharged ions and its application for diagnostics of h temperature plasmas. This group now consists of 7 researchers (5 physicists and 2 engineers).

The main fields of investigations:

A. creation of Bragg and Bragg-Fresnel optic elements for high-resolution X-ray spectroscopy
B. high-precision X-ray spectroscopy of multicharged ions (emission spectra observations, spectral line identification, accurate wavelength measurements) ($\lambda = 1 \div 26$ A)
C. creation of X-ray spectroscopy diagnostic methods and its applications for measurements of differer plasma object parameters (laser-produced plasma, Z- and X- pinches, plasma focus)
D. creation of database on spectra of atoms and ions (database "SPECTR")

The database "SPECTR":

The database SPECTR (DB "SPECTR"), on the one hand, is a great number of data characteristics of atoms and ions, and, on the other hand, is the software allowed to find fast information needed, to browse it on the screen and to make its hard copy.

The information stored in DB SPECTR may be divided on the two parts. The first part (and t the greatest one) is the data on properties of isolated atoms and ions, that is, the data on energy le structure, wavelengths of radiative transitions and its probabilities. The second part is the data characteristics of collision processes. The main difference between these two parts is the following. first part deals with the set of constants, while the second one -- with the set of functions. That is, if any radiative transition its wavelength, radiative probability, energies of upper and lower levels are some numerical quantities, then its collisional characteristics are the functions of the colliding part relative velocity. This difference causes the some difference in software used to operate with these dat different types.

The DB "SPECTR" software:

The database "SPECTR" software is based on FoxPro Database Management System. The information is stored in well-known DBF-format and can be transferred easily into another formats.

The DB "SPECTR" data:

The quantitative characteristics (4 May 1997):

Data on spectral lines	397 885 records
Data on energy levels	75 100 records
Data on ionization potentials	2 292 records
Data on excitation cross sections and rates	4 932 records
Data on ionization cross sections and rates	145 records
Data on dielectronic recombination rates	276 records
Data on references	504 records
The total number of records	**481 134**

The qualitative characteristics:

1). Now DB "SPECTR" is really database on characteristics of isolated atoms and ions, i.e. on spectr lines (wavelengths and radiative probabilities) and energy levels. The small number of collisional data wer inputted practically only for to test software developed.

2). Because of MISDC research team works in the field of X-ray spectroscopy, the main part of dat (about 75%) refers to the multicharged ions.

3). Data sources:

1. Published experimental data. For X-ray region database contains practically all publishe experimental data, for UV and visible regions - only some data.
2. Own experimental data for multicharged ions. This research group produc experimental data on X-ray spectra of multicharged ions during more than 20 years. Fo example only during last 5 years they have produced new accurate data on satellite lin caused by radiative transitions in He-, Li-, Be-, B-, C-, N-, O-, F-, Na-, Mg- like ion on high-n transitions in He- and Ne-like ions. Producing this kind of information is th main field of scientific interest of MISDC group. For this purpose they create a ne types of X-ray high-resolution spectrographs (with a spherically bent crystals, f example) and develop the new methods allowed to improve the accuracy of waveleng measurements.
3. Theoretical data, both published (not all, of course) and calculated especially for D "SPECTR" in some Russian (or Soviet) institutes: Institute of Physics of Lithuani Academy of Science, Voronezh State University, Uzgorod State University. Data f ions with small number of electrons were calculated by V.Pal'chikov (VNIIFTRI) w

the help of relativistic perturbation theory taking into account quant electrodynamics corrections.

The DB "SPECTR" performance:

The search operations are executed fast enough, some examples are presented in this table:

Database SPECTR
(4 May 1997)
The total number of records 481 134
Pentium-133, 16 MB RAM

	QUERY	SEARCH TIME	THE NUMBER OF RECORDS SELECTED
1	Lines of copper ions in spectral region 10.1 - 10.11 Å	2 s	9
2	Lines of silver ions in spectral region 10 - 15 Å	5 s	94
3	Lines of H-like and He-like silicon	4 s	3192
4	3d-2p transitions in Ne-like and Na-like silver	2 s	313
5	$1s2p\ ^1P_1$ - $1s^2\ ^1S_0$ transition in He-like uranium	2 s	2
6	$2s2p^63p$ - $2s^22p^6$ transitions in Ne-like ions	1 s	411
7	Lines of OI atom	1 s	441
8	Lines of O-like and N-like iron	3 s	998

The DB "SPECTR" applications:

Now DB "SPECTR" is used in:

1. Arzamas-16 (Russia)
2. Chelyabinsk-70 (Russia)
3. Livermore Lawrence National Laboratory (Livermore, USA)
4. University of Central Florida (Orlando, USA)
5. Max Plank Institute (Jena University, Germany)
6. Max Born Institute (Berlin, Germany)
7. Institute of Applied Physics and Computational Mathematics (Beijing, China)

Multicharged Ions Spectra Data Center (MISDC): A. Fayenov, I. Skobelev, V. Pal'chikov + 2 physicists and 2 engineers

4S-4P -3

Fe II $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s$ 1500

Ca II $1s^2 2s^2 2p^6 3s^2 3p^6 3d^0 4s$ 5

675 ENERGY LEVELS

$3d^7$ $3d^6(^ML)nl$ $3d^5(^ML)nln'l'(^{M'}L')$

$3d^4 4s^2 nl$

LAKIĆEVIĆ I. 1983, A&A, 127, 37

$a^6D - z^6D^o$

DIMITRIJEVIĆ, M.S. 1988 in Physics of Formation of Fe II lines outside LTE, Astrophys. Space Sci. Library, 138, D. Reidel p.c. 211

Solar

$a^4H - z^4F^o$

$a^6D - z^6D^o$

$a^4F - z^4F^o$

15 lines

$b^4P - z^4F^o$

$b^4F - z^4D^o$

$b^4P - z^4D^o$

MANNING, J.T. et al. 1990, Spectrochim Acta 45B, 1031

$a^4D - z^4D^o$

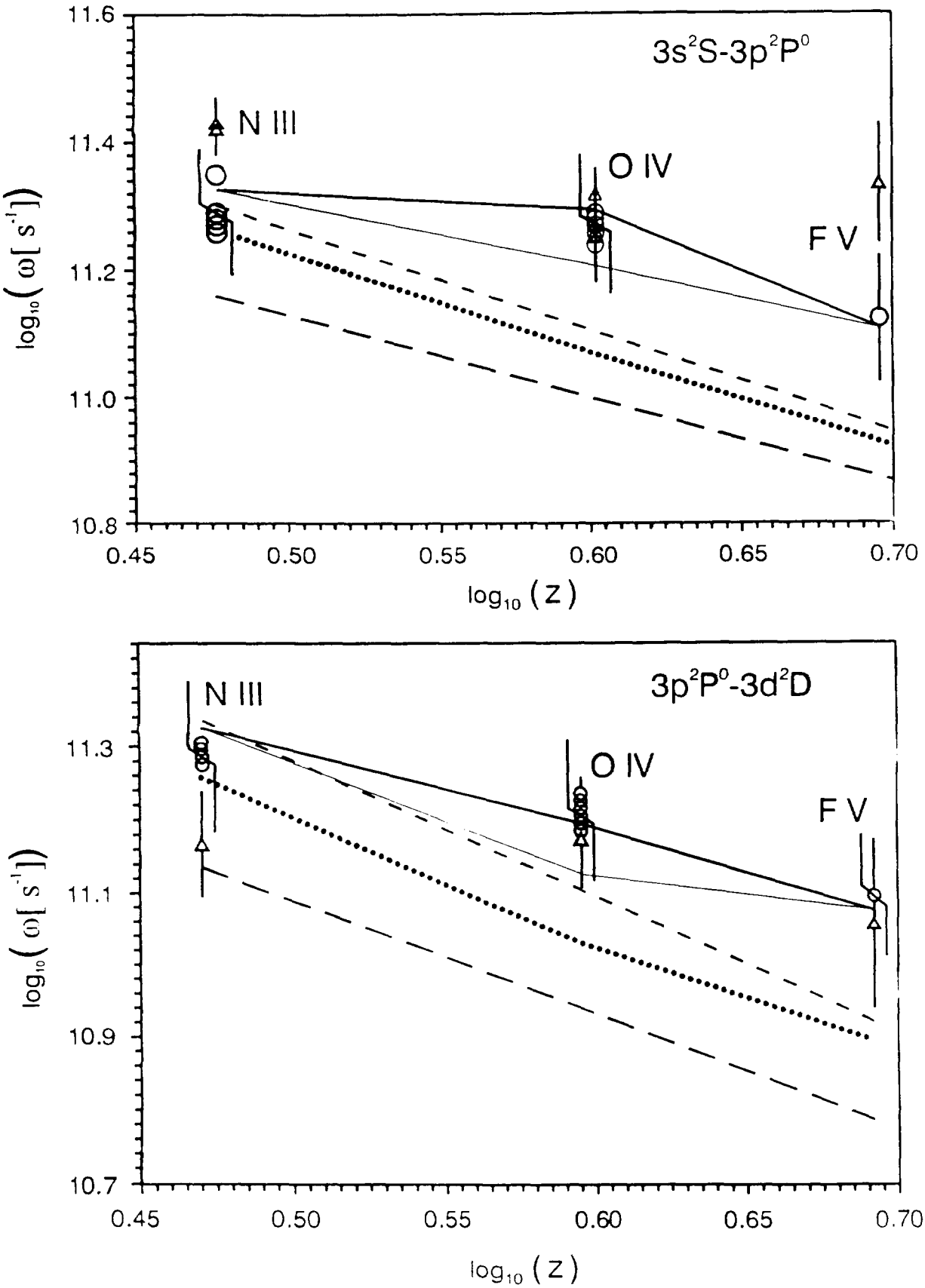
PURIĆ, MILLER, LESAGE, 1993, ApJ 416

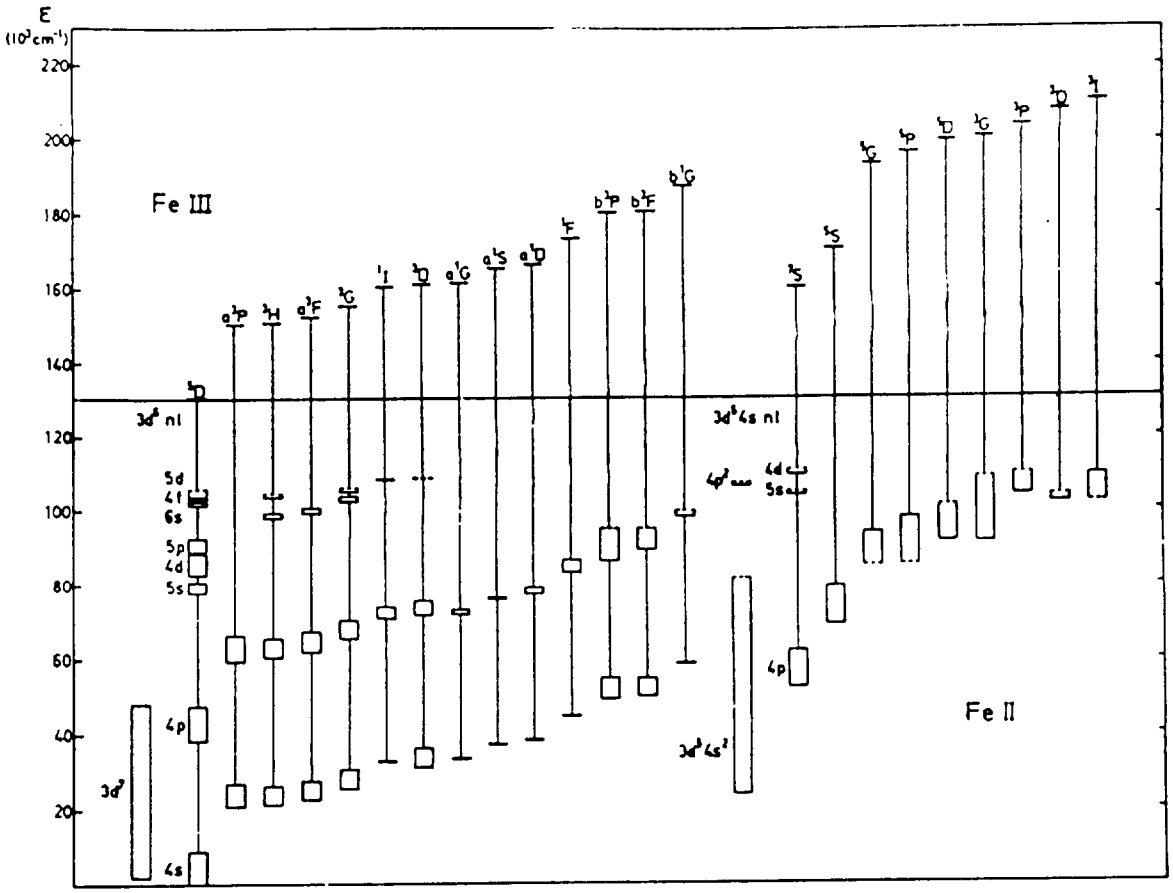
PURIĆ, DJENIŽE, SREĆKOVIĆ, BUKVIĆ PIVALICA, LABAT 1993, A&S 102, 607

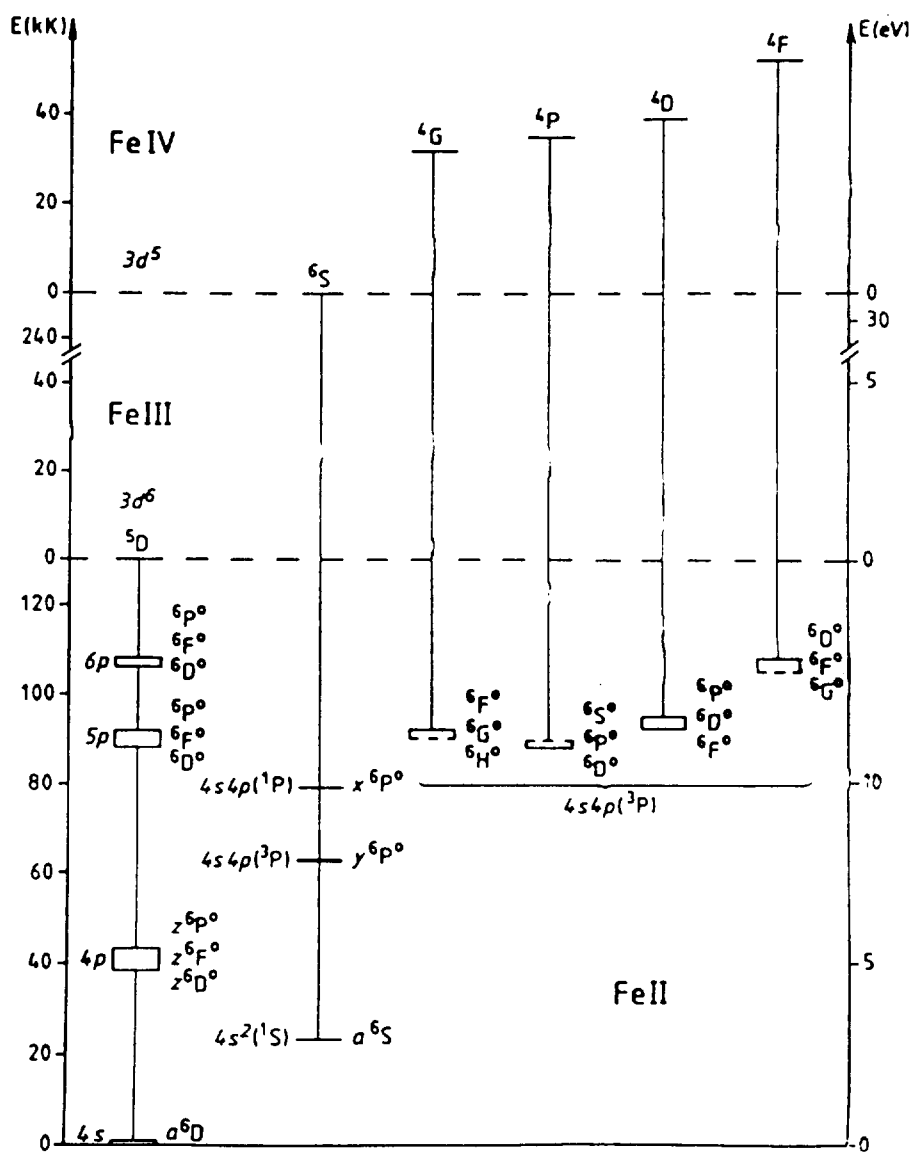
14 line $a^6D - z^6D^o$

$a^6D - z^6F^o$

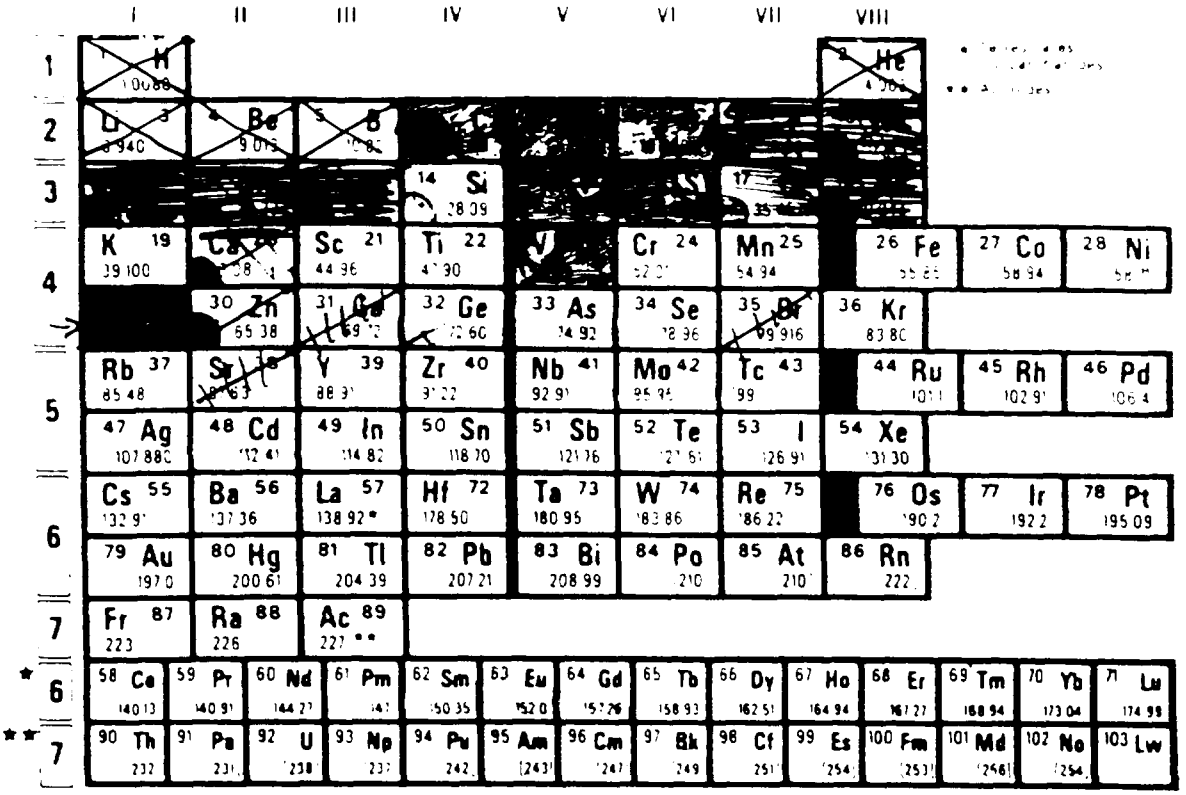
Fig. 5


3s²S-3p²P⁰
N III
O IV
F V
log₁₀(ω[s⁻¹])
log₁₀ (Z)
11.6
11.4
11.2
11.0
10.8
0.45
0.50
0.55
0.60
0.65
0.70
3p²P⁰-3d²D
N III
O IV
F V
log₁₀(ω[s⁻¹])
log₁₀ (Z)
11.3
11.1
10.9
10.7
0.45
0.50
0.55
0.60
0.65
0.70

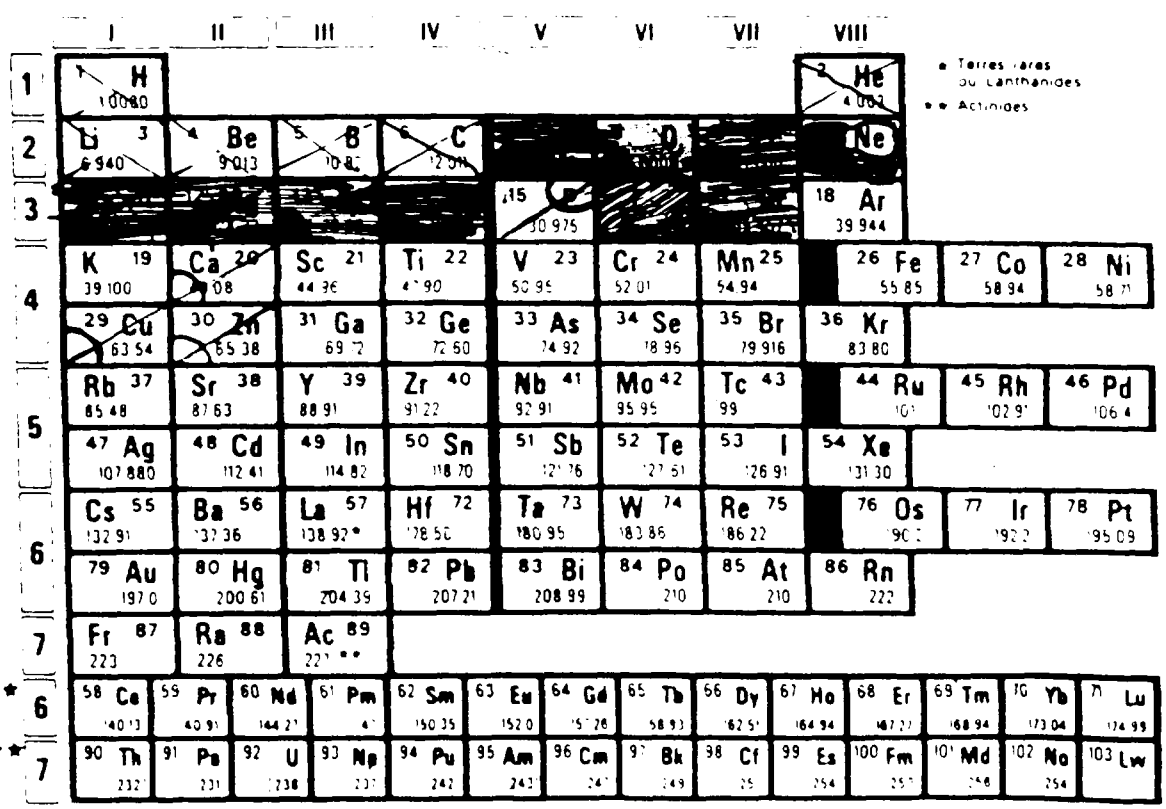

E
(10³cm⁻¹)
220
200
180
160
140
120
100
80
60
40
20
Fe III
3d⁶ nl
5d
4f
6s
5p
4d
5s
4p
3d⁶
4s
3d⁵4s nl
4p⁶ ---
4d
5s
4p
3d⁵4s²
Fe II


E(kK)
E(eV)
Fe IV
3d⁵
⁶S
⁴G
⁴P
⁴D
⁴F
0
240
30
5
Fe III
3d⁶
⁵D
6p
5p
4p
4s
⁶P°
⁶F°
⁶D°
⁶S°
4s4p(¹P) x ⁶P°
4s4p(³P) y ⁶P°
4s²(¹S) a ⁶S
4s4p(³P)
10
Fe II

CLASSIFICATION PÉRIODIQUE DES ÉLÉMENTS

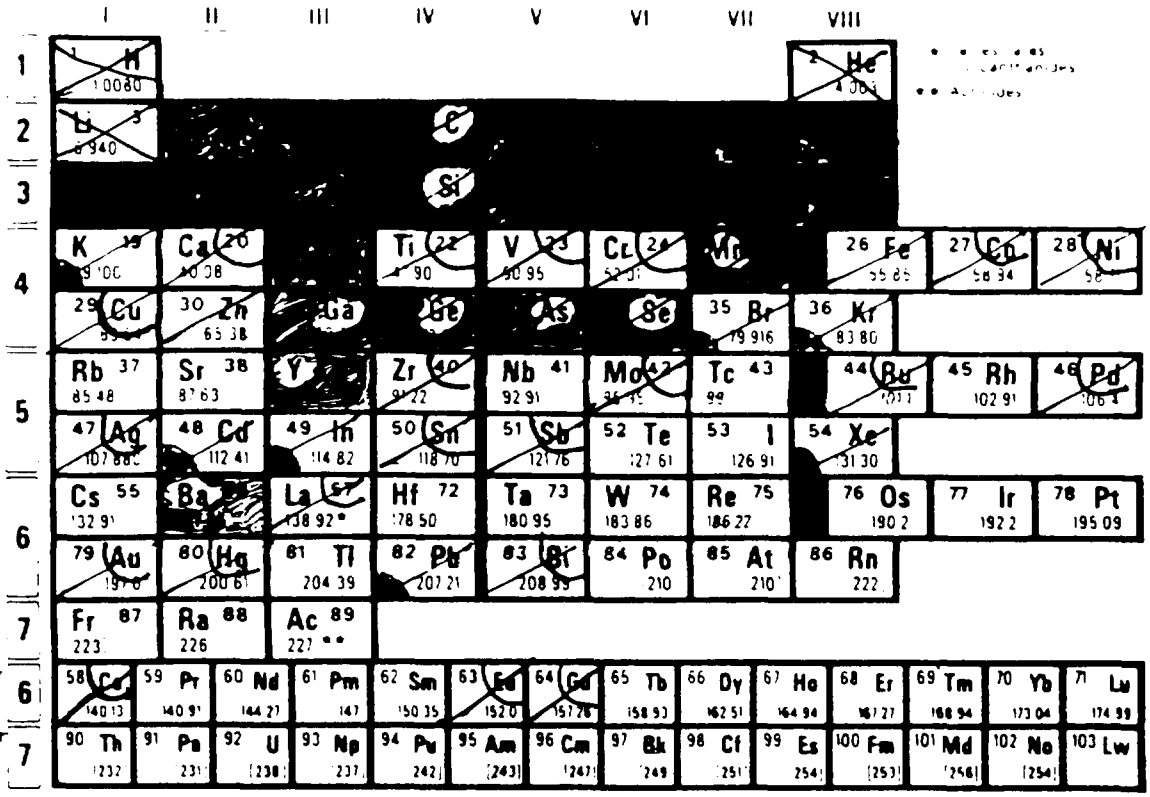


CLASSIFICATION PÉRIODIQUE DES ÉLÉMENTS

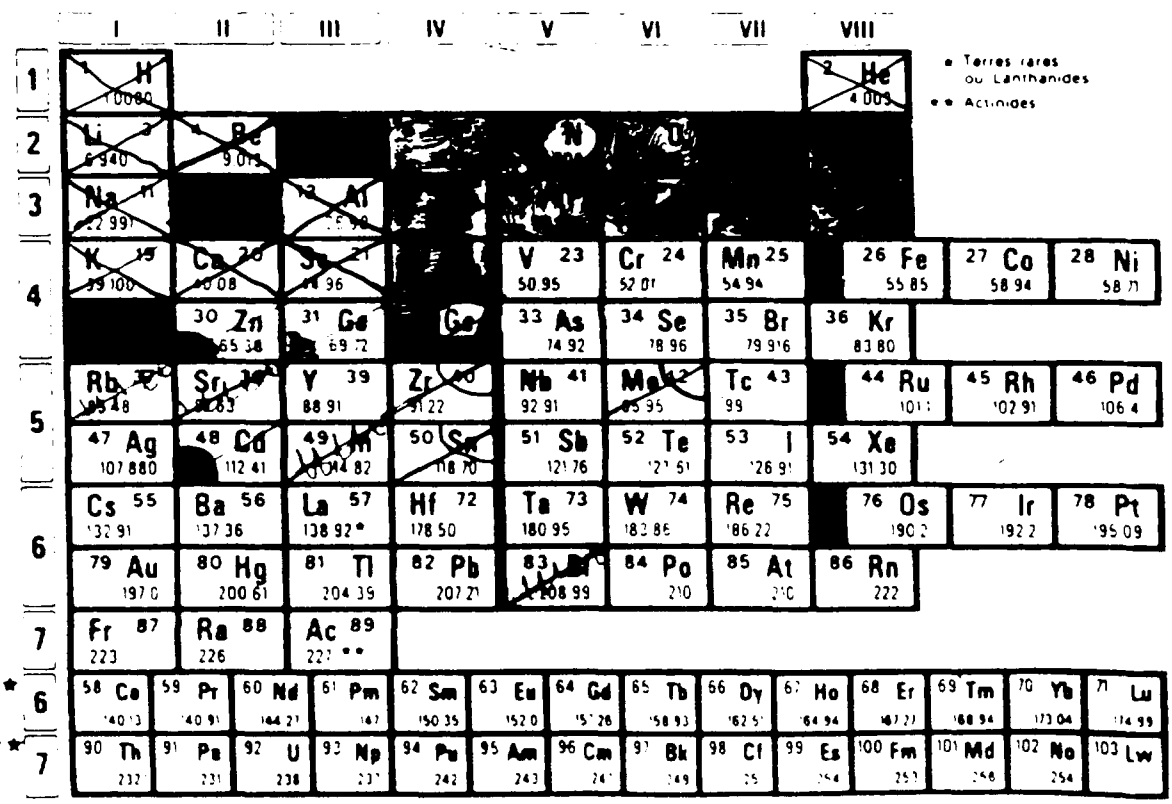


Cl VII Ca IX Ca X Si XI V XIII

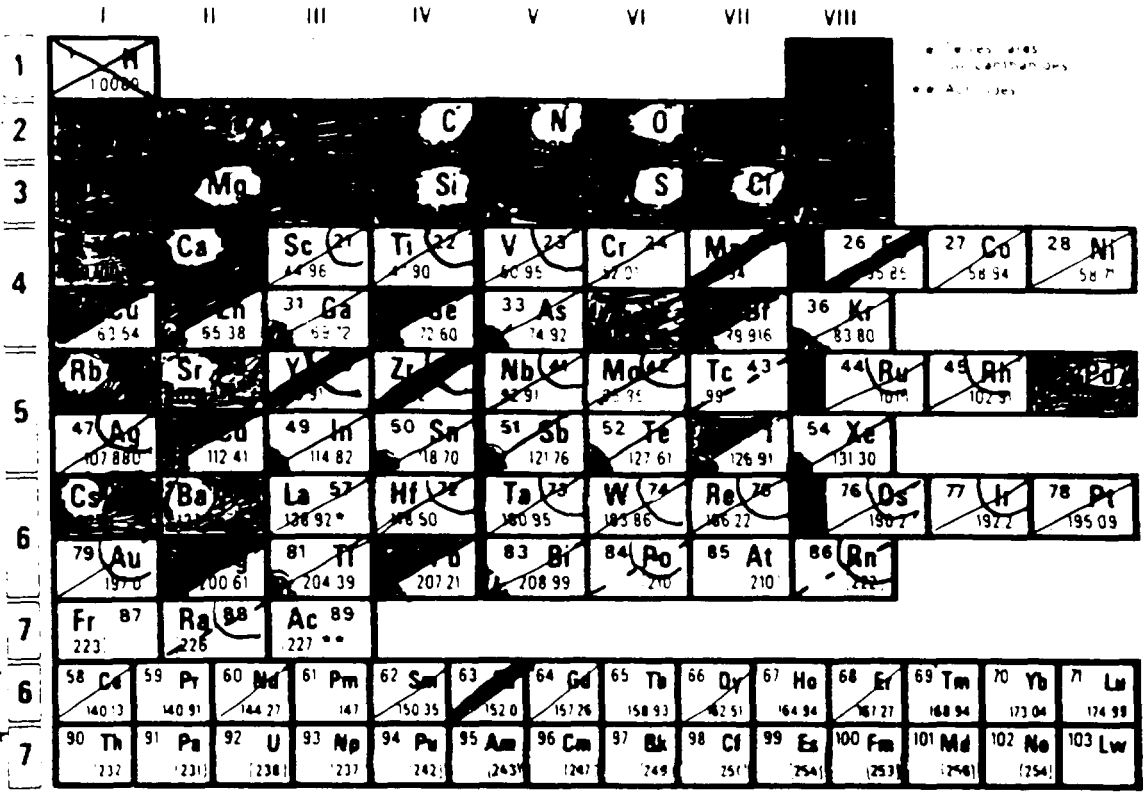
CLASSIFICATION PÉRIODIQUE DES ÉLÉMENTS



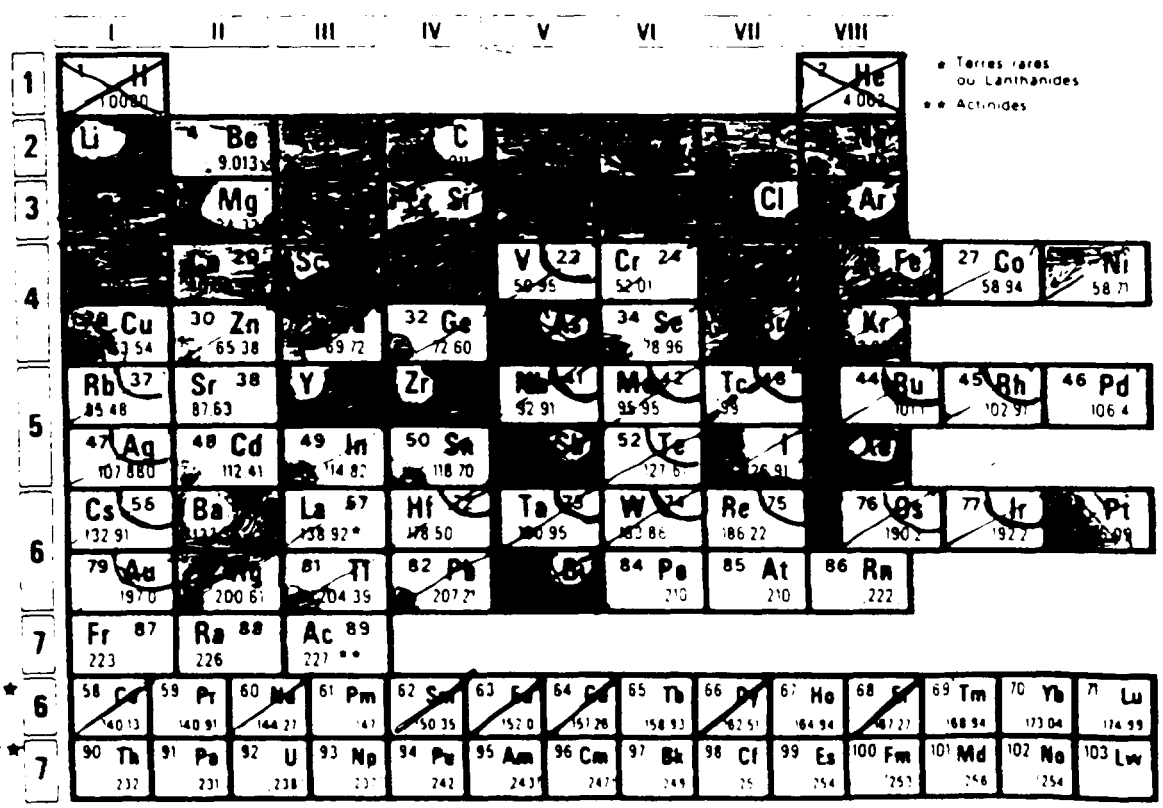
CLASSIFICATION PÉRIODIQUE DES ÉLÉMENTS



CLASSIFICATION PERIODIQUE DES ELEMENTS



CLASSIFICATION PERIODIQUE DES ÉLEMENTS



Transition	T(K)	WDSB (A)	WJBG (A)	WS (A)	dDSE (A)	dJBG (A)	ds (A)
2s-2p	5000	0.0801	0.144	0.0407	-0.0101	-0.0604	-0.0191
	20000	0.0445	0.0832	0.0286	-0.00499	-0.0347	-0.0121
2s-3p	5000	0.0555	0.0912	0.0598	0.00283	0.0358	0.00278
	20000	0.0420	0.0608	0.0397	0.00414	0.0214	0.00157
2p-3s	5000	0.133	0.155	0.127	0.0621	0.0789	0.0409
	20000	0.0723	0.102	0.0766	0.0371	0.0525	0.0220
2p-3d	5000	0.123	0.144	0.0978	0.00809	-0.0521	0.0104
	20000	0.0708	0.0870	0.0541	0.00183	-0.0278	0.00630
3s-3p	5000	11.0	12.2	8.54	-1.66	2.23	-0.522
	20000	7.56	8.34	6.21	-0.732	1.32	-0.332
3s-4p	5000	1.90	2.72		0.190	1.13	
	20000	1.57	2.18		0.151	0.753	
3p-4s	5000	3.60	3.84		1.50	1.77	
	20000	2.68	3.22		1.08	1.36	
3p-5s	5000	2.65	3.08		1.49	1.76	
	20000	2.14	2.92		1.12	1.48	
3p-3d	5000	336.	432.	280.	-22.6	-180.	-7.22
	20000	234.	302.	188.	-23.2	-113.	-4.34
3p-4d	5000	5.14	8.24		-0.507	1.32	+0.583 at 10^{13} cm^{-3}
	20000	4.74	5.38		-0.139	0.360	+0.231
3d-4f	5000	3.33	6.60		0.583	-1.65	
	20000	2.49	3.96		0.231	-0.756	

Be II

-0.0771
-0.0852 at 10^{13} cm^{-3}

Se I $4p^4 3p - 5s^3S^0$

T = 20000 K

$N_e = 10^{17}$ cm^{-3}

$W_{DSB} = 0.047$ A°

$W_L = 0.055$ A°

$d_{DSB} = 0.040$ A°

$d_1 = 0.033$ A°

TABLE IV. Average accuracy of different theoretical methods compared to Stark width and shift experimental data for helium lines. The results in parentheses are obtained by excluding the $2p\,^3D-3d\,^3D$ line which exhibits a strong unexplained difference between d_m and the calculated shift (especially for d_{DSB} and d_{BO}).

	All experiments included	Experiments with C and D accuracy excluded
$(W_m/W_{DSB})_{av}$	1.17±0.04	1.17±0.02
$(W_m/W_{BCW})_{av}$	1.07±0.04	1.07±0.04
$(W_m/W_{BO})_{av}$	0.92±0.04	0.93±0.02
$(d_m/d_{DSB})_{av}$	1.20±0.13 (1.07±0.04)	1.13±0.03
$(d_m/d_{BCW})_{av}$	1.23±0.08 (1.27±0.07)	1.34±0.09
$(d_m/d_{BO})_{av}$	1.14±0.07 (1.07±0.04)	1.14±0.03

perimental problems. Total uncertainties (in electron density and Stark width or shift measurements) are subdivided into four ranges and coded by letters.[8,9] The letters represent the following uncertainties: A, within 15%; B,

Table I

The list of spectral lines of Belgrade program for solar activity monitoring

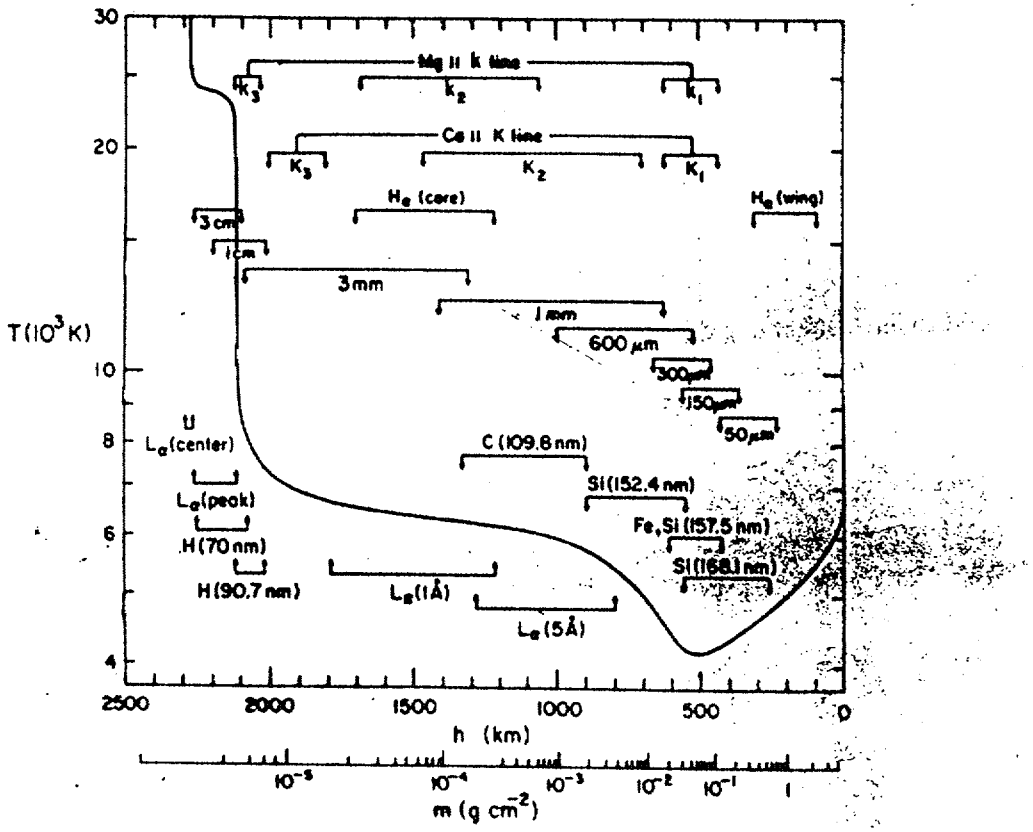
No	Element	λ(nm)	W(F)	Ep(eV)	g	Spot	Multiplet
1	MgI	518.36	303.0	2.72	-	S	$3^3P^\circ-4^3S$
2	NiI	519.72	4.8	3.90	-	u	
3	FeII	519.76	15.4	3.23	0.700	w	$a^4G-z^4F^\circ$
4	FeI	519.79	7.1	4.20	-	u	$y^5F^\circ-f^5P$
5	FeI	519.87	19.7	2.30	-	s	$a^5P-y^5P^\circ$
6	CrII	523.73	9.4	4.07	-	w	
7	ScII	523.98	10.5	1.45	-	w	
8	FeI	525.02	11.6	0.12	3	s	$a^5D-z^7D^\circ$
9	CaI	526.17	20.0	2.52	-	s	$3^3D-3d4p^3P^\circ$
10	FeI	527.32	19.5	3.29	-	s	
11	FeI	527.34	19.8	2.48	-	u	$a^3P-y^3D^\circ$
12	CrI	529.67	17.7	0.98	-	S	
13	CrI	529.74	16.4	2.90	-	s	
14	CrI	529.80	15.7	2.90	-	S	
15	CrI	529.83	20.8	0.98	-	S	
16	CrII	530.59	4.7	3.83	-	w	
17	FeI	530.74	16.6	1.61	-	S	$a^3F-z^3F^\circ$
18	TiII	533.68	12.9	1.58	1.071	w	
19	MnI	539.47	7.3	0.0	-	S	
20	FeI	539.83	14.1	4.44	0.333	s	$z^5G^\circ-f^5G$
21	FeII	542.53	8.8	3.20	-	w	a^4G-z^4F
22	MnI	543.25	8.5	0.0	-	S	
23	FeI	543.45	34.0	1.01	0.0	S	$a^5F-z^5D^\circ$
24	FeI	550.68	23.0	0.99	2.0	S	a^5f-z^5D
25	ScII	552.68	13.8	1.77	1.0	u	
26	FeI	557.61	21.9	3.43	0.0	u	$z^5F^\circ-e^5D$
27	CaI	558.20	16.7	2.52	1.5	S	$3^3D-3d4p^3D^\circ$
28	CaI	560.13	17.8	2.52	-	S	$3^3D-3d4p^3D^\circ$
29	NaI	568.26	18.5	2.10	1.067	s	$3^2P^\circ-4^2D$
30	NaI	568.82	22.3	2.10	-	S	$3^2P^\circ-4^2D$

S - The line is greatly strengthened in the spot spectrum

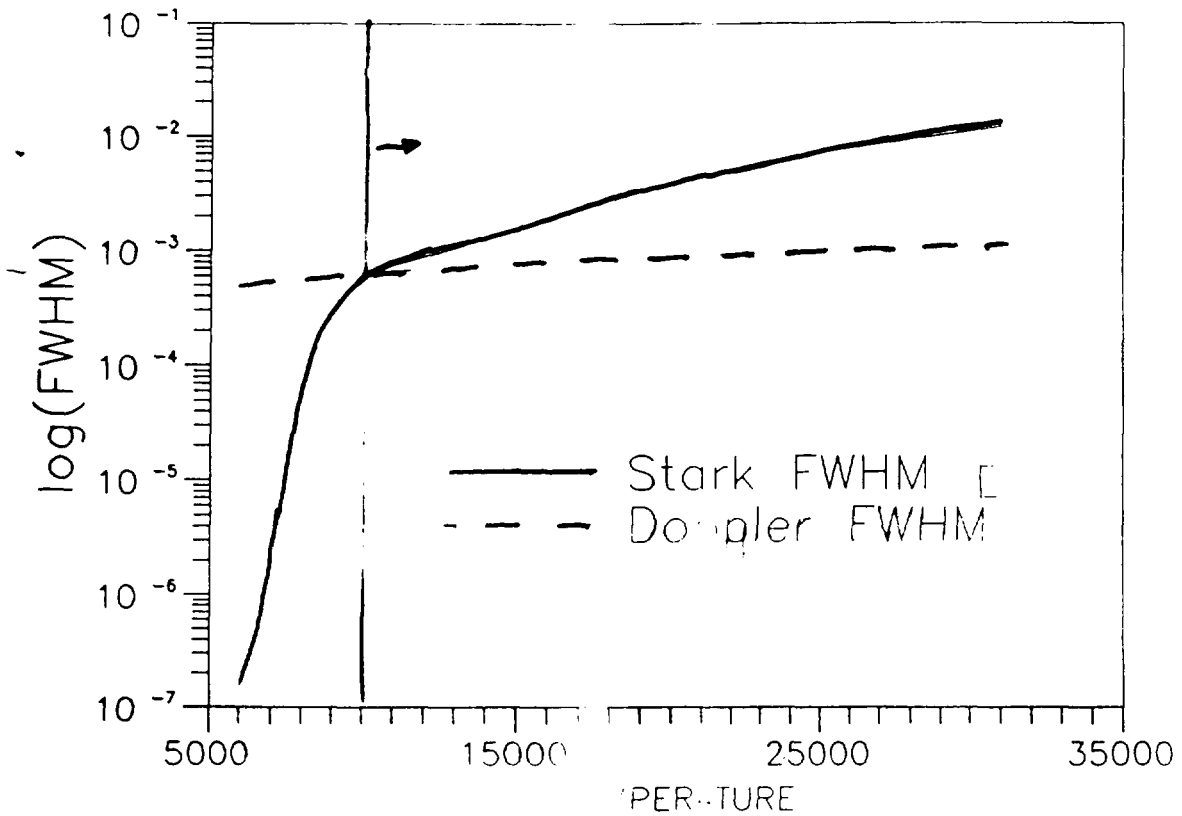
s - The line is strengthened in the spot spectrum

u - The line is unchanged in intensity in the spot spectrum

w - The line is weakened in the spot spectrum


T(10³K)
30
20
10
8
6
4
Mg II k line
K3
K2
K1
Ca II K line
K3
K2
K1
Hα (core)
Hα (wing)
3cm
1cm
3mm
1mm
600 μm
300μm
150μm
50μm
U
Lα(center)
Lα(peak)
H(70nm)
H(90.7nm)
Lβ(1Å)
Lα(5Å)
C(109.8nm)
Si(152.4nm)
Fe,Si(157.5nm)
Si(168.1nm)
2500
2000
1500
1000
500
0
h (km)
10⁻⁵
10⁻⁴
10⁻³
10⁻²
10⁻¹
1
m (g cm⁻²)

THERMAL DOPPLER AND STARK WIDTHS FOR $\lambda = 437.9$ (YII) LINE AS FUNCTIONS of TEMPERATURE AND OPTICAL DEPTH FOR AN A STAR ($T_{eff} = 10000$ K, $\log g = 4.0$)



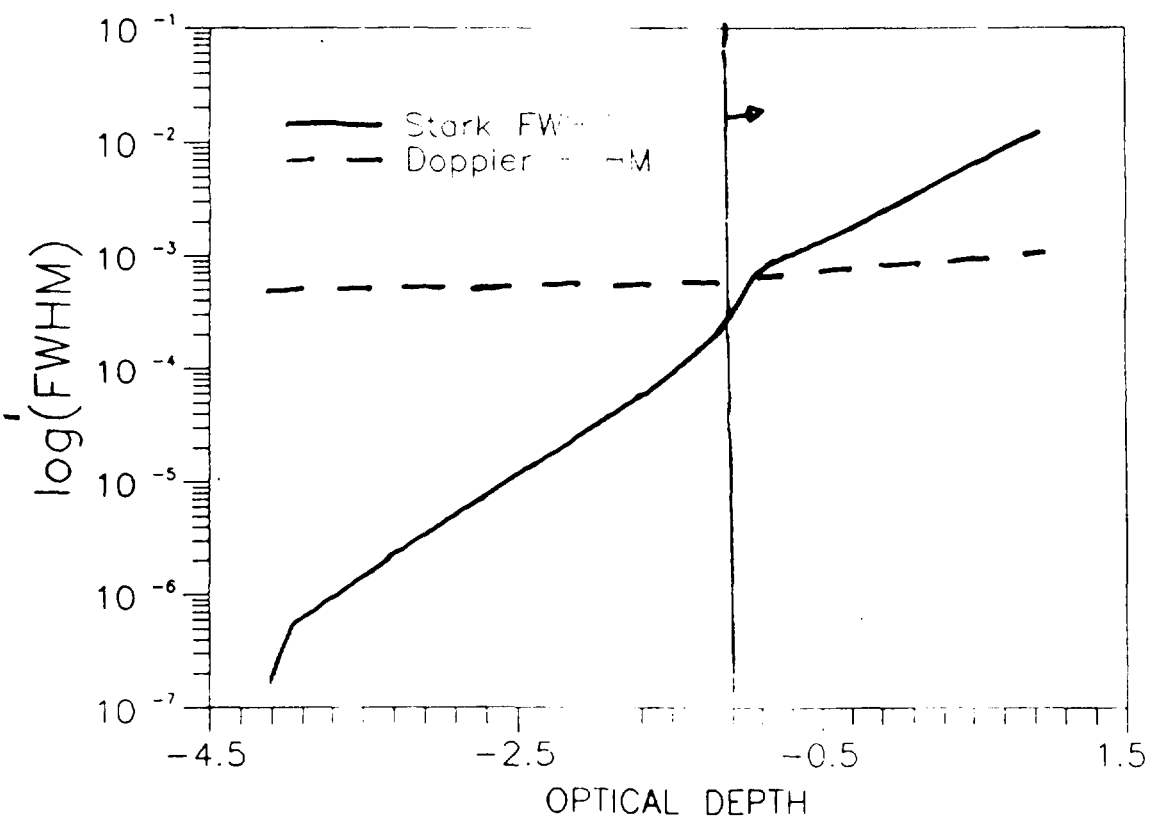


Table 3. Line identification list for the programme stars. These lines were identified in all stars if not indicated otherwise (labels: a=PG1159-035, b=PG1520+525, c=PG1424+535, d=PG1707+427). Doubtful identifications are marked by colons. Predicted line positions arising from some ions of interest which are, however, not observed are bracketed. Lines occuring in unresolved blends are marked by asterisks.

wave-length	ion	tran-sition	wave-length	ion	tran-sition
1168.9[ad]	C IV	3d-4f	1198.6[a]	C IV	3d-4p
1210.6[a]	C IV	4s-7p	1230.0[a]	C IV	3p-4s
1240.1[ac]	N V	2s-2p	1261.9[ab]	O VI	5p-7d
1289.9[ab]	O VI	5d-7f	1291.9[ab]	O VI	5f-7g etc
1302.5[a]	O VI	5d-7p	1303.8[a]	O VI	5p-7s
1315.7	C IV	4p-7d	1351.2	C IV	4d-7f
1353.0	C IV	4f-7g	1358.5[a]	C IV	4d-7p
1371.3[acd]	O V	$2p^1P^o$-$2p^1D$	(1413.7)	O VI	6d-10p
1423.[ab]	O VI	6d-10f etc.	1440.3[ac]	C IV	4s-6p
(1545.3)	O VI	6s-9p	1549.1	C IV	2s-2p
1585.9	C IV	4p-6d	(1637.6)	C IV	4d-6f
(1638.6)	O VI	6d-9f	1640.1*	C IV	4f-6g
1640.4*	He II	2-3	1640.9*	O VI	6f-9g
1641.1*	C IV	4f-6d	1641.2*	O VI	6g-9h etc
1653.9	C IV	4p-6s	(1860.4)	N V	5f-7g etc
3312.4[ab]	O VI	6p-7d	3423.2[ab]	O VI	6d-7f
3432.6[ab]	O VI	6f-7g	3433.9[ab]	O VI	6g-7h etc
3689.7[ab]	C IV	6f-9g etc	3811.3[ab]	O VI	$3s-3p_{3/2}$
3834.2[ab]	O VI	$3s-3p_{1/2}$	3934.7[ab]	C IV	5s-6p
(4100.1)	He II	4-12	(4101.7)	H I	2-6
(4199.8)	He II	4-11	4219.2	C IV	6s-8p
4231.3	C IV	7-12	4338.7[cd]	He II	4-10
(4340.5)	H I	2-5	4440.7	C IV	5p-6d
4493.7[ab]	O VI	8-10 trough	(4519.8)	N V	7f-9g etc
4542.9	He II	4-9	4554.1	C IV	6p-8d
(4603.7)	N V	$3s-3p_{3/2}$	(4620.0)	N V	$3s-3p_{1/2}$
(4632.)	O IV	multiplet 19	4646.8	C IV	5d-6f
4657.2	C IV	5f-6g	4658.9	C IV	5g-6h
4664.8	C IV	5f-6d	4677.8	C IV	6d-8f
4684.7*	C IV	6f-8g	4685.2*	C IV	6g-8h
4685.4*	C IV	6h-8i	4685.5*	C IV	6h-8g
4685.6*	C IV	6g-8f	4685.7	He II	3-4
4688.0	C IV	6f-8d	(4687.7)	O VI	9-12 trough
(4691.2)	C IV	7-11 trough	4736.2	C IV	6d-8p
(4773.2)	O VI	7s-8p	4786.2	C IV	5d-6p
4789.2	C IV	6p-8s	4859.3	He II	4-8
(4861.3)	H I	2-4	(4945.3)	N V	6f-7g etc.
5017.2	C IV	5p-6s	(5083.5)	O VI	7p-8d
5269.9[ab]	O VI	7d-8f	5288.7[ab]	O VI	7f-8g
5290.6[ab]	O VI	7g-8h etc.	5356.9	C IV	7p-10d
5411.5	He II	4-7	5470.7	C IV	7-10 trough
(5519.0)	C IV	7p-10s	5801.3[ab]	C IV	$3s-3p_{3/2}$
5812.0[ab]	C IV	3s-3p	(5864.6)	C IV	8-13 trough
(6560.)	C IV	8-12	(6560.)	O VI	12-18
6560.2	He II	4-6	(6562.8)	H I	2-3
6589.9	C IV:	6s-7p			

PG 1159 PRE WHITE DWARFS

T 100.000 – 170000 K

C/He ≈ 0,5

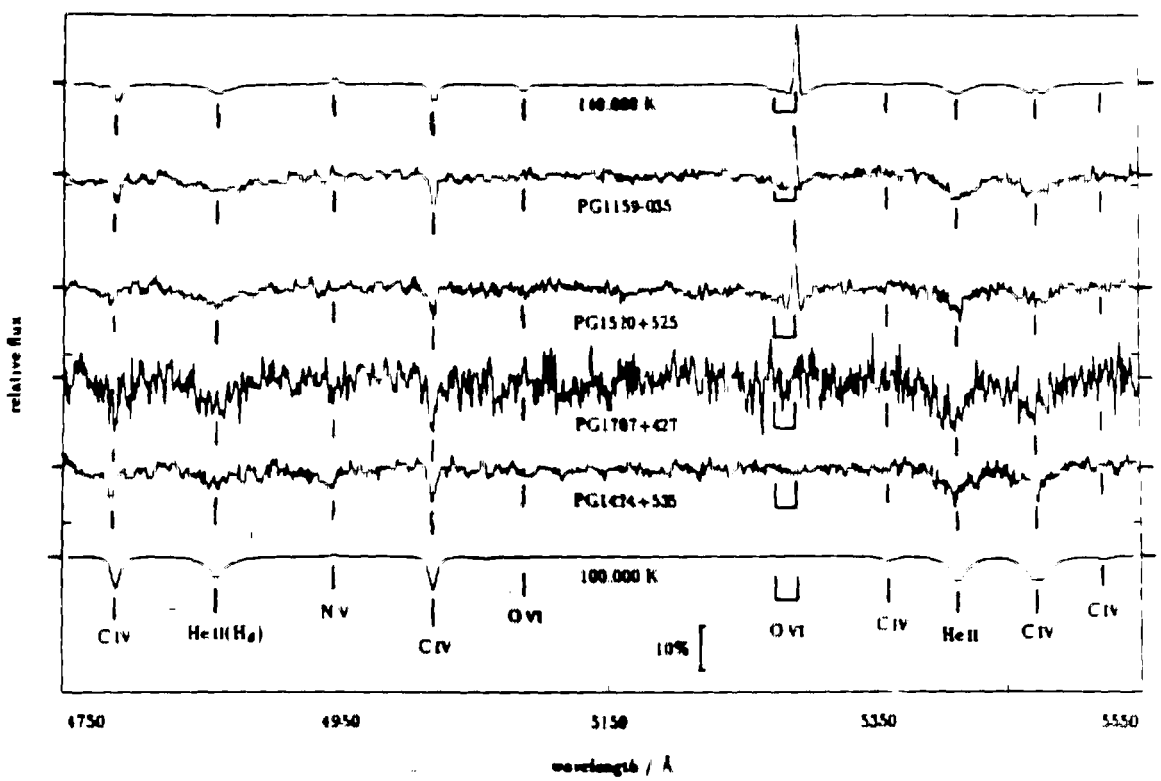


Fig. 1b. Continuation of Fig. 1a up to 5550Å. The spectral resolution is about 1Å. The O VI emission at 5291Å is prominent in PG1159-035 and PG1520+525

K. WERNER ET AL. ASTRON. ASTROPHYS. 244, 437 (1991)

=XV.

IRONS 1973 – Laser irradiation of polyethylene foil

IGLESIAS, GRIEM, 1988

WANG, GRIEM, IGLESIAS, 1989 } laser produced plasma

IEOR.

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McLEAN, STAMPER, MANKA, GRIEM, DROEMKE, RIPIN, Phys. Fluids 27, 1327 (1984)

1. The number of spectral lines of various atomic species taken into account for opacity calculations for classical cepheid models, by Iglesias, Rogers and Wilson [8].

Element	Number of spectral lines
H	45
He	45
C	638
N	54
O	2390
Ne	16030
Na	50170
Mg	105700
Al	145200
Si	133700
Ar	12560
Fe	11530000

QUANTUM MECHANICAL

Li I (2S-2P) DIMITRIJEVIC, FERLUTRIER, SAHAL-BRECHOT 198

Ca II 4S-4P BARNES, PEACH 1970
3D-4P BARNES 1971

Mg II 3S-3P BARNES, 1971; BELY, GRIEM 1970

Be II 2S-2P SANCHEZ, BLAHA, JONES 1983

42 TRANSITIONS in Li-LIKE Be II, B III, C IV, O VI, Ne VI
SEATON 1988

$2s^2\,{}^1S - 2s2p\,{}^1P$
$2s2p\,{}^3P^o - 2p^2\,{}^3P$
$2s2p\,{}^1P^o - 2p^2\,{}^1D$
$2s2p\,{}^1P^o - 2p^2\,{}^1S$

} C III, O V, Ne VII SEATON 1987

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