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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA CONSULTANTS' MEETING:

9th MEETING OF ATOMIC AND MOLECULAR DATA CENTRES

AND ALADDIN NETWORK

Vienna, September 20 and 21, 1990

SUMMARY REPORT

Prepared by R.K. Janev

November 1990

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

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SUMMARY REPORT

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Abstract

This Summary Report contains the proceedings and the conclusions of the IAEA Consultants' Meeting: 9th Meeting of Atomic and Molecular Data Centres and ALADDIN Network, convened on September 20 and 21, 1990, at the IAEA Headquarters in Vienna. The Progress Reports of national atomic data centres and reports on the ALADDIN status and developments are also included as appendices to the present Report.

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1. INTRODUCTION

On September 20 and 21, 1990, the IAEA Atomic and Molecular Data Unit (AMDU) convened at the IAEA Headquarters in Vienna the 9th Meeting of the Atomic and Molecular Data Centre Network (A+M DCN) together with the ALADDIN Users Network. The objectives of this year meeting were to exchange information on and discuss the current activities in the national A+M data centres for fusion and the IAEA AMDU, co-ordinate in future A+M data compilation and evaluation programmes (particularly in view of the ITER physics long-term R+D plans), to discuss the status of ALADDIN implementation in the A+M DCN practices and its further developments, and to analyze the manpower situation in the data centre network in relation with the urgency of some of the ITER R+D programmes. The detailed Meeting Agenda is given in Appendix 1.

The Meeting was attended by 17 participants (including three from the IAEA) and 4 observers. The List of Participants and Observers is given in Appendix 2. Of the 15 data centres co-operating within the A+M DCN only the JILA Information Center and the A+M Data Group of the Chinese Nuclear Data Centre were not represented at the Meeting. The ALADDIN Users Network, outside the A+M DCN, was represented by Dr. R. Hulse (Princeton Plasma Physics Laboratory) and Dr. R.E.H. Clark (Los Alamos National Laboratory).

2. MEETING PROCEEDINGS

The Meeting was opened by Dr. J.J. Schmidt, Head of the IAEA Nuclear Data Section. The work of the Meeting then proceded in the following sessions:

1) Current activities and near-future plans of the A+M data centres,
2) Status of ALADDIN, its implementation and further developments,
3) Priorities in the future A+M data compilation/evaluation activities and the DCN manpower situation,
4) Formulation of meeting conclusions and recommendations.

A brief account of the presentations and the discussions in these sessions is given below.

2.1. Current Data Centre Network Activities

All the representatives of national A+M data centres presented progress reports about their data compilation, evaluation and publication activities during the past year. Each of the reports covered finalized work, work in progress and work plans for the next year. The presented progress reports are given in Appendix 3. Included in this Appendix is also a brief report obtained from Dr. Yao Jinzhang on the last year activity of the A+M Data Group of the Chinese Nuclear Data Centre in Beijing. The A+M Group of the Nuclear Data Centre in Obninsk (USSR) is still in the process of consolidation (both in terms of staff and programmes) and no written report was provided. It was, however, reported that the Obninsk A+M Data Group has adopted and already implemented ALADDIN in its work.

On the basis of presented progress reports and discussions at the meeting, the following major characteristics of the current A+M DCN activities can be identified:

a) Bibliographic database: The bibliographic A+M data information for fusion is adequately covered by the ORNL CFADC. This information, supplemented by additional input from the Kurchatov Institute Data Centre, GAPHYOR (non-systematic check-ups) and the IAEA AMDU, is the basis for the semi-annual "International Bulletin on A+M Data for

Fusion", issued by the IAEA AMDU. This Bulletin now provides also information on the ALADDIN formatted A+M data files stored at the IAEA and available from the IAEA AMDU on request. It is felt that a more rigorous cross-checking between the GAPHYOR and ORNL CFADC bibliographic databases would be useful.

b) Compilation activity: This activity is being pursued by most of the data centres and is related to the specific programmes carried out by the centres. On a systematic basis, the data compilation activity is pursued by the data centres at NIST (Gaithersburg), NIFS (Nagoya), JAERI, VNIIFTRI (Mendeleevo) and recently by CRAAMD. It should be noted that particle-surface interaction (PSI) data are becoming an increasing part of this activity (NIFS, JAERI, Kurchatov Institute, IAEA AMDU).

c) Data evaluation activity: Important data evaluation work during the last year was performed in most of the data centres (ORNL CFADC, NIST, Belfast, NIFS, JAERI, Bologna, Kurchatov Institute, CRAAMD, IAEA AMDU), covering both A+M and PSI data. Among the highlights of this activity is the ORNL Redbook vol. 1: "Collisions of H, H_2, He and Li atoms and ions with atoms and molecules" (ORNL-6086, 1990), and several publications on spectroscopic data by NIST. Data evaluation is also being carried out within the Co-ordinated Research Programme on "A+M data for fusion edge plasmas".

2.2. Status of ALADDIN (implementation and developments)

The ALADDIN system currently contains three types of data: collisional, spectroscopic and PSI data. The oral reports by the data centre representatives indicated that ALADDIN is being used in most of the data centres. Data centres having other systems for internal data management have also a capability to convert the data into ALADDIN format. The information contained in the new ORNL Redbook vol. 1 is also ALADDIN formatted. The IAEA AMDU, ORNL CFADC, CRAAMD operate (store or exchange data) using only the ALADDIN system.

The spectroscopic part of ALADDIN has been developed by Dr. R.E.H. Clark (Los Alamos National Laboratory) and proved to be adequate. The PSI data part has been developed by the IAEA AMDU (in co-operation with Prof. E.W. Thomas, Georgia Institute of Technology). These developments will be included in the second version of the ALADDIN System Manual, the preparation of which is underway in the IAEA AMDU. The new version of ALADDIN manual will also incorporate the suggestions made at the last DCN meeting regarding some minor modifications in the system.

Since the ALADDIN format proved to be acceptable from practical point of view, the meeting participants felt that it will be useful to keep the basic ALADDIN structure and format "frozen" for certain period of time, until more experience is accumulated. Necessary additions in the ALADDIN dictionaries to accommodate for new types of data within the presently established categories should be co-ordinated with the IAEA AMDU.

The written reports presented at this session of the Meeting are given in Appendix 4. (The basic article on ALADDIN by R. Hulse is also included in this Appendix).

2.3. A+M Data Priorities Related to ITER Long-Term R+D Programme

The ITER Team has recently formulated the Long-Term Physics R+D Programme (up to 1995) in support to the ITER Engineering Design Activities (EDA). An analysis of the tasks in this programme revealed that in several critical R+D areas the atomic and particle-surface collision data are important ingredients in the underlying physics

problems. Such areas are the edge plasma physics, particle and power exhaust issues, impurity control, neutral beam heating and current drive, erosion and thermo-mechanical properties of plasma facing materials, and alpha particle diagnostics. The R+D investigations in these area involving atomic and particle-surface interaction data, as well as the required atomic physics information, are specified in Appendix 5.

Among the highest A+M and PSI data priorities imposed by the urgent tasks in the ITER physics R+D programme are:

- database for the plasma edge A+M processes (for plasma and neutral gas transport modelling, hydrogen recycling, edge plasma diagnostics, helium transport and exhaust),
- databases for impurity transport and radiation losses (accurate cooling rates for the common and metallic impurities, viability of the "radiative layer" concept for power exhaust),
- database for the net erosion rates of plasma facing materials (including all erosion and redeposition processes),
- complete databases for Be, B and certain medium- and high-Z impurities (Si, Ti, Cr, Fe, Ni, Mo and W),
- database for energetic He-beam penetration into plasmas (for alpha particle diagnostics).

The generation of significant part of the required evaluated data is already underway or planned within the existing (or planned) DCN and co-ordinated research programme (CRP) activities (the CRPs on A+M data for fusion edge plasmas, on erosion rates, on metallic impurities). However, some goal-oriented actions have to be undertaken by the IAEA AMDU in the near future to meet the urgent ITER data needs (e.g. for He-beam penetration, Be and B, hydrogen recycling, etc).

2.4. Data Centre Network Manpower Situation

The manpower and funding situation in the Data Centre Network was discussed in Session 4 in a historical prospective and in view of the current fusion A+M data needs and those inherently contained in the ITER long-term R+D programmes. Despite the increase of the DCN membership during last two years, a slight decline of funding and manpower is being observed in most of the national data centres.

A breakdown of the present manpower situation in the A+M Data Centre Network is given in Appendix 6. The A+M data generation capabilities of the individual data centres are also shown in that Appendix. (These capabilities are an important segment of the data centre potential in terms of both generation of urgently needed data and the required expertise for data evaluation). As evidenced by the Table in Appendix 6, the present DCN manpower potential is insufficient for prompt responds to urgent data demands from the fusion community. This is particularly true for the data evaluation work, which is directly related to the availability of funds (since data evaluation is usually done with the assistance of external consultants). The present level of DCN manpower and funding is also clearly insufficient to respond to the A+M needs of ITER R+D programme. An increase in DCN manpower/funding of at least 50% (on average) will be required as soon as the implementation of the ITER R+D programme starts. A stronger interaction of the data centres with the "home" ITER teams was suggested as potentially useful in resolving the funding problem and for direct involvement in the ITER R+D programmes.

2.5. Other Items

The Meeting was informed that the association of J.J. Smith with the IAEA A+M Data Unit will terminate in March 1992 for administrative

reasons. The Meeting participants expressed high appreciation for Jim's contribution to the IAEA AMDU activity and particularly in the process of establishment and implementation of ALADDIN.

The character of the DCN Meeting within the present IAEA Meeting classification scheme was also discussed. Its current classification as a "consultants' meeting" has become rather inadequate after the significant increase of the number of A+M data centres and A+M data groups co-operating within the Network in last several years and the recent IAEA reduction of the number of supported consultants to five. To preserve the active participation in the future DCN meetings by all data centres and groups, it has been recommended the IAEA considers the re-classification of these meetings as Advisory Group Meetings. This re-classification would also reflect one of the basic functions of the meetings: to advise the IAEA AMDU in technical matters related to the establishment and maintenance of numerical A+M databases for fusion.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

1) The presentations and discussions at the Meeting have indicted that despite of certain problems in the area of manpower and funding, the Data Centre Network still successfully responds to the A+M data demands from the fusion research community. The adequate level data compilation and evaluation activities is maintained as result of better organization, use of internal resources, work co-ordination and active collaboration within the A+M Data Centre Network. The new members of the Network (CRAAMD, Obninsk, CNDC/AMD Group, VNIIFTRI) are still in a stage of internal consolidation and/or adaptation to the programmatic scope of the A+M DCN, but their contribution is becoming significant and is expected to increase in future.
2) With inclusion of the spectroscopic and particle-surface interaction parts in the ALADDIN structure, the system now covers all types of data from the scope of DCN activities. It has been concluded that the next version of ALADDIN Manual (which will implement all the suggestions for improvements given at the last DCN Meeting) should be kept "frozen" for a longer period of time to further consolidate the system.
3) The recently formulated long-term ITER R+D plans set a general framework for the priorities in the data compilation, evaluation and generation activities of the A+M Data Centres. More specific guidelines in this respect are expected from the IFRC Subcommittee on A+M Data for Fusion in nearest future. It was also concluded that the current programme of activities is well within the ITER priority framework (A+M data for fusion edge plasmas, data for metallic impurities, erosion rates of plasma facing materials, database for H-beam penetration into plasmas, etc), but new specific actions have to be taken in the immediate future for establishing complete databases for Be and B, He-beam penetration into fusion plasmas, and Mo and W.
4) The present DCN manpower and funding situation is inadequate to carry on efficiently and timely the full scale programmes on A+M/PSI data for fusion. This inadequacy will particularly affect the required A+M data support to the urgent tasks of ITER R+D plans. Interaction of national data centres with the "home" ITER teams could be beneficial in this respect.
5) Due to the recent increase of DCN membership and enhanced advising role of DCN in technical matters of IAEA AMDU, it has been strongly recommended that IAEA AMDU investigate all administrative possibilities for re-classification of the DCN Consultatns' Meeting into an Advisory Group Meeting.

IAEA Consultants' Meeting:
9th Meeting of Atomic and Molecular Data Centres and ALADDIN Network

September 20 and 21, 1990, Vienna, Austria

MEETING AGENDA

Thursday, September 20

09:30 - 09:45: Opening
Adoption of Meeting Agenda

Session 1: Current activities and near-future plans of A+M Data Centres
Chairman: Delcroix

09:45 - 11:00: Reports from Data Centres:
Wiese (NIST), Abramov (Moscow), Smith (Belfast)

11:00 - 11:15: Coffee break

11:15 - 12:30: Reports from Data Centres:
Phaneuf (ORNL), Tawara (Nagoya), Shirai (JAERI)

12:30 - 14:00: Lunch

Session 1: (Cont'd)
Chairman: Abramov

14:00 - 15:45: Reports from Data Centres:
Delcroix/Katsonis (GAPHYOR), Menapace (Bologna), Piksaikin (Obninsk)

15:45 - 16:00: Coffee break

16:00 - 18:00: Reports from Data Centres:
Sun Yongsheng (CRAAMD), Faenov (VNIIFTRI), Janev (IAEA)

Friday, September 21

Session 2: Status of ALADDIN system, its implementation in data centre practices and further developments
Chairman: Hulse

09:00 - 10:30: Comments of Hulse and Reports from IAEA AMDU, A+M Data Centres and other ALADDIN users

10:30 - 10:45: Coffee break

10:45 - 12:00: Further ALADDIN developments and next version of ALADDIN Manual (Hulse, Clark, Faenov, J.J. Smith, other ALADDIN users)

12:00 - 14:00: Lunch

Session 3:	Priorities in the future A+M data compilation/evaluation activities and the DCN manpower situation
Chairman:	Janev
14:00 - 15:30:	a) A+M data compilation/evaluation priorities following from the ITER physics R+D programme (1991-95) b) Analysis of the DCN funding and manpower situation
15:30 - 16:00:	Coffee break
Session 4:	Meeting conclusions and recommendations
Chairman:	Janev
16:00 - 17:30:	- Formulation of Meeting conclusions and recommendations - Adoption of Meeting conclusions and recommendations

Appendix 2

List of Participants

Dr. Jia Baolin	Institute of Applied Physics and Mathematics, P.O. Box 8009, Beijing, Peoples Republic of China
Dr. Sun Yongsheng	Institute of Applied Physics and Computational Mathematics, No. 6 Huayuan Road, Hai-Dian District, P.O. Box 8009, Beijing, Peoples Republic of China
Dr. J.L. Delcroix	GAPHYOR, Laboratoire de Physique des Plasmas, Université de Paris XI (Paris-Sud), Batiment 212, 15, Rue G. Clemenceau, F-91405 Orsay Cedex, France
Dr. K. Katsonis	GAPHYOR, Laboratoire de Physique des Plasmas, Université de Paris XI (Paris-Sud), 15, Rue G. Clemenceau, F-91405 Orsay Cedex, France
Dr. E. Menapace	ENEA-C.R.E. "E. Clementel", Viale Ercolan 8, I-40138 Bologna, Italy
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Dr. H. Tawara	Data and Planning Centre, National Institute for Fusion Science, Nagoya 464-01, Japan
Dr. V.A. Abramov	Institut Atomnoi Energii I.V. Kurchatova, Ploshchad, I.V. Kurchatova, Moscow D-182, 123182, USSR
Dr. V. Belyaev (Observer)	Institut Atomnoi Energii I.V. Kurchatova, Ploshchad, I.V. Kurchatova, Moscow D-182, 123182, USSR
Dr. A. Faenov (Observer)	All Union Research Institute for Physical Technical and Radiotechnical Measurements, VNIIFTRI, 141570 Mendeleevo Moscow Region, USSR
Dr. V. Piksaikin	Centr Po Jad. Dannym, Fiziko-Energeticheskij Institut, Ploschad Bondarenko, 249 020 Obninsk, Kaluga Region, USSR
Dr. F.J. Smith	The Queen's University of Belfast, Department of Computer Science, Belfast BT7 1NN, Northern Ireland, United Kingdom
Dr. R.E.H. Clark	Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87545, USA
Dr. R.A. Hulse (Observer)	Plasma Physics Laboratory, Princeton University, James Forrestal Campus, P.O. Box 451, Princeton, NJ 08544, USA
Dr. R. McKnight	U.S. Department of Energy, Division of Applied Plasma Physics, Washington, D.C. 20545, USA
Dr. R.A. Phaneuf	Oak Ridge National Laboratory, Bldg. 6003, MS 6372, P.O. Box 2008, Oak Ridge, TN 37831, USA

Dr. E.W. Thomas (Observer)	Georgia Institute of Technology, Atlanta, Georgia 30332, USA
Dr. W.L. Wiese	National Institute for Standards and Technology, United States Dept. of Commerce, Gaithersburg, MD 20899, USA
Dr. R.K. Janev	IAEA, Atomic and Molecular Data Unit, Wagramerstrasse-5, P.O. Box 100, 1400 Vienna, Austria
J.J. Smith	IAEA, Atomic and Molecular Data Unit, Wagramerstrasse-5, P.O. Box 100, 1400 Vienna, Austria
Dr. J.J. Schmidt	IAEA, Nuclear Data Section, Wagramerstrasse-5, P.O. Box 100, 1400 Vienna, Austria

Appendix 3

Progress Reports of the National A+M Data Centres and the IAEA AMDU

Activities of the Data Centers on Atomic Spectroscopy at the National Institute of Standards and Technology

W.L. Wiese

		Director	Workforce
1.	Atomic Energy Levels and Wavelengths	W.C. Martin	2 Professionals
2.	Atomic Transition Probabilities	W.L. Wiese	$1\frac{1}{4}$ Professionals
3.	Spectral Line Shapes and Shifts	W.L. Wiese	Occasional Guest Scientists, Contractors

NIST Data Centers on Atomic Spectroscopy

	Energy Levels	Wavelengths	Transition Probabilities
Recent Work Areas: (compilations last 2 years)	S, Sc, Cu, Mo	Mg, Sc, Fe	Iron-group elements, selected heavy elements
Work in Progress:	OII, Mg, Cr, Co, Ge, Kr	OII, Na, Al, Co, Cu	Be-sequence C-sequence, NI
Selected Future Plans:	Volume on H, D, T, He, C, N and O for ORNL "Red Book" series		
	M-Shell elements (Na-Ar), Zw	Na, Al, Si, V, Cr	Selected heavier elements
			N-sequence O-sequence B-sequence

In-House Databases at NIST

1. Literature references (Bibliographic database):

   All recent literature references (for AEL, since 1985; ATP, since 1980) are entered into a database utilizing ORACLE software and HP 9000 computer. (Assistance by NIST Office of Standard Reference Data in design).

2. Numerical Data:

   A general spectroscopic database has been designed by OSRD personnel. Database contains wavelengths, energy levels and transition probabilities in a unified format. Evaluated data on Fe-group elements loaded into database. Again, ORACLE software has been used.

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Staff: W. C. Martin, Director
J. Sugar
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Scope: Critical evaluation and compilation of data on atomic energy levels and spectra. Data on levels, g-values, calculated eigenvectors, wavelengths and line classifications, ionization energies. Bibliographic files also include references for Zeeman effect, Stark effect, hyperfine structure, isotope shift, and related theoretical results. Responds to user requests for data, literature references, and technical information.

References for Atomic Energy Levels (arranged by spectra)

*H I, D, T	(1972)	[13]
*He I	(1973)	[14]
	(1987)	[45]
*C I–VI	(1970)	[8]
*N I–III	(1975)	[18]
*N IV–VII	(1971)	[10]
*O I	(1976)	[19]
*O II	(1990)	[51]
*O III	(1985)	[35]
*O IV	(1982)	[29]
*O V	(1980)	[25]
*O VI–VIII	(1979)	[23]
Na I–XI	(1981)	[28]
Mg I–XII	(1980)	[24]
Al I–XIII	(1979)	[22]
Si I–XIV	(1983)	[30]
P I–XV	(1985)	[33]
S I–XVI	(1990)	[37]
Cl I–XVII	(1990)	[50]
Fe-Period, K–Ni, (Z=19–28)	(1985)	[36]
Cu I–XXIX	(1990)	[42]
Kr I–XXXVI	(1990)	[49]
Mo I–XLII	(1988)	[38]
Rare-Earths, La–Lu, (Z=57–71)	(1978)	[21]

Older Data: "Atomic Energy Levels", Vols I, II, III

H–V, (Z=1–23), (1949, reissued 1971) [9]
Cr–Nb, (Z=24–41), (1952, reissued 1971) [9]
Mo–La, (Z=42–57), Hf–Ac, (Z=72–89) (1958, reissued 1971) [9]

[ ] The numbers in brackets refer to the publications list at the end.

* Data compiled include a line list or multiplet table for each spectrum.

Wavelength Tables and Multiplet Tables Covering Many Elements

[3] Ultraviolet Multiplet Tables originally issued 1950-1952.
[12] Multiplet Tables originally issued in 1945.
[15] Reference Wavelengths, 15 Å to 25000 Å
[17] Has 39,000 lines of 70 elements, mainly first and second spectra, arranged by element and in a finding list, 2000–9000 Å.
[27] Has 47,000 lines, first through fifth spectra of all elements, by spectra and in a finding list, all wavelength regions.
[31] The first part of the tables in [27], with the lines arranged by spectra, were published in the 60th (1979) and later editions of the CRC Handbook. Some corrections have been included in later editions.
[39] 2000 observed and predicted wavelengths and transition probabilities of magnetic dipole lines for the configurations ns^2np^k, $n=2$ and 3, $k=1$ to 5, for beryllium through molybdenum.
♦[48] A compilation of vacuum ultraviolet wavelengths for the elements hydrogen through krypton. Wavelength tables include intensities, upper and lower energy levels, and classifications arranged separately by element and by wavelength.

Wavelength Tables and Multiplet Tables for Particular Elements or a Few Elements

[1] A critical compilation of energy levels (now superseded by [30]) and multiplet table for Si I.
[2] A critical compilation of energy levels (now superseded by [30]) and multiplet tables for Si II–IV
[8] A critical compilation of energy levels and multiplet tables for C I–VI.
[10, 18]
Critical compilations of energy levels and multiplet tables for N I–VII.
[13] A critical complilation of energy levels and multiplet tables for H I, D, T.
[19, 23, 25, 29, 35, 51]
Critical compilations of energy levels and multiplet tables for O I–VIII.
[34] A collection of recent spectroscopic data tables for iron; ionization energies, wavelengths, atomic energy levels, and atomic transition probabilities.
[41] A collection of recent spectroscopic data tables for titanium, chromium, and nickel; ionization energies, wavelengths, atomic energy levels, and atomic transition probabilities.
[43] A critical compilation of wavelengths, classifications, and intensities for molybdenum ions, Mo VI–XLII.
[44] A critical compilation of wavelengths, energy levels, level classifications, oscillator strengths, and radiative transition probabilities for nickel ions, Ni IX–XXVIII. Grotrian diagrams are also included.
[47] A critical compilation of wavelengths, classifications, intensities, and transition probabilities for iron ions, Fe VIII – Fe XXVI.
[46] A critical compilation of wavelengths and energy level classsifications for all scandium spectra.
[52] A critical compilation of wavelengths, classifications, intensities, and transition probabilities for copper ions, Cu X–Cu XXIX. Grotrian diagrams are also included.
[53] A critical compilation of wavelengths and energy level classifications for all magnesium spectra.

Bibliographies

[4, 6, 11, 20, 26, 32, 40] Cover literature since "Atomic Energy Levels", Vols I-III [9] through December 1987.
Literature since January 1988 are cataloged in the center's database.

♦Tables published by R. L. Kelly (retired), Naval Postgraduate School, Monterey, CA.

1. Moore, C. E., "Selected Tables of Atomic Spectra" (Si II–IV), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 1 (1965). (AEL)

2. Moore, C. E., "Selected Tables of Atomic Spectra" (Si I), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 2 (1967). (AEL)

3. Moore, C. E., "An Ultraviolet Multiplet Table", Natl. Bur. Stand. (U.S.), Circ. 488, Sec. 1 (1950) and Sec. 2 (1952); Secs. 3, 4, 5 (1962), (reprinted 1968). (AEL)

4. Moore, C. E., "Bibliography on the Analyses of Optical Atomic Spectra", Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sec. 1 (1968). (AEL)

5. Moore, C. E., and Merrill, P. W., "Partial Grotrian Diagrams of Astrophysical Interest", Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 23 (1968). (AEL)

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8. Moore, C. E., "Selected Tables of Atomic Spectra" (C I–VI), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 3 (1970). (AEL)

9. Moore, C. E., "Atomic Energy Levels", Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 35, Vol. I, Vol. II, and Vol. III (1971).(Reprint of NBS Circ. 467, originally issued in 1949, 1952, and 1958). (NTIS)

10. Moore, C. E., "Selected Tables of Atomic Spectra" (N IV–VII), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 4 (1971). (AEL)

11. Hagan, L., and Martin, W. C., "Bibliography on Atomic Energy Levels and Spectra, July 1968 through June 1971", Natl. Bur. Stand. (U.S.), Spec. Publ. 363 (1972). (AEL)

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14. Martin, W. C., "Energy Levels of Neutral Helium (⁴He I)", J. Phys. Chem. Ref. Data 2, 257-266 (1973). (ACS)

15. Kaufman, V., and Edlen, B., "Reference Wavelengths from Atomic Spectra in the Range 15 Å to 25000 Å", J. Phys. Chem. Ref. Data 3, 825-895 (1974). (ACS)

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17. Meggers, W. F., Corliss, C. H., and Scribner, B. F., "Tables of Spectral-Line Intensities, Part I - Arranged by Elements, Part II - Arranged by Wavelengths", Natl. Bur. Stand. (U.S.), Monogr. 145 (1975). (NTIS)

18. Moore, C. E., "Selected Tables of Atomic Spectra" (N I–III), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 5 (1975). (AEL)

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♦Tables published by R. L. Kelly (retired), Naval Postgraduate School, Monterey, CA.

Availability of NIST Publications

Following each publication is a source code symbol in parentheses, e. g., (ACS). This code denotes the availability of each publication and how it may be obtained.

Source Ordering Codes:

ACS
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National Institute of Standards and Technology
Physics Building, Room A167
Gaithersburg, MD 20899
Telephone: (301) 975-3221

ALS
Data Center on Atomic Line Shapes and Shifts
National Institute of Standards and Technology
Physics Building, Room A267
Gaithersburg, MD 20899
Telephone: (301) 975-3204

ATP
Data Center on Atomic Transition Probabilities
National Institute of Standards and Technology
Physics Building, Room A267
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Telephone: (301) 975-3204

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National Technical Information Service
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5285 Port Royal Road
Springfield, VA 22161
Telephone: (703) 487-4650

O
Out of print--no longer available

Data Centers on Atomic Transition Probabilities and Line Shapes

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Scope: Collects, catalogs, and evaluates data on transition probabilities and oscillator strengths as well as line shape parameters of atoms and atomic ions in the gas phase, as well as radiative lifetimes of atomic and ionic levels. Publishes critical reviews and tables of critically evaluated data, as well as annotated bibliographies. Responds to user requests for data, literature references, and technical information.

References on Critically Evaluated Transition Probabilities

(arranged by spectra)

H - Ne	(Z = 1-10)	(1966)	[1]
Na - Ca	(Z = 11-20)	(1969)	[2]
Sc - Mn	(Z = 21-25)	(1988)	[10]
Fe - Ni	(Z = 26-28)	(1988)	[11]
Ba I-II	(Z = 56)	(1969)	[3]
63 elements (about 8300 spectral lines)		(1990)	[9]

[] The numbers in brackets refer to the publications list numbers on the following pages.

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Activities Related to the Collection, Evaluation and Dissemination of Atomic and Molecular (A+M) Data for Nuclear Fusion at the Kurchatov Institute of Atomic Energy

V.A. Abramov

I.V. Kurchatov Institute of Atomic Energy
Moscow 1990

The more reliable and extensive atomic and molecular data for some elementary processes in the main (hot core) and edge plasmas are required to consider the Conceptual Design and Engineering Design of ITER. The data concerning the process of penetration fast atom beams used for plasma heating and current drive (E > 100 keV/amu) are also of interest. Therefore, the activities in the Palsma Physics Department of the I.V. Kurchatov Institute of Atomic Energy concerning the (A+M) data problems have been directed, mainly, on the analysis of processes involving low Z elements (divertor -relevant processes) and elements such as W, Ga (these elements are interesting as candidate materials for the divertor plates and the so-called liquid-metal divertor) and on the processes which affect the neutral beam penetration.

At present, the activities concerning the collection of bibliographic (A+M information are in progress. These data are transmitted semiannually to the IAEA for the publication in the International Bulletin on Atomic and Molecular Data for Fusion. The copies of the "International Bulletin on Atomic and Molecular Data for Fusion" which we received from the IAEA are circulated by us to a number of organizations in the USSR. The exchange of (A+M) data information with the different scientific centres is in progress: ORNL, Data Information Centre of the NIFS (Nagoya), Queen University (Belfast), Culham Laboratory (Culham), NIST (Gaithersburg). We believe this exchange will be continued and developed.

We are currently engaged in the compilation of (A+M) data for some processes. It is necessary to put forward the recommendation data set. The comparison of data for the processes involving carbon ions has been given in [1]. Analogous study has been performed in [2] for some metallic elements present in the hot plasmas of magnetic confinement devices. The results of extensive calcualtions of the sputtering yield for different target plus projectile combinations are collected in [3,4]. It should be noted that these results are twice averaged: over energy distribution (the distortion of the Maxwellian distribution function is taken into account) and over incidence angle.

Apart from the collection and the dissemination of the available bibliographic and numerical data, in the I.V. Kurchatov Institute the experimental activity concerning the fusion-relevant processes are being carried out. The total electron capture cross-sections for C^{+q} + H reactions in the energy range 1 eV - 1 keV have been measured by Dr. V.A. Belyaev et al. at the "ATOS" device. These measurements have been made within the framework of the IAEA CRP: "Atomic data for fusion edge plasmas". Dr. M.I. Guseva and her collaborators have measured the sputtering yields for composite materials. We believe that this activity will be included in CRP "Atomic and Molecular Data for Plasma-Surface Interactions".

The effect of A+M database accuracy on the beam energy deposition function and the induced current distribution when fast hydrogen beam is injected in ITER has been investigated. The database proposed by Prof. R.K. Janev has been taken as the reference database. It is shown that the variation of some

important cross-section (within the range ± 10%) may lead to substantial variation of the non-ohmic currently density distribution (up to 50% in the plasma centre). The plasma stability may be substantially affected by the corresponding redistribution of the current density.

At present the most important problem is the exchange of (A+M) data between the national centres and the centres and IAEA due to tremendous required data files. It seems to us that after some modernization the ALADDIN format may be used to data exchange in the future.

All aspects of the (A+M) data problem require the consolidation of international cooperation between the national centres and IAEA. The experience of international cooperation during the last several years shows that the requirements that have been formulated by the fusion community for ITER project as well as for other programs (such as analysis of fusion systems with alternative fuels) may be successfully solved if the international cooperation is strong enough and if new forms of the cooperation (especially, for such important problem as the problem of the evaluation of available data could be used.

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The Atomic and Molecular Data Centre at The Queen's University of Belfast

Progress Report
F.J.Smith, September 1990

During the past year, we have been involved with two main projects:

(i) Electron impact ionisation of atoms and ions.

The third in our series of reports on this topic has been completed. As a continuation of the earlier work on H - Li,[1] and F - Ni,[2] we now have recommended cross sections and rates for electron impact ionisation of atoms and ions for Cu - U.[3] However, largely due to the sparsity of data for many species, it was not possible to use scaling techniques to predict cross-sections values for all cases.

This report is being prepared for submission to the Journal of Physical and Chemical Reference Data for publication as a supplement.

(ii) Electron impact ionisation of molecules relevant to plasma edge studies.

A preliminary report on this topic was presented at the IAEA Specialist Meeting on Atomic and Molecular Data for Plasma Edge Studies, Vienna, July 8-10,1987.[4] It contained a compilation of data for a large group of molecules including H_2, O_2, CO, CH_2, and CH_4, covering the processes of total, single, double and dissociative ionisation. In each case, a recommendation was made for the choice of most reliable data with a view to providing fit parameters at a later stage.

In order to bring the content of the report up-to-date, an extensive literature search has been carried out for the period April '87 to March '90 and all the relevant material included in our database.

Following the recommendations made, the process of fitting the data has begun. We aim to provide recommended cross-sections and rate coefficients for all of these plasma edge molecules within the coming year.

[1] "Recommended Cross Sections and Rates on the Electron Impact Ionisation of Atoms and Ions: Hydrogen to Helium"
K.L.Bell, H.B.Gilbody, J.G.Hughes, A.E.Kingston, and F.J.Smith
J.Phys.Chem.Ref.Data 12, 891 (1983)

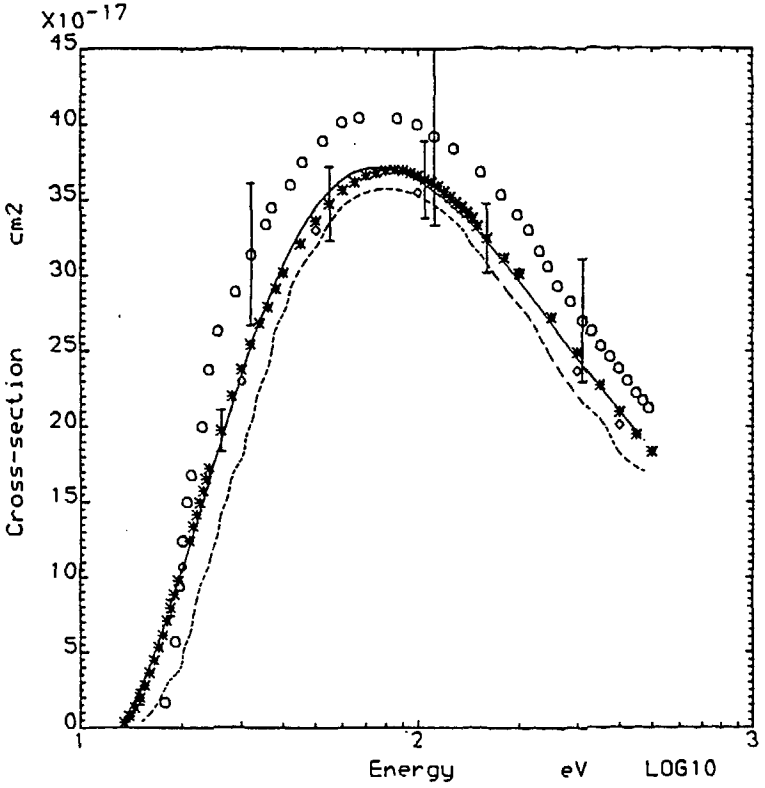
[2] "Recommended Cross Sections and Rates on the Electron Impact Ionisation of Atoms and Ions: Fluorine to Nickel"
M.A.Lennon, K.L.Bell, H.B.Gilbody, J.G.Hughes, A.E.Kingston, M.J.Murray and F.J.Smith
J.Phys.Chem.Ref.Data 17,1285 (1988)

[3] "Recommended Cross Sections and Rates for Electron Impact Ionisation 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 and F.J.Smith.
Culham Report CLM-R294 (1989)

[4] "Recommended Data on Electron Impact Ionisation of Molecules in the Plasma Edge" (preliminary report)
M.A.Lennon, A.Crowe, D.S.Elliott, J.G.Hughes, and F.J.Smith

PROCESS : Total ion production.

REACTION: e + CH4 -> I(+)

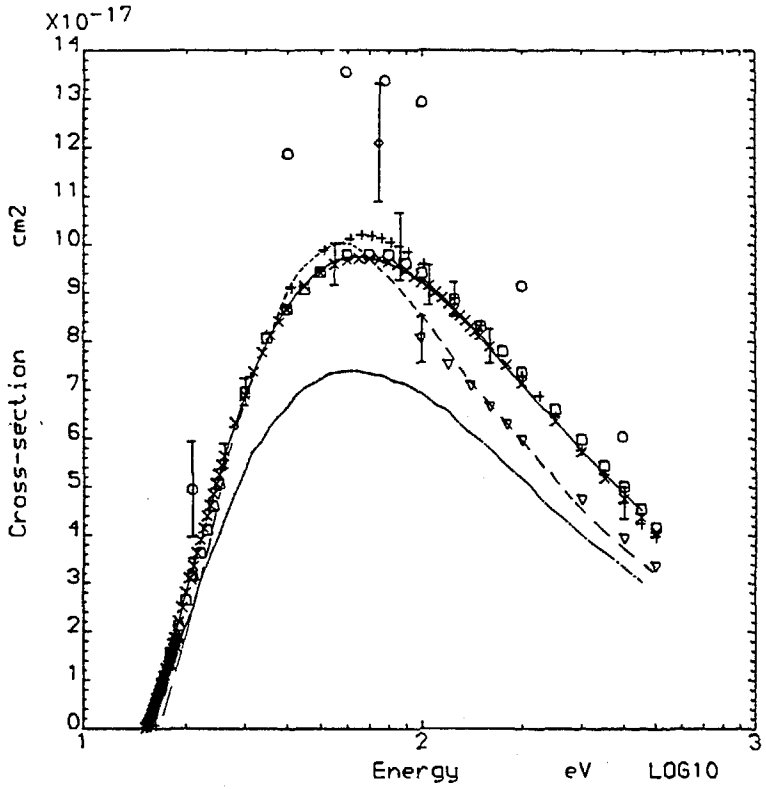


KEY:

—— Higgins M.J. et al(1988)
✱ Rapp D. (1965)
o Orient O.J. et al(1985)
– – Jain D.K. et al(1976)
◇ Chatham H. et al(1984)

PROCESS : Total ion production.

REACTION: e + H2 -> I(+)



KEY:

—— Higgins M.J. et al(1988)
✱ Briglia D.D.(1965)
– – Khare S.P. et al(1970)
o Harrison H.(1956)
◇ Lampe F.W. et al(1957)
□ Cowling I.R. et al(1973)
× Rapp D. et al(1965)
+ Tate J.T. et al(1932)
▽ Schram B.L. et al(1966)
–·– Shingal R. et al(1974)

CONTROLLED FUSION ATOMIC DATA CENTER
Oak Ridge National Laboratory

Progress Report, October, 1989 - September, 1990

R.A. Phaneuf

1. Data Compilation/Evaluation Activities

During this period, the major activity in the ORNL Controlled Fusion Atomic Data Center has been the completion, publication and distribution of the compilation of recommended data, entitled: "Atomic Data for Fusion, I: Collisions of H, H_2, He and Li atoms and Ions with Atoms and Molecules," by C.F. Barnett. This volume contains evaluated and recommended data for 321 different heavy-particle collision processes. The breakdown according to type of process is as follows:

Total electron capture (36 reactions)

State-Selective Electron Capture (74 Reactions)

Direct Excitation and Spectral Line emission (75 reactions)

Ionization and Charged-Particle production (50 reactions)

Electron Loss or stripping (15 reactions)

Electron Detachment from Negative Ions (17 reactions)

Dissociation of Molecules and Molecular Ions (33 reactions)

Heavy-Particle Interchanger reactions (21 reactions)

Cross-section data as a function of collision energy are presented for all reactions. Rate coefficients have also been calculated from the cross-section data for the case of two interacting Maxwell-Boltzmannn velocity distributions, and also for a mono-energetic beam interacting with a Maxwell-Boltzmann velocity distribution. Rate coefficients are presented as a function of temperature only for those reactions for which cross-section data are available over a sufficiently wide energy range to permit their accurate determination. Beam-Maxwellian rate coefficients are presented only for neutral particle beams.

The recommended data for each reaction are presented in the form of tables, graphs and Chebyshev polynomial fitting coefficients. The estimated accuracy of the recommended data, references to original data sources, and comments or notes are given for each reaction. The rms uncertainty of the polynomial fit and the maximum percent deviation from the actual data are also given.

An ALADDIN database was also created for this volume, and distributed on a PC-DOS diskette along with a copy of the ALADDIN program (IAEA Version 1.0) to 150 of the 500 recipients of ORNL-6086. Due to the cost of production, the diskette was supplied only to those who requested it by returning a questionnaire. In

the course of creating the ALADDIN data base, several new process labels were added to the dictionary, in co-ordination with the IAEA Atomic and Molecular Data Unit. A "README" help file was also created and distributed along with the diskette, to facilitate the adoption of the ALADDIN system by users.

At the request of the IAEA Atomic and Molecular Data Unit, cross-section data for ion-atom collision processes which play important roles in the edge plasma of magnetically-confined fusion devices were surveyed and reviewed. A manuscript was also prepared for inclusion in a Special Supplement to Nuclear Fusion, which is being co-ordinated by the Data Unit. The species considered include H, He, Li, Be, C, O, Ne, Al, Si, Ar, Ti, Cr, Fe, Ni, Cu, Mo, W and their ions. The most important ion-atom collision processes occurring in the edge plasma are charge-exchange reactions. Excitation and ionization processes are also considered. The scope is limited to atomic species and to collision velocities corresponding to plasma ion temperatures in the 2-200 eV range. Sources of evaluated or recommended data are presented where possible, and deficiencies in the data base have been indicated.

A collaboration was initiated with T. Shirai of JAERI on the development of an improved analytical scaling formula for ionization of H, H_2 anf He by multiply charged ions. This work addresses the deficiency of existing scaling formulae in the low-energy region. A manuscript on this work has been prepared for submission to Nuclear Instruments and Methods in Physics Research.

2. Bibliographic data Base

The on-line bibliographic data base has been kept up-to-date, and now contains 22,500 categorized and indexed references from 120 journals, covering the period from 1978-present. Input from 4 ORNL atomic physics staff members and 5 consultants under contract is entered regularly. Access for on-line searching is available via a local area personal-computer network. Semi-annual updates were supplied on diskette to the data centers at the IAEA, for inclusion in the Bulletin, and also to NIFS-Nagoya and JAERI.

3. Planned Data Compilation Activities

Data compilation activities planned for the CFADC include the preparation of a "Redbook" compilation of evaluated and recommended data, entitled "Atomic Data For Fusion, Volume 2: Collisions of Electrons with Atoms and Molecules," by C.F. Barnett, J.W. Gallagher and D.C. Gregory. The scope of this compilation, which will include an ALADDIN data base, is as follows:

e + H, H_2, He, Li, C, O, O_2, N, N_2, Li, Fe, CH_4, H_2O

Ionization (24 reactions)

Excitation (62 reactions)

Dissociation (24 reactions)

Dissociative Excitation (6 reactions)

Radiative recombination (5 reactions)

Electron Attachment (5 reactions)

Elastic Scattering [differential] (10 reactions)

Inelastic scattering [differential] (5 reactions)

A high priority for the next year will be given to the creation of an evaluated ALADDIN database for dielectronic recombination involving C and O ions. Improved radiative cooling rates for C and O will also be calculated from these data, and from the recommended excitation data in the ORNL-6086 "Redbook" compilation.

Plans also call for the CFADC to establish a user area on the NERSC Cray computer network, where the ALADDIN databases will be available.

4. Manpower

The CFADC regrets the departure of H.T. Hunter during the past year to the ORNL Engineering Physics Division. The present CFADC staff and manpower levels are organized as follows:

Clerical/Information Specialist:	M. I. Kirkpatrick	1.00 PY
Scientific/Technical:	R.A. Phaneuf	0.20 PY
	D.C. Gregory	0.10 PY
	F.W. Meyer	0.05 PY
	C.C. Havener	0.05 PY
Consultants Under Contract:	H.B. Gilbody	0.05 PY
	E.W. McDaniel	0.05 PY
	M.S. Pindzola	0.05 PY
	T.J. Morgan	0.05 PY
	E.W. Thomas	0.05 PY
TOTAL		1.65 PY

5. Recent Publications

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

Atomic Data for Fusion, Volume 6: "Spectroscopic Data for Titanium, Chromium and Nickel," W.L. Wiese and A. Musgrove, ORNL-6551 (September, 1989).

ACTIVITY REPORT 89/90
at Data and Planning Center (DPC), National Institute of Fusion Science (NIFS)

Hiro Tawara
National Institute of Fusion Science
Nagoya 464-01, Japan

Introduction

Since establishing the present new National Institute of Fusion Science (NIFS) in May, 1989, activities on atomic and molecular data have been transferred to Data and Planning Center from Research Information Center, Nagoya University. Presently two full time scientists (one working both in AM and surface, the other in AM) are involved in AM data activities, with the help of a student part timer for data input into computer and programming. The funding provided through NIFS amounts to about 1.5 M¥ (10k $) per year (excluding the running cost) and is addressed to the travel expense of collaborating volunteer scientists who are the main contributors and helpers for compilation/evaluation of AM data at NIFS. Unfortunately no money has been allotted to domestic as well as international travels of the NIFS staffs and that hinders a lot our efficient AM data activities.

Activities in 1989-1990

1) Data compilation and evaluation of collisions of electrons with hydrocarbon molecules and molecular ions have recently been completed and reported in NIFS-DATA-6.
2) Using special funding in 1989, we have begun to develop data base handling system which incorporates ALADDIN for easy use of the evaluated data (cross sections and rate coefficients) and are still testing it.
3) Possible applications of polarization phenomena to plasma diagnostics have been surveyed and will be reported in NIFS report soon.
4) As Be and B have recently been found to be very effective materials as the inner wall of fusion apparatus, we have started to survey collision data for these elements and to calculate (probably measure) the cross sections for electron transfer (in particular, (n,l) distributions) and ionization processes.

International collaboration

Dr.J.Safronova and Dr.L.Vainshtein, Academy of Sciences, USSR, visited and stayed with us to work on calculations of various parameters of transitions

involving highly ionized ions which are useful for plasma diagnostics. Also this November, Dr.P.Hvelplund of Univ. Aarhus is coming to our institute to discuss ion-atom collision processes and related data.

Reports published

a) Internal reports

1) Y.Yamamura, T.Takiguchi and H.Tawara ; Data compilation of angular distributions of sputtered atoms
   NIFS-DATA-1 (Jan., 1990)
2) T.Kato, J.Lang and K.E.Berrington ; Intensity ratios of emission lines from O V ion for temperature and density diagnostics
   NIFS-DATA-2 (Mar., 1990)
3) T.Kaneko ; Partial electronic straggling cross sections of atoms for protons
   NIFS-DATA-3 (Mar., 1990)
4) T.Fujimoto, K.Sawada and K.Takahata ; Cross sections for production of excited hydrogen atoms following dissociative excitation of molecular hydrogen by electron impact
   NIFS-DATA-4 (Mar., 1990)
5) H.Tawara ; Some electron detachment data for H^- ions in collisions with electrons, ions, atoms and molecules - an alternative approach to high energy neutral beam production for plasma heating
   NISF-DATA-6 (Apr., 1990)
6) H.Tawara, Y.Itikawa, H.Nishimura, H.Tanaka and Y.Nakamura ; Collision data involving hydrocarbon molecules
   NIFS-DATA-6 (July, 1990)
7) H.Tawara ; Bibliography on electron transfer processes in ion-ion/atom/molecule collisions
   NIFS-DATA-7 (August, 1990)

b) Published papers

8) H.Tawara ; Atomic and molecular data needed in space, fusion and related researches
   Molecular Processes in Space (ed. T.Watanabe et al., Plenum Press, 1990)
9) T.Kato, J.Lang and K.E.Berrington ; Intensity ratios of emission lines from O V ions for temperature and density diagnostics and recommended excitation rate coefficients
   At. Data & Nucl. Data Tables 44 (1990) 133
10) H.Tawara, Y.Itikawa, H.Nishimura and M.Yoshino ; Cross sections and related data for electron collisions with hydrogen molecules and molecular ions
    J. Phys. Chem. Ref. Data 19 (1990) 617

11) T.Kusakabe, Y.Mizumoto, K.Katsurayama and H.Tawara ; Electron capture by C^+, N^+ and O^+ ions in collisions with H_2 molecules and He atoms at low keV energies
J. Phys. Soc. Japan 59 (1990) 1987

Progress report for 1989-90 at AMDU/NDC/JAERI

Toshizo Shirai
Japan Atomic Energy Research Institute

A four-year program from 1988 for the third edition of Evaluated Atomic and Molecular (A+M) Data Library (JEAMDL-3) is now in progress. This program has been carried out at the A+M Data Unit (AMDU) of Nuclear Data Center (NDC) in cooperation with the Research Committee on A+M Data of JAERI. Data compilation and evaluation work is in progress for cross section data for heavy particle collisions involving low-Z atomic ions, and spectral data for highly ionized ions of particular interest to the fusion community. For particle-surface interaction processes, data compilation has been made of elementary processes for hydrogen recycling, and stopping power for heavy ions.

Collaborations with H. Hunter and R. Phaneuf (ORNL) and J. Sugar and W.L. Wiese (NIST) have been made in evaluation of collision cross section data and spectroscopic data, respectively, under the US-Japan fusion cooperation program.

1. A+M Unit Manpower

T. Shirai		
M. Sataka	(10% of his time)	A+M Physics Laboratory
S. Nagai	(10% of his time)	Department of Development
T. Tabata	Consultant	University of Osaka Prefecture
H. Nakamura	Consultant	Institute for Molecular Science

A. Ichihara	Postdoctoral Fellow	April 1990 -
A. Mengoni	Visiting Scientist, ENEA/Bologna	March 1990 - September 1990
Y. Zou	Visiting Scientist, IAPCM/Beijing	October 1990 -

2. Recent Activities and Work in Progress

Semiempirical Formula for Collision Cross Section Data

"A semiempirical formula for single-electron-capture cross sections of multiply charged ions colliding with H, H_2 and He", Y. Nakai, T. Shirai, T. Tabata, and R. Ito, Phys. Scripta T28, 77 (1989).

"Partial cross sections for single-electron capture of hydrogen ions colliding with gaseous atoms and molecules", T. Tabata, R. Ito, Y. Nakai, T. Shirai, and Y. Funatake, Osaka Prefect. Radiat. Center Tech. Rep. No. 11 (1990).

"Extended scaling cross-sections for the ionization of H, H_2, and He by multiply-charged ions", T. Tabata, T. Shirai, R. Ito, Y. Nakai, H. Hunter, and R. Phaneuf.

Spectroscopic Data

"Spectral data and Grotrian diagrams for highly ionized iron, Fe VIII - Fe XXVI", T. Shirai, Y. Funatake, K. Mori, J. Sugar, W.L. Wiese, and Y. Nakai, J. Phys. Chem. Ref. Data 19, 127 (1990).

"Spectral data and Grotrian diagrams for highly ionized copper, Cu X - Cu XXIX", T. Shirai, T. Nakagaki, Y. Nakai, J. Sugar, K. Ishii, and K. Mori, J. Phys. Chem. Ref. Data (1990) in press.

"Spectral data and Grotrian diagrams for highly ionized cobalt, Co VIII - Co XXVII", T. Shirai, A. Mengoni, Y. Nakai, J. Sugar, W.L. Wiese, K. Mori, and H. Sakai.

Particle-Surface Interaction Data

"Role of reflection and sputtering in ion impact desorption of gases from solid surface", T. Oshiyama, S. Nagai, and K. Ozawa, J. Nucl. Matter. 168, 162 (1989).

3. Numerical Database and Data Exchange

Systematic data compilation is being made of experimental data for charge changing processes of H and He atoms and their ions in collisions with atoms and molecules, and also for electron capture and ionization by atomic ions incident on H, H_2 and He. The data collected have been stored into the A+M Data Storage and Retrieval System (AMSTOR).

Parametrization of evaluated data for 125 kinds of heavy particle collision has been so far completed. The results written in ALLADIN format were already sent to J. Smith (IAEA).

The ALLADIN system (version 1.0) distributed by the IAEA is working on the mainframe computer FACOM M780 without any essential problems.

4. Activity Plans for 1990 to 1991

Collision Cross Section Data

Data compilation of all processes between H^+, H, H_2 and He, He^+, He^{2+} is planned not only for analysis of hydrogen and helium plasmas but also elucidation of He-ash transport phenomena. Recent experimental data available at present are first surveyed and compiled with reference to ORNL redbook Vol. 1 provided by C.F. Barnett. In cases where the accumulation of data is enough, we will make analytical empirical formula for each process.

Spectroscopic data

Critical compilation of wavelengths belonging to the V and Cr ions will be completed in joint work with NIST.

Particle-Surface Interaction Data

Efforts are being made for data evaluation of stopping power for heavy ions.

GAPHYOR DATA CENTRE
Progress Report 1989-1990

J-L DELCROIX, K. KATSONIS

Centre de Données GAPHYOR, Université de Paris-Sud, Bat. 212
91405 ORSAY CEDEX, FRANCE - FAX. 694117844

1. SOME STATISTICS.

As of the 15th of September 1990, the total number of entries in the files was distributed as follows :

a) The entries for one, two, three and four elements files for each section are given in Table 1.

b) The number of entries contained in each process is given in the Table 2, separately for each of the five sections

c) At the last meeting we described the methods used now in GAPHYOR for covering five "New fields :

Shell structure description
Neutral or ionized clusters
Interaction of Atoms and Molecules with Solids
Isoelectronic series
Homonuclear sequences

The statistics of GAPHYOR in these new fields is shown in Table 3

2 NEW METHODS OF DATA COLLECTION

2.1 Working methods

The working methods used to produce GAPHYOR Data Base are summarized in Table 4.

A recent development is the use of Excel by some experts and the "direct entry" of the data. An expert using Excel on its own microcomputer (Macintosh or PC) creates directly a spreadsheet . An example of such a sheet is shown on Table 5.These sheets are registered on a disket which is directly entered into the validation procedure.

This new working method has many advantages:

Smaller number of errors
Continuous updating of the Data Base
Shorter time delay for availability of data.

2.2 Actualisation rate

As a result of the present working methods it is interesting to look at the speed of up-dating of GAPHYOR. It is convenient to specify this by a coefficient that we call the "actualisation rate":

AR = Actualisation rate = (4/5)*(F89+F90)/AV with the following notations:

Σ=Total number of entries
F89 = Number of entries for publication year = 89
F90 = Number of entries for publication year = 90
NY = Number of effective years
AV = Average number of entries per year=Σ/NY
Cla= ranking of journals by annual average number of entries

Table 1: Number of entries by sections and number of elements

SECTION 1 Structure	SECTION 2 Coll. photon.	SECTION 3 Coll.electron.	SECTION 4 Coll.atom.mol.	SECTION 5 Prop.macro.	TOTALS
38030	6572	11789	6857	4353	67601
48118	5310	4468	34509	7125	99530
22050	2321	802	19016	2554	46743
4655	461	87	5446	785	11434
112853	14664	17146	65828	14817	225308

Table 2: Number of entries by process in each section
(see for instance [1] for the process code)

SECTION 1 Structure		SECTION 2 Coll.photon.		SECTION 3 Coll.electron		SECTION 4 Coll.atom.mol.		SECTION 5 Prop.macro.	
EN	63519	AN	1697	SN	1054	SN	1019	PV	1043
CP	258	SN	493	SC	431	SC	559	FT	1574
DP	3052	SC	273	EL	1607	EL	764	VR	154
NP	805	EL	172	EX	4229	EN	1753	ZT	122
PE	2432	FF	80	ER	498	EX	2456	CO	131
VR	28557	EX	1576	DX	183	ER	1110	DN	584
TR	10840	ER	398	XX	355	DX	7594	VI	683
IN	762	DX	96	DO	41	XX	2175	CT	803
DT	209	XX	64	IN	4542	DO	279	TD	280
DS	1584	DO	84	RC	200	TE	2047	PE	267
XX	44	IN	5735	RR	147	IN	6686	EN	2464
EA	791	DT	464	RE	89	DT	933	DM	57
Σ	112853	DS	3100	RO	63	RI	450	RN	934
		NL	138	RD	419	10	5014	FE	343
		PR	294	RS	553	20	204	CE	158
		Σ	14664	AT	1550	LN	3093	ME	615
				DT	53	MP	146	DE	173
				DS	820	LP	3790	PI	483
				BS	213	IR	13544	AT	448
				PR	99	AS	3996	DT	69
				Σ	17146	DS	2589	PC	67
						IH	905	FI	29
						AH	190	MI	867
						DH	107	DI	179
						KE	647	DA	40
						PR	3095	RC	91
						IA	86	RR	84
						ID	597	RE	20
						Σ	65828	RO	7
								RD	3
								RS	0
								RI	4
								LA	912
								MD	94
								ST	1035
								Σ	14817

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

Table 3: Number of entries in "New fields" (1-09-90)

	Multicharge ions	**Isoelectronic series**	**Internal shell structure**	**Exotic atoms and molecules**	**Clusters**	**Gas-wall interactions**
	Info=Q or i=n+	Info=I	Info=:	Fam=EE or Mol="M.n"	Info=8	Info=/ or -
1 élément	8225	1549	264	94	121	247
2 éléments	4058	84	35	17	131	1863
3 éléments	51	0	0	1	222	782
4 éléments	0	0	0	0	74	286
Totaux	12334	1633	299	112	548	3178

The normal value of the actualisation rate is 100. The differences between the actual value of actualisation rate and this normal value is the object of the comments in the last column of Table 5 :

Direct entry	Excellent situation and short delay
***	Excellent situation
**	Good situation
*	Fair situation
New expert	A new expert has been recently elected to improve the situation
Expert N?	GAPHYOR is looking for a new expert

2.3. On-line Retrieval

GAPHYOR can be consulted on-line via the standard data networks from everywhere in the world seven days a week on a 24 hours basis, except for a few maintenance interruptions. This consultation can be made easily at home through the french VIDEOTEX system using a telephone extension (MINITEL), in France and in a number of european countries.

Table 4 Working methods and direct entry

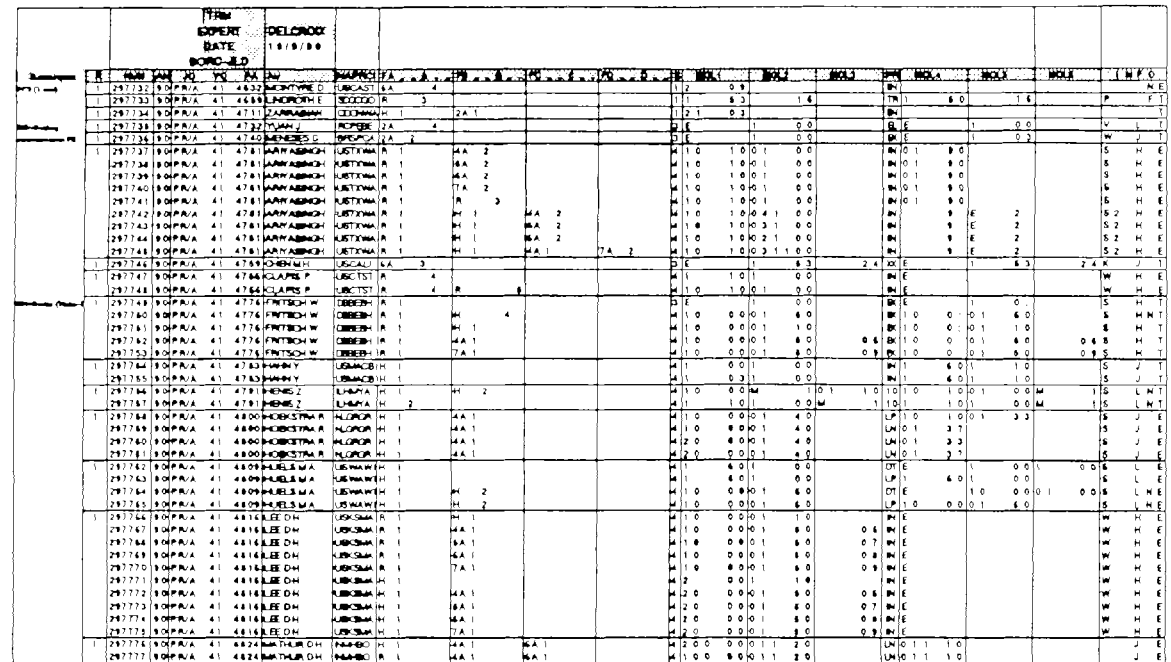
15 "EXPERTS" (France,Italy,Portugal)	CENTRAL UNIT (Orsay)
reading journals	
Bristol cards (personal document,natural language,archivs)	
Data collection and coding "internal" language formerly: paper sheets(bordereaux) formerly: floppy disk typing 1990: **Microsoft Excel** 1990: **Direct entry**	
	Data validation Automatic error tests Temporary listing Reading and manual corrections
special corrections	
	Final entry Translation to natural language **Quaterly bulletin publication**

SEMI-ANNUAL MEETING
Improvement of methods
Homogeneity maintenance

Table 4: Actualisation rate (see text for notations)

Cla.	JOURNALS		Σ	F89	F90	NY	AV	AR	Comments
1	JCP	*J.Chem.Phys.*	40545	1624	240	15	2703	55	**
2	PR/A	*Phys.Rev. A*	12608	1288	426	15	841	163	Direct entry
3	JPC	*J.Phys.Chem.*	12051	1685	0	15	803	168	Change of scope
4	CHPL	*Chem.Phys.Letters*	11731	0	0	15	782	0	New expert
5	JP/B	*J.Phys. B*	11555	0	0	15	770	0	New expert
6	JMSC	*J.of mol.struct.(Theo-chem)*	5333	892	232	8	667	135	Direct entry
7	JRD	*J.of Phys.Chem.Ref.Data*	9494	395	128	15	633	66	Direct entry
8	ZP/D	*Z.Phys. D (At.Mol.Clust.)*	2106	726	120	4	527	129	Direct entry
9	ADND	*Atom.data,Nucl.tables*	7338	1042	978	14	524	308	Direct entry
10	JACS	*J. of the Am.Chem.Soc.*	5503	132	26	15	367	34	**
11	IJMS	*Int.J.Mass spectr.,Ion Phys.*	4960	202	0	15	331	49	**
12	JMSP	*J.Molec.spectroscopy*	4774	91	0	15	318	23	*
13	CHPH	*Chem.Phys.*	4187	0	0	15	279	0	New expert
14	JFII	*J.Chem.Soc.Faraday trans. II*	3284	96	0	15	219	35	**
15	MOL	*Molecular Physics*	3254	20	0	15	217	7	*
16	THCA	*Theor.Chem.Acta*	3142	0	0	15	209	0	Expert: N?
17	PSC	*Physica Scripta*	2918	367	0	15	195	151	***
18	JMSR	*J.of mol.struct.*	2800	345	114	15	187	197	***
19	IJCK	*Int.J.Chem.Kinetics*	2440	282	94	15	163	185	***
20	IJQC	*Int.J.Quantum Chem.*	2413	35	0	15	161	17	*
21	IPPJ	*Inst.Plas.Phys.Nagoya Rep.*	2309	17	0	15	154	9	Change of title
22	OASK	*Optik i Spektr.+engl.transl.*	2021	0	0	15	135	0	Expert: N?
23	CJCH	*Can.J.Chem.*	2002	4	0	15	133	2	*
24	JQS	*J.of Q.Spectr.Radiation transf.*	1906	0	0	15	127	0	Expert: N?
25	ZFKH	*Zh.Fiz.Khim.*	1891	68	0	15	126	43	**
26	JOSA	*J.of the Opt.Soc.Am.*	1560	0	0	15	104	0	Expert: N?
27	PRL	*Phys.Rev. Letters*	1515	179	0	15	101	142	Direct entry
28	PL/A	*Phys.Lett. A*	1409	0	0	15	94	0	New expert
29	CJP	*Can.J.Phys.*	1405	0	0	15	94	0	Expert: N?
30	JESP	*J.Electron.sp.relat phen.*	1244	32	0	15	83	31	*
31	BCSJ	*Bull.Chem.Soc.Jap.*	1203	26	0	15	80	26	*
32	BBUN	*Ber.Bunsen Phys.Chem.*	1189	14	0	15	79	14	*
33	INOR	*Inorg.Chem.*	1165	131	30	15	78	166	***
34	JFI	*J.Chem.Soc.Faraday trans. I*	1119	34	0	15	75	36	**
35	ZN/A	*Z.Naturforschung A*	1070	0	0	15	71	0	Expert: N?
36	APL	*Appl.Phys.Letters*	1029	0	0	15	69	0	Expert: N?
37	JDP	*J.de Phys.*	974	16	33	15	65	60	Direct entry
38	JCPB	*J.de Chim.phys.Chim.bio.*	964	115	0	15	64	143	***
39	APJ	*Astrophys.J.*	954	0	0	15	64	0	New expert
40	KNCT	*Kinetics and Catalysis*	877	43	0	15	58	59	**
41	ZETF	*Z.E.T.P.+engl.transl.*	875	0	0	15	58	0	Expert: N?
42	JAPH	*J.of Appl.Phys.*	805	12	1	15	54	19	Expert: N?
43	OPTC	*Opt.Communic.*	795	0	0	15	53	0	New expert
44	JDPC	*J.de Phys.Colloques*	778	441	0	15	52	680	Direct entry
45	JPHT	*J.of Photochem.*	737	0	0	15	49	0	New expert
46	JPJ	*J.of the Phys.Soc.Jap.*	701	0	0	15	47	0	Expert: N?
47	IJPP	*Ind.J.Pure appl.Phys.*	698	0	0	15	47	0	New expert
48	USPN	*Usp.Fiz.Nauk+engl.transl.*	694	0	0	15	46	0	Expert: N?
49	EUPL	*Europhys.Letters*	130	24	0	3	43	44	Direct entry
50	SPCA	*Spectrochim.Acta A*	517	21	0	15	34	49	**
51	ZSKH	*Zh.Strukt.Khim.*	433	0	0	15	29	0	Expert: N?
52	JP/D	*J.Phys. D*	405	0	0	15	27	0	Expert: N?
53	HTSU	*High temperatures*	334	0	0	15	22	0	New expert
54	APPA	*Acta phys. Pol. A*	322	0	0	15	21	0	Expert: N?
55	CR/B	*Comptes Rendus Ac.Sc. B*	318	0	0	15	21	0	New expert
56	PCPP	*Plasma Chem.Plasma Process*	180	0	0	9	20	0	New expert
57	ASAR	*Astron. and Astrophys.*	287	0	0	15	19	0	New expert
58	LTFS	*Litov.Fis.Sbor.*	264	0	0	15	18	0	Expert: N?
59	IVZF	*Izvest.Vys.Uchebn.zaved.Fis.*	134	0	0	15	9	0	Expert: N?
		Totals	193276	10400	2422	15	12885	80	

Table 5: A recent example of direct entry (Phys.Rev.**41**-9,1 may 1990)



3. NUMERICAL DATA EVALUATION.

A numerical calculation research project was developed in our Data Centre (K. Katsonis, G. Maynard) in collaboration with R. K. Janev. Our Classical Trajectory Monte Carlo (CTMC) code for calculation of charge transfer and ionization cross sections (see Report GA-2, Progress Report 1988-89, presented at the previous DCN meeting) has been used to obtain ionization and n resolved charge transfer cross sections for the following collisions:

3.1. Neon ions colliding with Hydrogen atoms.

The results for single target ionization and for electron capture by Ne^{q+} (q = 1 to 10) are shown in Figs. 1 and 2. For the calculation concerning q = 1 to 8 ions, a model potential derived from the Thomas-Fermi model for a many electron positive ion has been used, as defined previously (M. R. C. McDowell and R. K. Janev, J. Phys. B 18, L295, 1985). For q = 9 and q = 10 ions the model potential was practically giving the same results as the pure Coulomb case; therefore we used the Coulomb potential to calculate the results for these cases.

For low ionization stages the view of the collision as a three-body problem becomes less accurate. The curves for q = 1 or q = 2 are expected to depart significally from the reality and are given here only for comparison with the q > 1 cases. Quantum calculations (multichannel Landau - Zener approximation) are under way in order to complete this data set.

The energy range over which the CTMC method is valid is not clearly established. Molecular effects are expected to be important at the lower energy range and tunneling at the higher. Moreover, the validity region is depending on the used model potential. We have extended our calculations down to 0.1 keV/amu for charge transfer and up to 10 MeV/amu for ionization. For lower energies, the time needed for calculating one trajectory grows very fast; for higher energies, the number of trajectories needed in order to obtain a satisfactory statistics becomes excessive.

It is to be noted (see Fig. 1) that the dependence of the ionization cross section on the ionization stage q becomes negligible in the medium energy region range (20 to 80 keV/amu) for sufficiently charged projectiles. Also, the asymptotic form of the charge transfer variation shown in the Fig. 2 curves, i.e. a plateau for lower energies and an exponential decay for higher energies is in agreement with the experimental results discussed in previous DCN meetings.

Tables containing the numerical values obtained for the hydrogen ionization (σ_i) and the charge transfer (σ_c) cross sections in πa_0^2 units are given in the internal GAPHYOR Report GA-5, where the results are evaluated. σ_c values when expressed in reduced coordinates (σ_c/q versus $E/q^{0.5}$) are giving the expected universal curve shown in Fig. 3 except for n = 1,2 as discussed.

Preliminary results for n resolved charge transfer cross sections were presented in the IAEA Advisory Group Meeting on "A+M Data for Metallic Impurities in Fusion Plasmas", Vienna, May 1990. Sample results for Ne^{6+} and H^+ collisions with H are given in Tables 6 and 7. A comprehensive set of the obtained results is included in Report GA-7.

3.2. Na- and Mg-like metallic ions (Z = 22 to 29) colliding with Hydrogen atoms

Extensive CTMC calculations have been done for metallic ions (Ti, V, Cr, Mn, Fe, Co, Ni and Cu) with 11 and 12 electrons

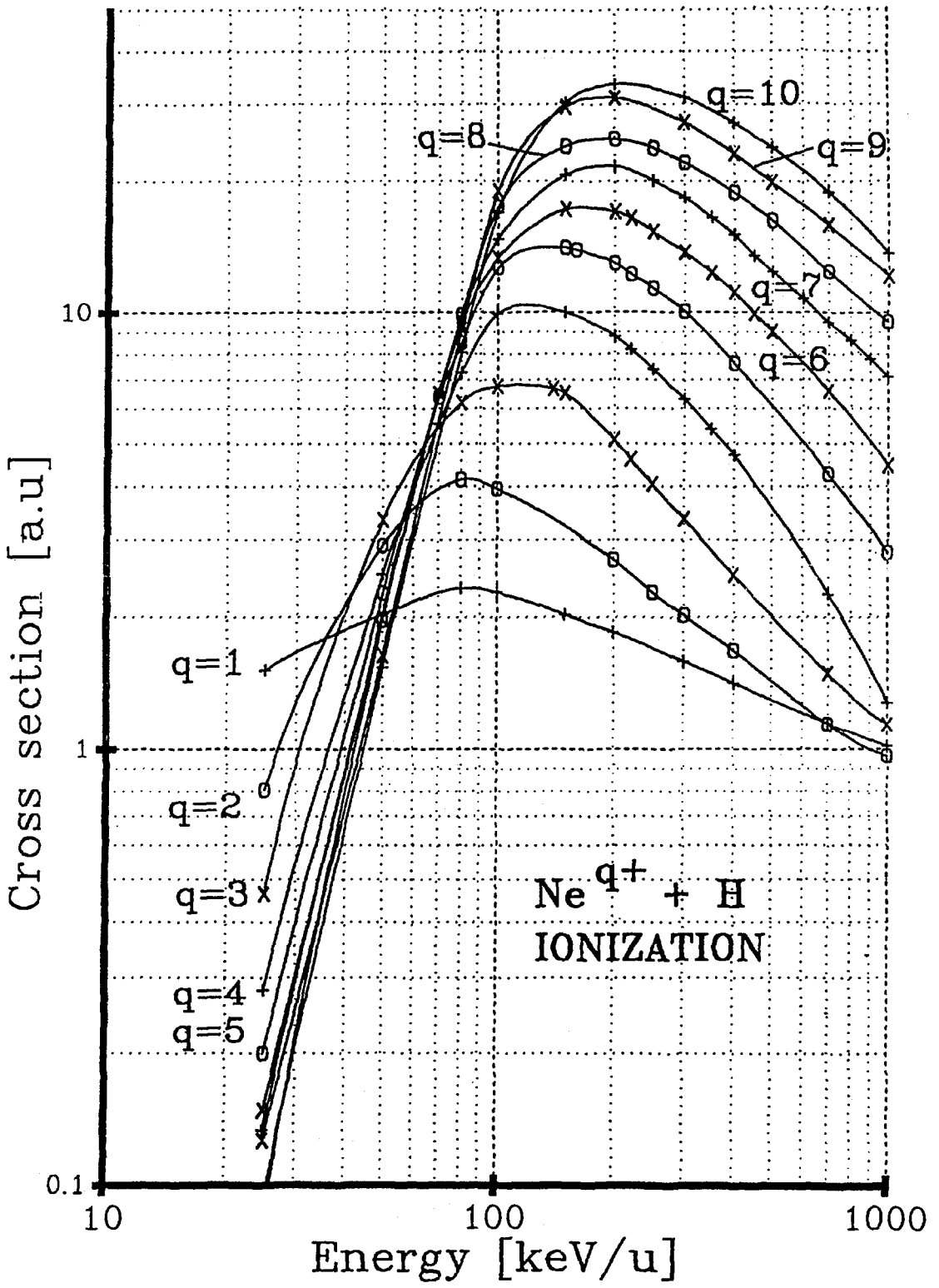


Fig. 1. Ionization cross sections in Ne^{q+} - H collisions.

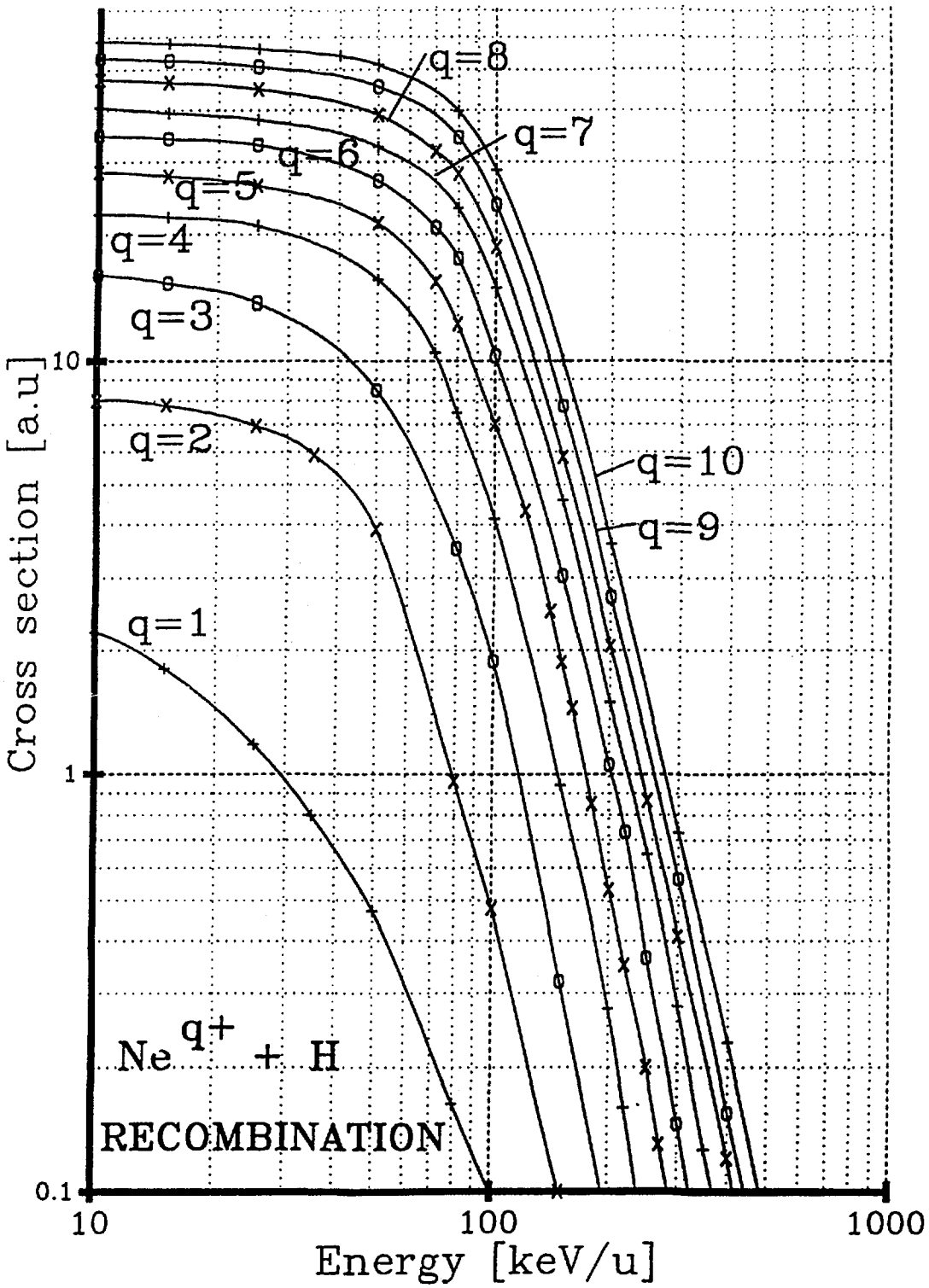


Fig. 2. Recombination cross sections in Ne^{q+} - H collisions.

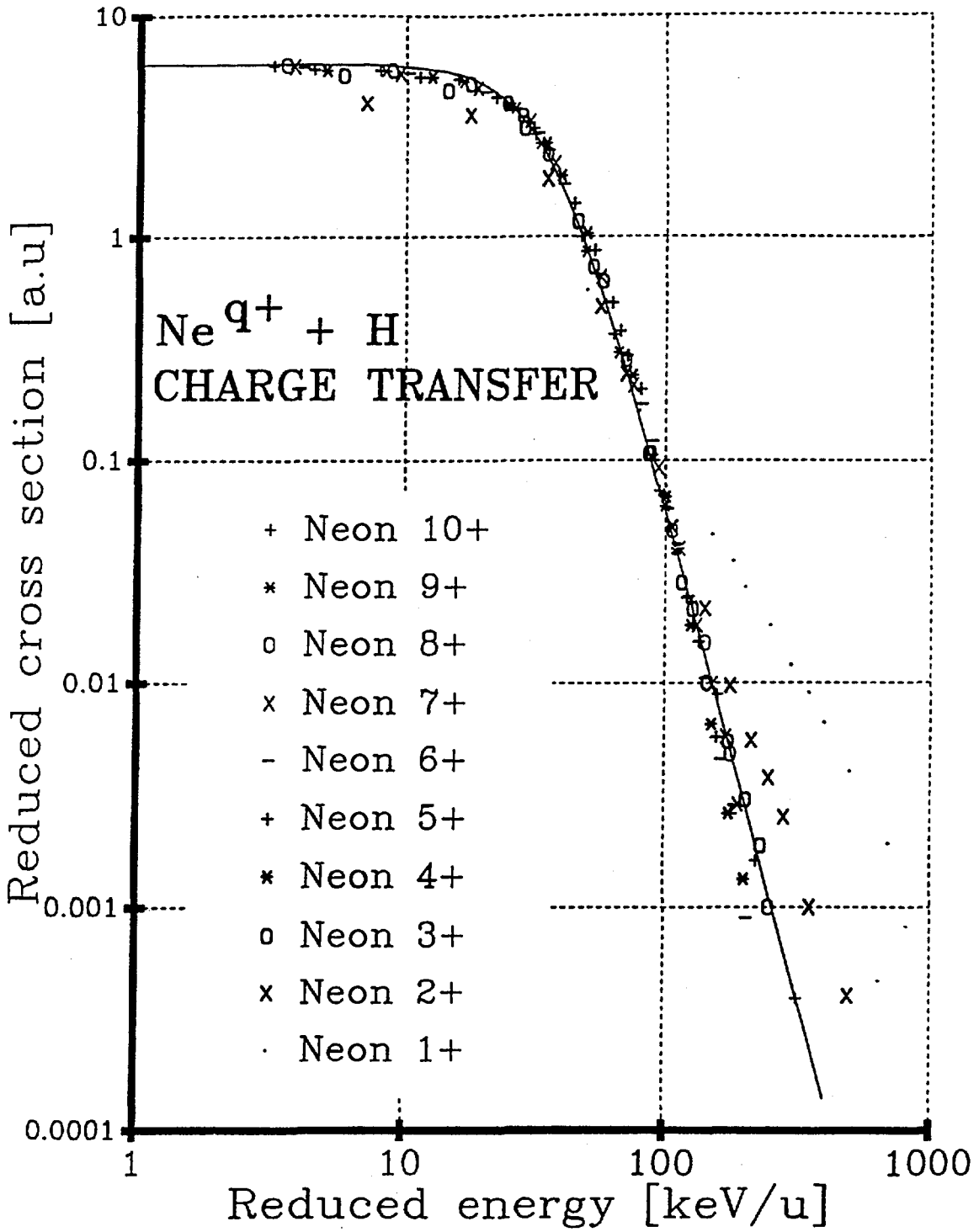


Fig. 3. Recombination cross sections in Ne^{q+} - H collisions in reduced coordinates (σ/q, $E/q^{0.5}$).

Table 6. n - resolved recombination cross sections in Ne^{6+} - H collisions.

Ne 6+, 25keV/a				
partial cross section				
n	r	s		
1	0,00	0,000		
2	0,43	0,023		
3	9,01	0,096		
4	18,78	0,127		
5	4,97	0,075	N moy.	3.60678
6	1,01	0,035	N^2 moy.	13.77915
7	0,38	0,021	E moy.	1.197279
8	0,17	0,014	E^2 moy.	1.634741
9	0,08	0,010	r tot	33.01
10	0,04	0,007		
11	0,03	0,006		
12	0,03	0,006		
13	0,01	0,004		
14	0,01	0,004		
15	0,01	0,004		
16	0,01	0,003		
17	0,00	0,002		
18	0 01	0,004		
19	0,01	0,003		
20	0,00	0,002		

Ne 6+, 80keV/a				
partial cross section				
n	r	s		
1	0,00	0,000		
2	0,29	0,031		
3	1,82	0,077		
4	2,80	0,095		
5	3,13	0,100	N moy.	5.440646
6	2,47	0,089	N^2 moy.	24.05646
7	1,66	0,074	E moy.	0.691802
8	1,18	0,062	E^2 moy.	0.823323
9	0,84	0,053	r tot	17.48
10	0,70	0,048		
11	0,45	0,039		
12	0,34	0,034		
13	0,34	0,034		
14	0,20	0,026		
15	0,15	0,023		
16	0,20	0,026		
17	0,17	0,024		
18	0,10	0,018		
19	0,06	0,015		
20	0,10	0,018		

Ne 6+, 200keV/a				
partial cross section				
n	r	s		
1	0,00	0,000		
2	0,06	0,005		
3	0,17	0,008		
4	0,17	0,008		
5	0,16	0,008	N moy.	4.844467
6	0,11	0,007	N^2 moy.	18.10713
7	0,06	0,006	E moy.	0 870262
8	0,06	0,005	E^2 moy.	1.382257
9	0,04	0,004	r tot	1.0528
10	0,03	0,004		
11	0,03	0,003		
12	0,02	0,003		
13	0,02	0,003		
14	0,02	0,003		
15	0,01	0,002		
16	0,01	0,002		
17	0,01	0,002		
18	0,01	0,002		
19	0,01	0,002		
20	0,00	0,001		

Table 7. n - resolved recombination cross sections in H' - H collisions.

H 1+, 25keV/a				
partial cross section				
n	r	s		
1	1.81	0.038		
2	1.09	0.030		
3	0.15	0.011		
4	0.05	0.007		
5	0.03	0.005	N moy.	1.304191
6	0.01	0.003	N^2 moy.	1.505081
7	0.01	0.002	E moy.	0.332708
8	0.00	0.002	E^2 moy.	0.140315
9	0.00	0.001	r tot	3.105
10	0.01	0.002		
11	0.00	0.001		
12	0.00	0.002		
13	0.00	0.001		
14	0.00	0.002		
15	0.00	0.000		
16	0.00	0.000		
17	0.00	0.001		
18	0.00	0.000		
19	0.00	0.000		
20	0.00	0.000		

H 1+, 80keV/a				
partial cross section				
n	r	s		
1	0.133	0.0048		
2	0.080	0.0041		
3	0.020	0.0018		
4	0.009	0.0013		
5	0.005	0.0009	N moy.	1.411487
6	0.002	0.0006	N^2 moy.	1.88052
7	0.001	0.0004	E moy.	0.295787
8	0.001	0.0004	E^2 moy.	2.347781
9	0.001	0.0004	r tot	0.2704
10	0.001	0.0004		
11	0.000	0.0000		
12	0.000	0.0002		
13	0.000	0.0002		
14	0.000	0.0003		
15	0.000	0.0003		
16	0.000	0.0000		
17	0.000	0.0002		
18	0.000	0.0003		
19	0.000	0.0002		
20	0.000	0.0000		

H 1+, 200keV/a				
partial cross section				
n	r	s		
1	0.007	0.0000		
2	0.003	0.0004		
3	0.001	0.0002		
4	0.000	0.0001		
5	0.000	0.0000	N moy.	1.212863
6	0.000	0.0000	N^2 moy.	1.339102
7	0.000	0.0000	E moy.	0.373308
8	0.000	0.0000	E^2 moy.	0.173308
9	0.000	0.0000	r tot	0.011
10	0.000	0.0000		
11	0.000	0.0000		
12	0.000	0.0000		
13	0.000	0.0000		
14	0.000	0.0000		
15	0.000	0.0000		
16	0.000	0.0000		
17	0.000	0.0000		
18	0.000	0.0000		
19	0.000	0.0000		
20	0.000	0.0000		

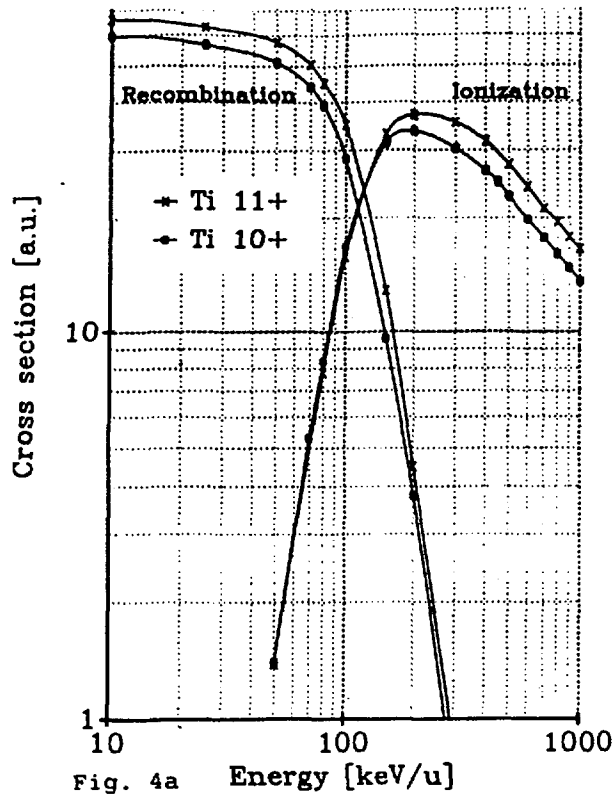


Fig. 4a

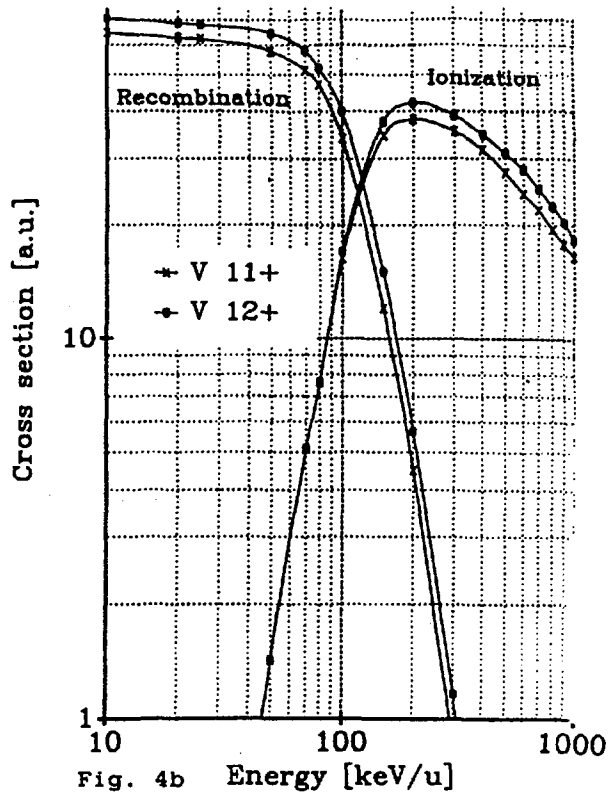


Fig. 4b

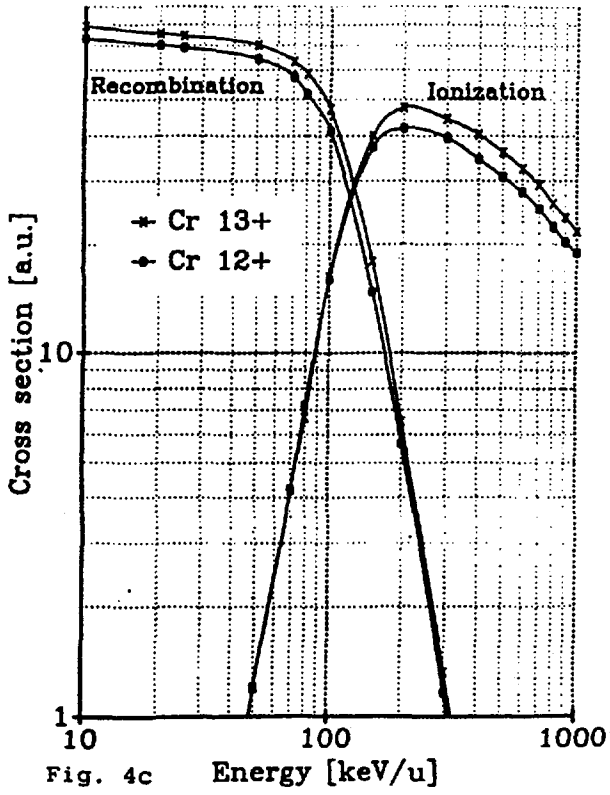


Fig. 4c

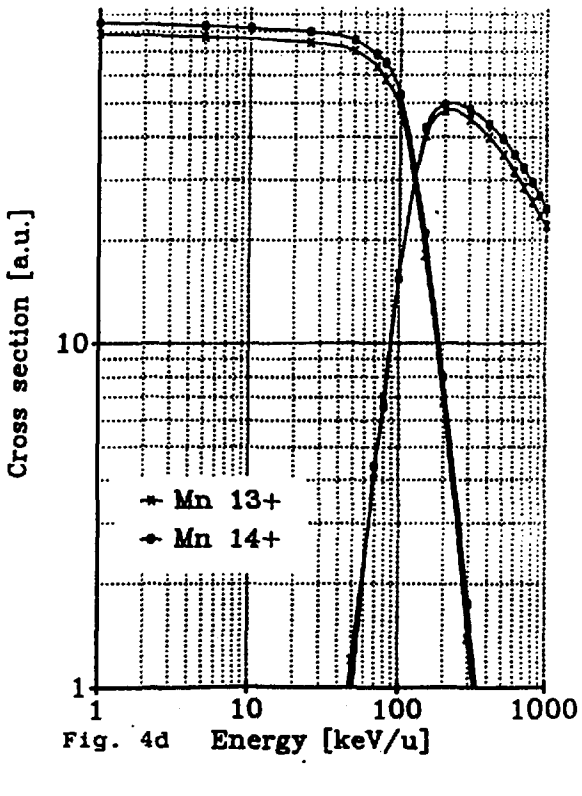


Fig. 4d

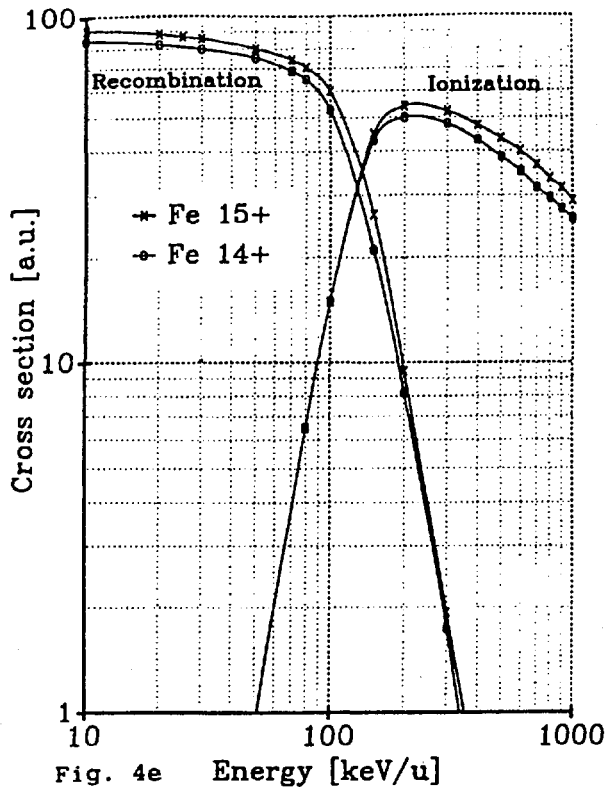


Fig. 4e

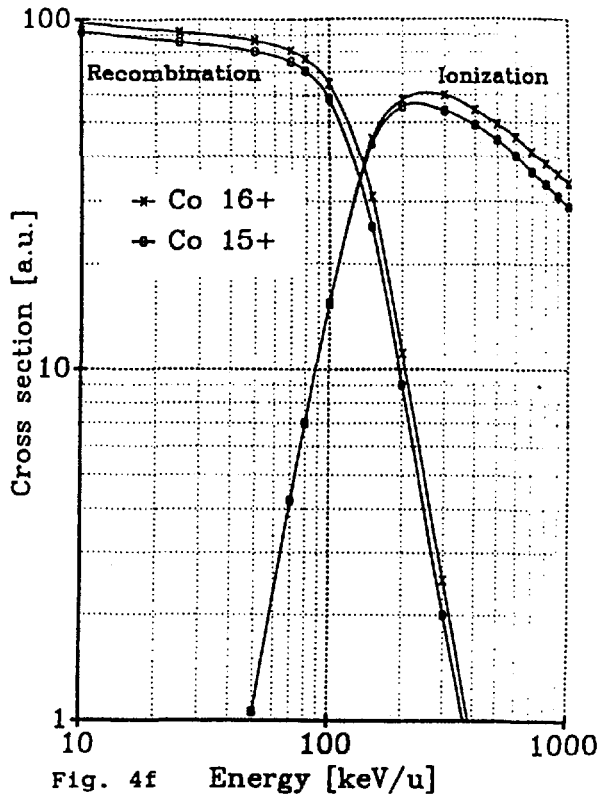


Fig. 4f

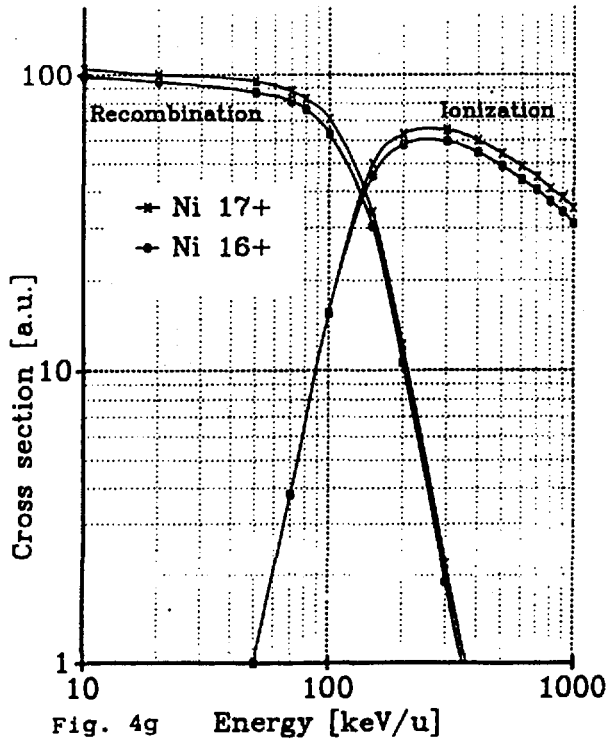


Fig. 4g

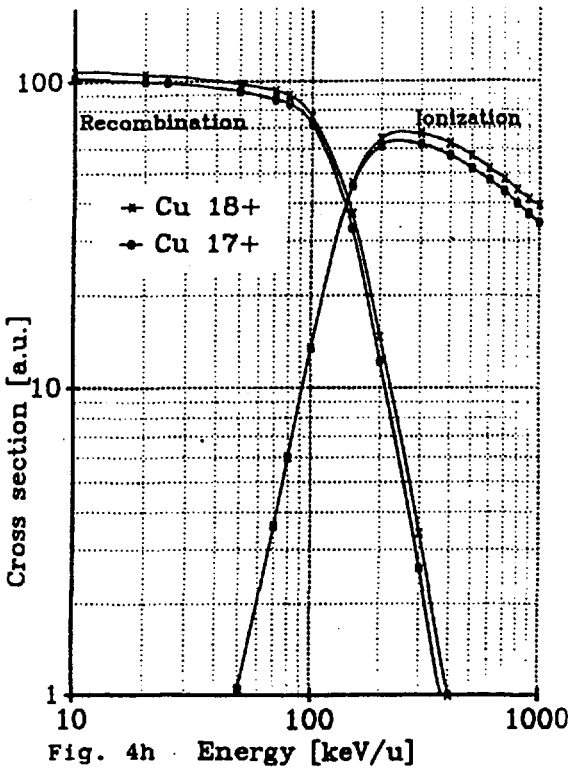


Fig. 4h

(iso-electronic series of Na and Mg) using the same model potential. The observations for the energy range given in 3.1 are also valid here. The results are presented schematically in Figs. 4a to 4h.

The general form of the curves is similar to those for neon ions. The ionization cross section for energies smaller than 30 - 50 keV/amu become too small to be calculated within the classical approximation. The cross sections given for the Na- and Mg-like ion of each element are slightly different. The addition of one electron results to an increase of the corresponding cross section except for ionization in the intermediate energy region. Also, the cross sections are increasing with Z. The σ_i maximum in units of πa_0^2 is increasing from 37 (Z = 2) to 68 (Z = 29) for an energy between 200 and 300 keV/amu. In the same units, the (σ_c) for 10 keV/amu is increasing from 68 to 108. n resolved charge transfer cross sections are presented and discussed in the aforementioned Report GA-7.

3.3. Current activities.

Work in progress includes CTMC calculations of ionization and charge transfer cross sections for heavier species. Preliminary results for I^{q+} ions colliding with hydrogen were presented recently (K. Katsonis and G. Maynard in "SFP, Deuxième Congres de la Division Plasma, Orsay, September 1990") and will be published elsewhere. These calculations are part of our collaboration with the SPQR group working on various aspects of inertial fusion research.

We obtained also results for ionization of excited hydrogen by Z = 1, 2, 6, 10, 13, 18 and 26 fully stripped ions . As expected, discrepancy with the first Born approximation for proton projectiles is reduced in comparison with previous calculations from Rivarola and collaborators. These results are contained in Report GA-8.

Collisions of metallic ions with helium are presently studied.

3.4. Near-future plans.

Our research project will continue with calculations of neon ions - atomic hydrogen collision cross sections for lower impact energies for the elaboration of a collisional - radiative model for neon diagnostics. Also, the CTMC code will be modified in order to calculate collisions involving He targets and a number of heavy and light ion projectiles. Substantial financial support will be necessary for the continuation of this project. Besides, an enlargement of the GAPHYOR team has been requested.

Activities in the A+M data at ENEA, Nuclear Data and Codes Laboratory, Bologna, Italy

by E.Menapace

1.Electron-ion collision excitation data

M.Frisoni [1], P.L.Ottaviani and G.C.Panini-ENEA, G.Rinaldi-NIER

The work about the systematic collection of experimental and theoretical data for electron-ion excitation for iron has been completed. For this process all the ions have been considered and the data were accordingly selected.

The collected data have been organized into a library which includes numerical data, references and various headings for identification purpose, for plotter and for high quality printing. Computer codes have been written to perform the tasks needed in order to properly manage the data. Primarily the codes have been used to create a data library, i.e. to write the numerical data and the associated references into a data base structure which includes counters, numerical flags and retrieval items too. Another code has been designed to retrieve the data from the library in order to obtain cross sections and rate coefficients, both in tabular and in graphical form suitable for easy comparison. Being in use for domestic purpose only, the code has no relevant interactive features.

As an example of the organization of the entire data base, we present here some criteria that have been adopted for the collection of data on electron impact excitation collision strengths of iron ions from Fe XXVI to Fe I:

1. For each ion the compilation has been limited to single electron transitions from the ground state term to excited terms that are in general the most important ones for radiation losses even though, in some ions, long-lived close metastable states can play a not negligible role.

2. Resonance cross sections are not easily handled for the purpose of tabulating, plotting and comparing, then non resonant collision strengths only were considered, whereas resonance effects were included in excitation rate coefficients.

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[1] Guest researcher

[2] Presented at the 9th Atomic and Molecular Data Centre Network Meeting, IAEA, Vienna, September 20-21, 1990

3. The data found in literature have been expressed in threshold energy units using the values given by the authors for ΔE_{ij}.

4. In the cases where fine structure calculations were available, the collision strength of the term has been derived using a weigthed energy threshold. The total contribution of a configuration is obtained summing over the different terms. In this way discrepancies in the results due to different term-mixing treatment can be neglected.

The data library has been structured into a home made format since no standard existed yet. Recently an effort has been made to convert the data into ALADDIN format in order to standardize them and make it possible the retrieval by means of the ALADDIN code itself. The work has been performed by means of a preprocessor which reads the source format and translates it into the ALADDIN structure, eliminating redundant information (such as some headings) and adopting the standard formulas defined in the code. For some references new formulas had to be added in ALADDIN to account for the algorithms which define the functions and that are not included among the ALADIN formulas (7 new formulas have been added).

During the work we had in mind to include in ALADDIN plotting facilities, but we discarded the project because:

excellent codes (e.g. PLOTTAB; see in the next page a graph from the library) exist which produce graphs of good quality and the inclusion of a similar software in ALADDIN will enormously enlarge the code so as it could no more easily fit into the DOS region; ALADDIN could output the numerical data directly in PLOTTAB format;

to add plotting facilities involves a deep modification in the structure of ALADDIN: in fact it is simple to retrieve one function and to plot it, but it is not to retrieve a certain number of curves and interactively plot different groups of them many times until the best set has been selected;

a problem of interface exists: the basic software to produce graphs on the screen has not yet come to a standard neither a standard hard copy feature is available; we developed a basic graphics software based upon the MICROSOFT compiler which allow mixed calls among different languages (i.e. FORTRAN calls Assembler, C, Basic and Pascal). The software is in use at our installation but not included in ALADDIN.

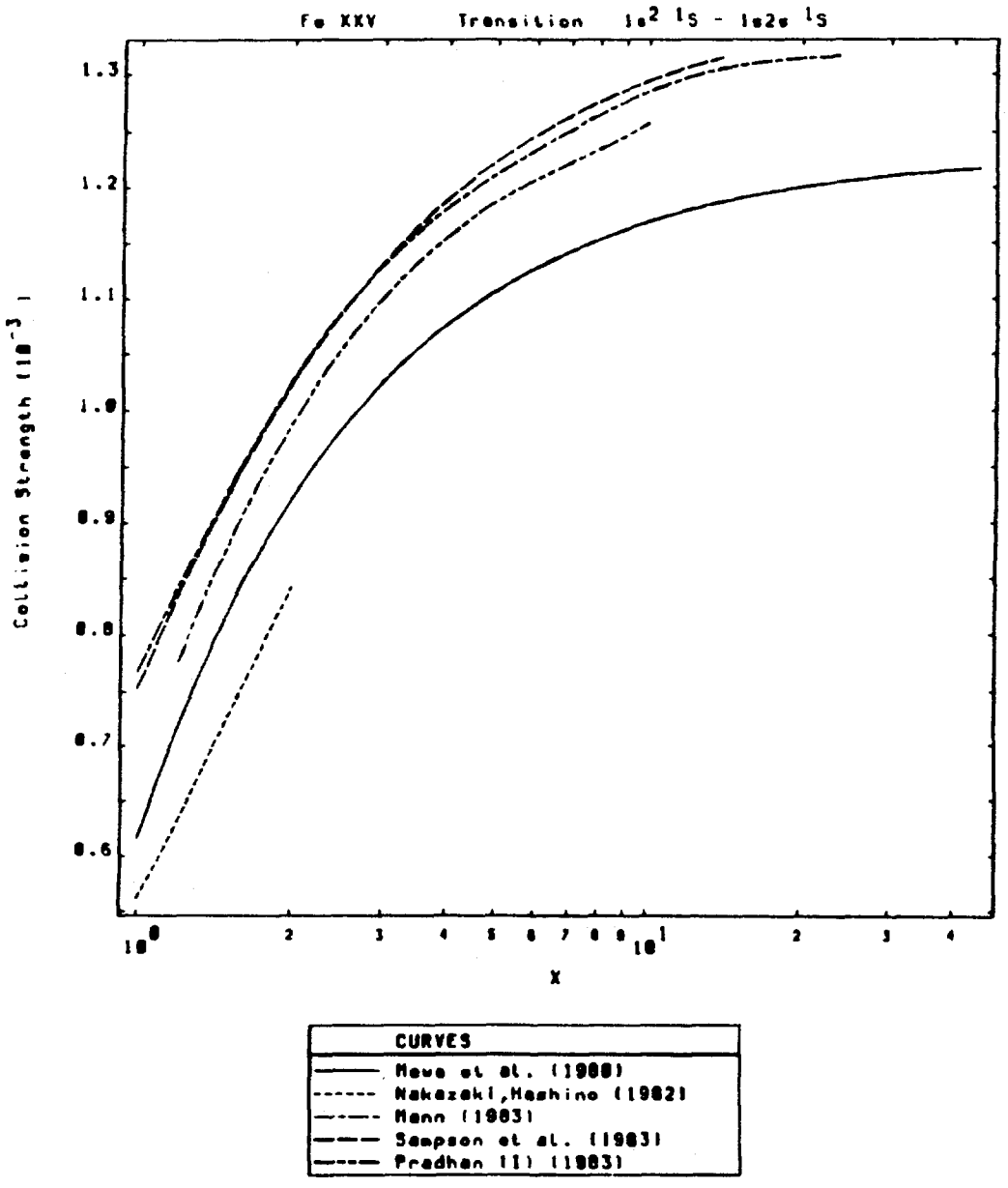
Some references (about 200) in the original library included experimental data only since the retrieval code is written to select point data as opposite to formula coefficients. ALADDIN does not allow the re-

trieval of point data neither any kind of fit, therefore these references have not yet included in the new ALADDIN formatted library. Work is in progress at ENEA to find suitable formulas to approximate experimental data when no recommended fitting formula exists.

References

M.Frisoni, P.L.Ottaviani, G.C.Panini : A collection of electron excitation collision strenghts for iron ions. I. Fe XXVI-Fe XVIII. RT/TIB/89/3

M.Frisoni, P.L.Ottaviani, G.C.Panini : A collection of electron excitation collision strengths for iron ions. II. Fe XVII-Fe I. RT/TIB/89/12



2.Electron-molecule collision data

A.Mengoni-ENEA (collaboration with T.Shirai JAERI-Nuclear Data Center)

Data calculations for $e^- +$ molecule collisions are in progress for molecules with high dipole momentum and collision energy from few eV up to tens of eV by an implemented computational technique based on the Vibron Model (Iachello et al.1981-82) algebraic description of the roto-vibrational states in conjunction with the Glauber diffractive theory.

This technique (suitable for a simple description of the scattering amplitude for rotational excitation of biatomic molecules) has been extended to the vibrational excitations too.

The calculation of E1 transition intensities among different vibrational bands of biatomic molecules was solved by a proper algebraic operator and the results were successfully compared with experimental measurements for molecules such as $H^{19}F$, $D^{19}F$, $H^{35}Cl$, $D^{35}Cl$, $H^{89}Br$ and $D^{89}Br$.

For the calculation of the scattering amplitude the difficulties arising from matrix inversion (when both vibrational and rotational transitions are considered) were overcomed by a simple approximated analytical expression and its validity was verified as generally good.

Considering that the Bijker and Amado (1986) approach leads to vibrational excitation cross sections several orders of magnitude smaller than the vibrational elastic one, at deviance with measurements showing a much less drop, the new dipole transition operator (inducing vibrational transitions) here adopted has been the one recently proposed by Iachello et al. (1990) for the calculation of infrared transition intensities.

Then the scattering cross section $e^- +$ HF has been calculated for collision energies ranging from 2 and 10 eV for the various vibrational elastic and inelastic ($V' = 1$, 2 and 3) channels.

From the comparison with experimental data one can deduce:

1. the rotational excitation is well described by the calculations for the vibrational elastic channel, the dominant interaction being the dipole one; in fact the results are in good agreement with experiments and "ab initio" technique predictions;

2. the vibrational excitation cross section is well approximated at small angles (dipole term dominant), but big discrepancies appear at high angles (due both to the importance of quadrupole short range contribute and to the less validity of Glauber approximation at high scattering angles).

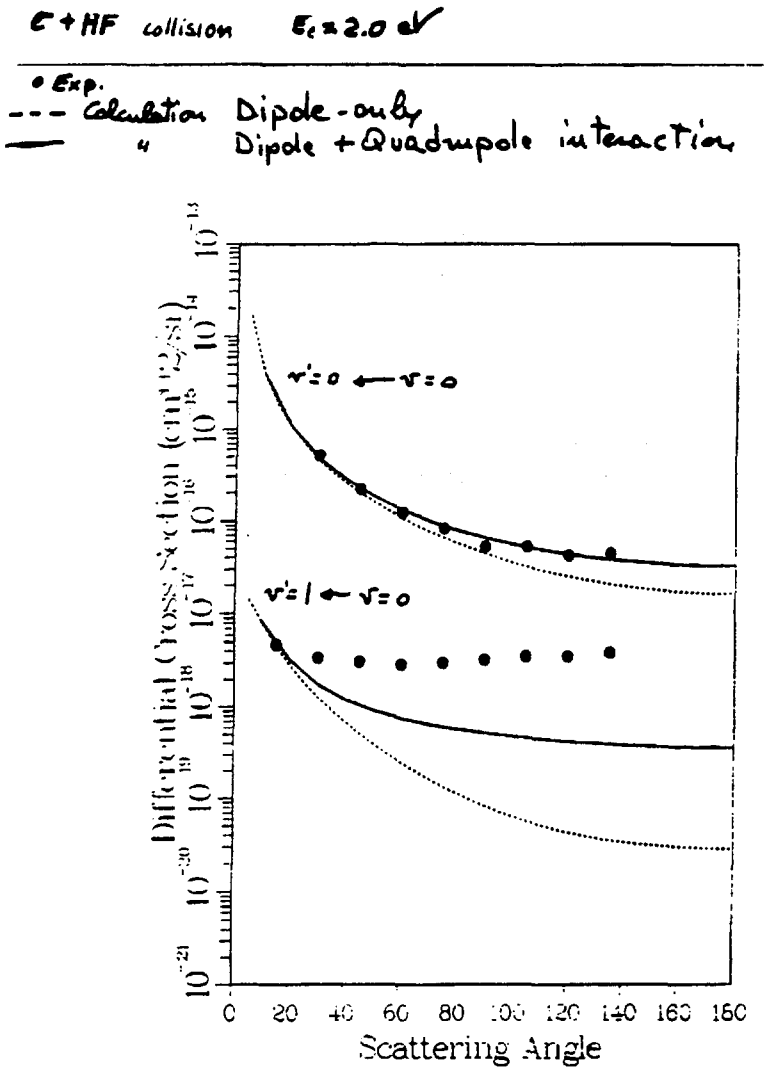
Then the quadrupole interaction potential has been included in the same algebraic model with the aim of improving the desription of the scattering at short distances.

In order to check the validity of the improved approach an example of calculations with respect to experimental data for $e^- + HF$ differential cross section of elastic and inelastic scattering involving vibrational states is given in Fig. 1 (to be published as in reference).

Trend for the future will concern the application of this both phenomenological and algebraic approach to the calculation of e^+ + more complex molecule collision data, taking into account the parameterization of the Vibron Model in the successful computational description of polyatomic molecules (by Iachello et al. 1989 and 1990).

References

A.Mengoni, T.Shirai : Algebraic-eikonal approach to the electron-molecule collision process: vibrational excitation and quadrupole interaction. To be publsished as JAERI and ENEA Reports.



Report From CRAAMD

(1989 - 1990)

Sun Yongsheng, Jia Baolin

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

September 1990

OUTLINE

Report from CRAAMD
(1989–1990)

Ⅰ. Overall Plan

Goal: for the sake of fitting the needs of MCF, ICF and X–ray Laser research work, we have already begun establishing A+M data base in China.

1. Contents of our data base

Our data base will include the following contents:

(1) Ionic, atomic and molecular energy levels.
(2) Electron impact excitation cross sections and rate coefficients of ions, atoms and molecules.
(3) Electron impact ionization cross section of ions, atoms and molecules.
(4) Wavelengths and oscillator strengths of the spectra.
(5) Photo–ionization cross sections.
(6) Transition probabilities rate for autoionization, dielectronic recombination.
(7) Cross sections of collision excitation, ionization and charge exchange between ions and atoms.
(8) Data for plasma–surface interactions, including: Reflection of light ions from solids, Sputtering, Secondary electron emission and so on.

The original data are collected, compiled, calculated and measured by ourselves. Besides these, we are also engaged in calculation methods research and programming computational softwares. All atomic scientists joining CRAAMD should jointly make their plans and coordinate their research works on A+M data.

Our data base is divided into two parts :

Part A consists of original data.
Part B recommended data and fitted formulas.

All of the data are formatted according to the ALADDIN system used by IAEA.

2. Man power: for A+M data in IAPCM: ~ 25 (full time).

The institutions joining CRAAMD are as follows:

(1) Institute of Physics, Academia Sinica(theory and experiment)
(2) Institute of Atomic and Molecular Physics, Jilin university (theoretical calculations)
(3) Department of Modern Physics, Fudan University (experiment)
(4) Institute of Low Energy Physics and Department of Physics, Beijing Normal University(theory and experiment)
(5) Nuclear Physics Division, Institute of Atomic energy (experiment)

(6) Institute of Atomic and Molecular Physics, Chengdu University of Science and Technology (theory and experiment)
(7) Department of Modern Physics,University of Science and Technology of China(theory and experiment)
(8) Institute No.207th, the Second Academy, Ministry of Aerospace, Beijing, China (theory)
(9) Department of Applied Physics, National University of Defence Technology(theoretical calculations)

Cooperating Institutions:
(1) Institute of Nuclear Science and Technology, Sichuan University (experiment)
(2) South–West Institute of Nuclear Physics and Chemistry (experiment)
(3) Department of Physics, Huaihai University(theory)

3. Fund:

For data centre (in IAPCM): ~ 100 thousand R.M.B. yuan (Chinese yuan) per year; for joining and cooperating Institutes, according to agreement signed by IAPCM with the menber institution of CRAAMD, the total amount of fund depends on the budget situation of CRAAMD, in the past three years, about 100 thousand R.M.B. yuan per year. More funds for data research work are supplied by National Natural Science Foundation of China.

Ⅱ. Annual progress (1989–1990)

Research works performed in the past year in CRAAMD:

1. Establishing A+M data base

Data collected,compiled and put in storage are as follows:

(1) Electron impact excitation collision strengths of Ne–like ions ($Z=22$–92). There are 89 energy levels of different configurations, the principal quantum numbers of excitation state is $n \leqq 4$. The original data are quoted from Los Alamos, they are fitted to analytic form before ALADDIN formatted.

(2) Electron impact excitation cross sections of Ne–like ions ($Z=26$, 34, 39, 42, 47). There are 37 energy levels.With the transitions between excited states ($n \leqq 3$), there are altogether 660 transitions. They are also fitted into analytic expressions, the original data are quoted from Livermore.

(3) Eletron impact ionization cross sections and rate coefficients of atoms and various ions ($Z=1$–28). The parameters of the fitted forms are from Belfast.

(4) We have compiled and evaluated electron impact excitation rate coefficients of Iron ions Fe^{+1}, Fe^{+9}, $Fe^{+14}$to Fe^{+25}etc.(see CRAAMD–AM–2).

(5) We have collected experimental cross sections of K–shell ionization of C to U atoms by electron impact, and these cross sections are tabulated according to target atomic number and incident electron energy (see CRAAMD–AM–4).

(6) We also collected experimental data of emission cross section for the collisions between ions and atoms. These data were measured by Institute of Physics, Academia Sinica during the last two years (see CRAAMD–AM–6).

2. Data calculation and Programming

(1) We have calculated atomic structure data and spectroscopic data for the Ne–like ions (Fe, Ni, Cu, Ge, Se), using the non–relativistic Hartree–Fork method including the relativistic mass–velocity and Darwin terms in the Hamiltonian (HFR) proposed by Dr.R.Cowan (see CRAAMD–AM–5).

In the same way, we have also calculated the above–mentioned data for the Na–like ions(Ge, Fe, Cu, Se), the Li–like ions (Al, S, Rb, Nb), the F–like ions (Ge, Se, Fe, Cu), the Be–like ions (Rb, Nb) and the He–like ions (Rb, Nb) etc.

(2) Using Plane–Wave–Born approximation, we have calculated electron impact excitation cross sections and rate coefficients for the following ions:

Li–like ions (Al, S), $n \leqq 4$;
Na–like ions (Fe, Cu, Ge, Se), $n \leqq 4$;
F–like ions (Fe, Cu, Ge, Se), $n \leqq 3$;
Ne–like ions (Fe, Cu, Ge, Se), $n \leqq 4$.

The incident electron energies adopted 1.01–100 times of the threshold energy. The data nearby threshold are not reliable to a factor of 2–3.

(3) Using the non–relativistic Hartree–Fork wavefunctions including relativistic effects, we have calculated dielectronic recombination cross sections for the Se, Ni, Cr, Ti, Fe ions.

(4) Using Grant's multiple configurations Dirac–Fork (MCDF) wave functions, we have made the computer program of electric dipole radiative transition probabilities (Jilin Univ.).

3. Experiments

Using LF–11$^{\#}$laser device, we have measured wavelengths of Ne–like ions (Fe, Ni, Cu, Ge, Zn) and compared them with theoretical calculations.

4. We are spreading ALADDIN system in CRAAMD and in China.

Ⅲ. Tentative Plan for Next Year

1. To continue collecting, evaluating data on electron impact excitation, ionization and dielectronic recombination etc. and speed up establishing A+M data base for fusion. (IAPCM)

2. We will calculate electron impact excitation and dielectronic recombination data more and better than we did last year. For low incident electron energy, we will use close–coupling (CC) approximation.(IAPCM)

3. We will speed up building experimental devices on electron impact in following institutions:

(1) Institute of physics,Academia Sinica (Prof. Liu Jiarui's group).

(2) Fudan Univ. (Prof. Yang Fujia's group).

(3) Chengdu Univ. of Science and technology (Prof. Wang Renguang's group).

(4) Univ. of Science and Technology of China(Prof. Xu Kezun's group).

4. Finally, we would like to undertake some research works on A+M data for fusion from IAEA.

Thank You !

Report on Activities of Atomic Data Research
Chinese Nuclear Data Centre
Institute of Atomic Energy
Beijing, China

Yao Jinzhang

I. Compilation

1) Yao Jinzhang, Yang Qing:
Emission cross sections in collision among He, Ne and Ar atoms and their ions (Report)

2) Yang Qing, Yao Jinzhang:
Electron impact ionization cross sections for atoms and ions with high Z (to be published)

3) Xiangquan Long, Mentian Liu et al:
Cross section for K-shell ionization by electron impact (Atomic and Nuclear Data Tables 45, 353 (1990))

4) Zhang Di:
Desorption cross sections for light ions incident on stainless steel surface (Report)

II. Experiment

1) Dong Zhi-Qiang, Li Jin-Wen, Hu Ai-Dong, Zhou Shu-Hua:
Charge distribution of phosphorus ion in gold foil at 99 MeV (to be published)

2) Hu Ai-Dong, Zeng Xian-Tang, Li Jin-Wen, Zhou Shu-Hua:
Two-electron-one photon transition in Cu^{q+} +Zn system at 80 MeV (Report)

3) Miao Jingwei et al:
Produce of H^- and D^- negative ions and measurements of charge exchange cross section in solid state (Report)

4) Yu Jinnan et al:
Radiation effects on the first wall material of fusion reactors
(Research contract is being supported by IAEA)

THE FACTOGRAPHIC DATABASE *on* ATOMIC SPECTROSCOPY "SPECTR-2" FOR INFORMATION SERVICE IN THE FIELD OF THERMONUCLEAR AND QUANTUM ELECTRONIC INVESTIGATIONS.

V.Yu.Bugaev, V.G.Pal'chikov, I.Yu.Skobelev, A.Ya.Faenov

Introduction. The atomic constants of multycharged ions are the main object of studies in the fields of high-temperature plasma physics, quantum radiophysics and nonatmospheric astronomy. It's mainly connected with three circumstances: First, the emission spectra of such ions carry fundamental information about the matter properties in the extreme conditions of super high temperature and pressure, Second, the knowledge of atomic constants is necessary for numerical plasma modeling of both laboratory and astrophysical sources, and Third, for theoretical and experimental studies with in the programmes of X-ray lasers development. (see Fig. 1)

The data about the spectra characteristics of multicharged ions may be obtained by three methods: subsequent quantum-mechanical calculation, experimentally, by means of semi-empirical methods, which use both experimental and theoretical information. Until now large material has been accumulated in this field which, however, is avalable in many original works and accessible to a very narrow circle of experts. A number of compilations of the US National Institute of Standards and Technology which are available for separate chemical elements ion spectra doesn't inprove the situation. Due to this fact the task of systematic accumulation and distribution of information on multicharged atomic constants is especially vital at the modern stage and it is obvious the information concentration in the data base DB must mean its critical estimation. It is natural that such DB should be built as automated base with the use if modern computing facilities, sinle the volume of information is very large and it is not possible to handle it "manually".

"Spectr-2" automated data base (ADB) is an extension of "Spectr-1" database developed in VNIIFTRI (USSR) for storage and rapid search of multicharged ions atomic characteristics.

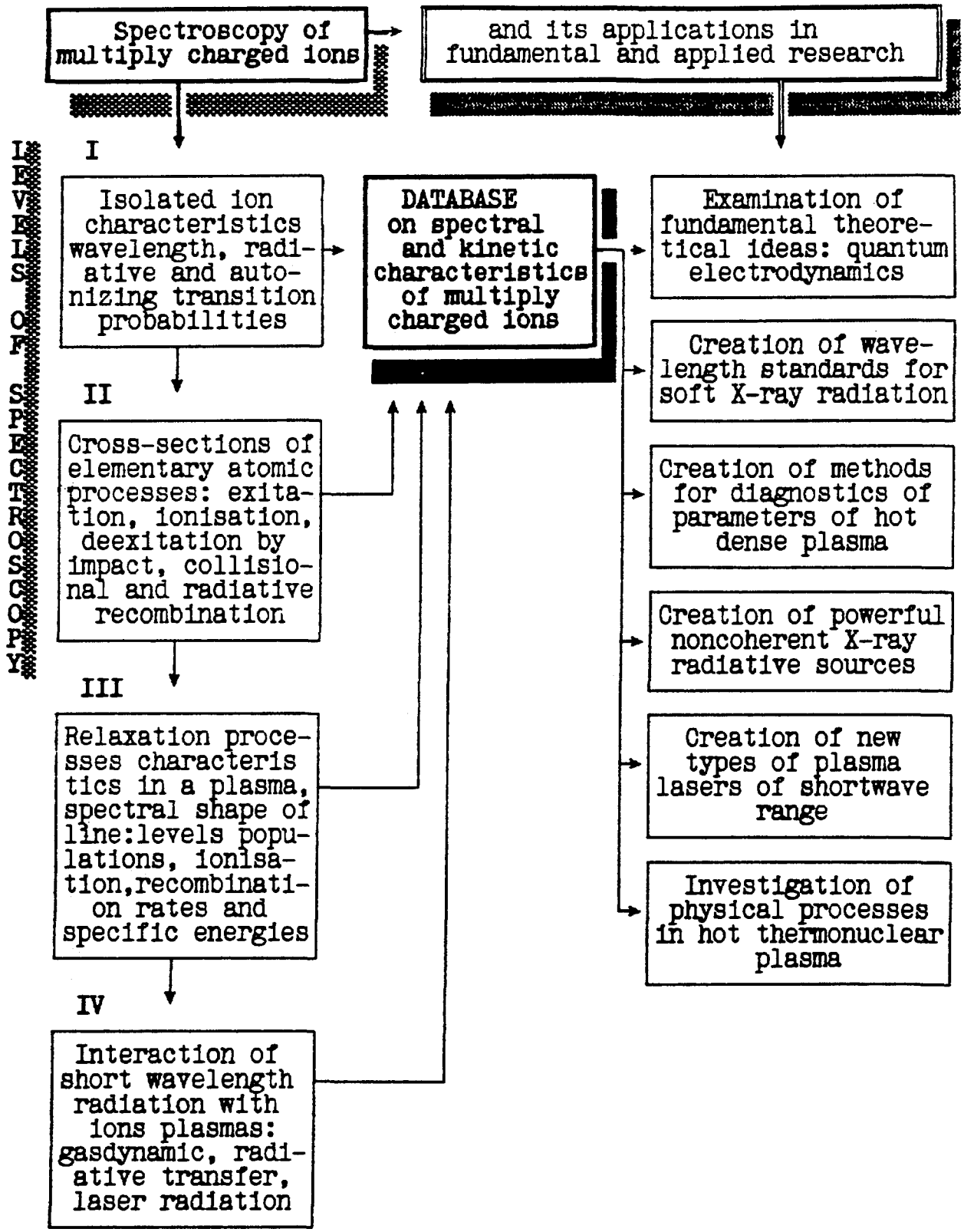
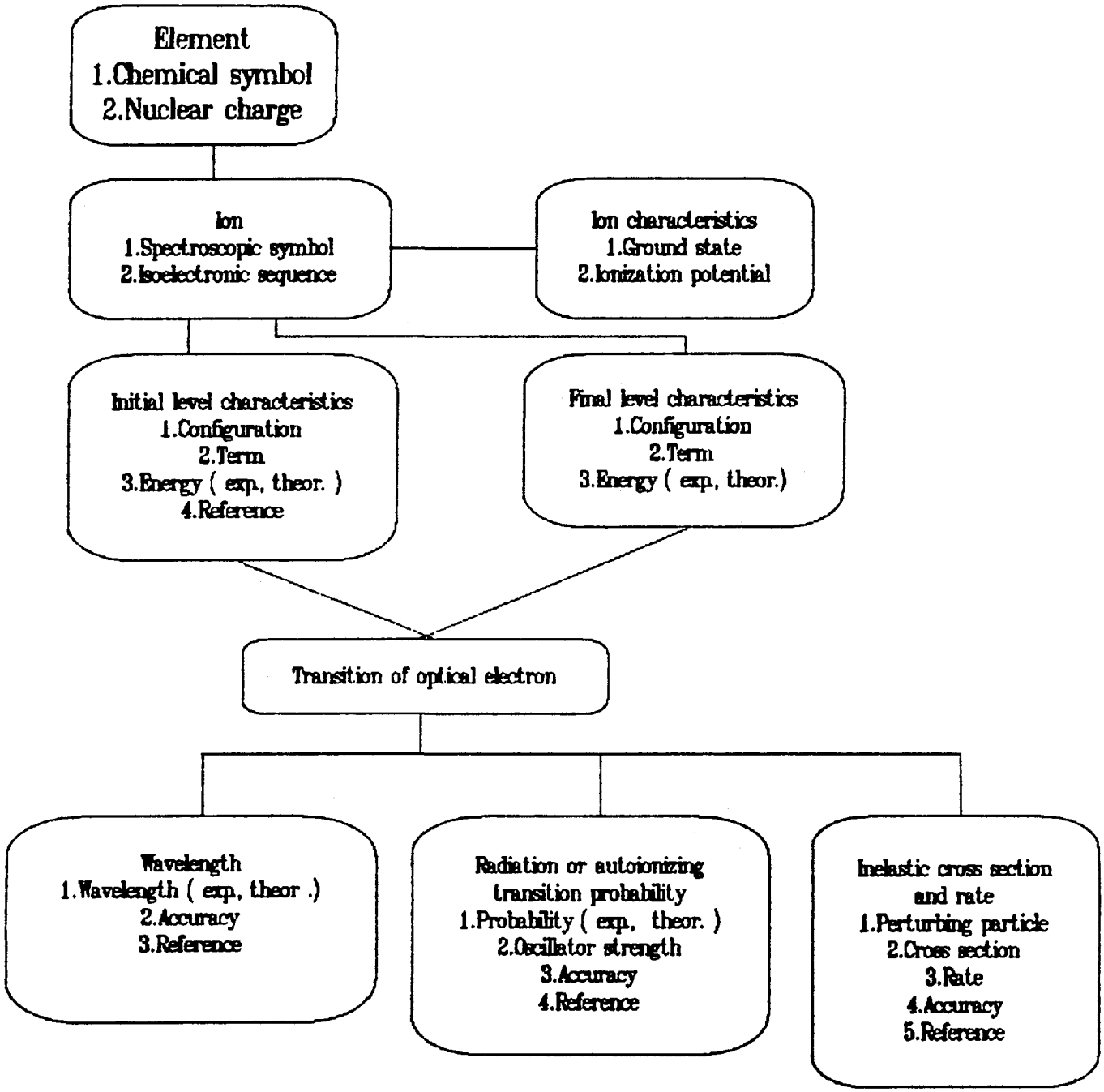

Spectroscopy of multiply charged ions
and its applications in fundamental and applied research
LEVELS OF SPECTROSCOPY
I
Isolated ion characteristics wavelength, radiative and autonizing transition probabilities
DATABASE on spectral and kinetic characteristics of multiply charged ions
Examination of fundamental theoretical ideas: quantum electrodynamics
Creation of wavelength standards for soft X-ray radiation
Creation of methods for diagnostics of parameters of hot dense plasma
Creation of powerful noncoherent X-ray radiative sources
Creation of new types of plasma lasers of shortwave range
Investigation of physical processes in hot thermonuclear plasma
II
Cross-sections of elementary atomic processes: exitation, ionisation, deexitation by impact, collisional and radiative recombination
III
Relaxation processes characteristics in a plasma, spectral shape of line:levels populations, ionisation,recombination rates and specific energies
IV
Interaction of short wavelength radiation with ions plasmas: gasdynamic, radiative transfer, laser radiation

Fig. 1



Information structure of database " SPECTR - 2 "

Fig. 2

The development of a new ADB version is linked with the necessity of including information about cross-section and excitation speeds of ions by different particles in ADB. On the other hand, large volume of information (more than 200000 transitions) accumulated on spectral characteristics (level energetic structures, wavelength, radiation transition probabilities etc) as well as the experience of utilizing "Spectr" ADB led to the necessity of changing formats of data presentation in both entry documents and files loaded for automatic search. The process of ADB servecing has also changed. A number of service packges providing a more flexible technology to support data base has been created.

"Spectr-2" DB information structure. The main unit of information presentation in "Spectr-2" ADB is a document. Every document contains segments which incorporate data or texts. In order to distinguish one data from another they are given a unique tree-symbol label. The data having one label in "Spectr-2" DB may differ by its position within the segment.

Combinations of practically any symbols may serve as data for "Spectr-2" DB. One data from another is separated by at least one blank. Terms indicating element chemical symbols, energy level configuration, nucleous charge levels energy, transition wave length, radiation probabilities, etc serve as data in "Spectr-2" (Fig.2)

The documents contained in "Spectr-2" ADB may be found with the help of terms which are referred to as search terms. The search terms fully identify the information contained in the document. For this purpose every document should feature informational completeness property, i.e. the document should contain all terms by means of which it can be found.

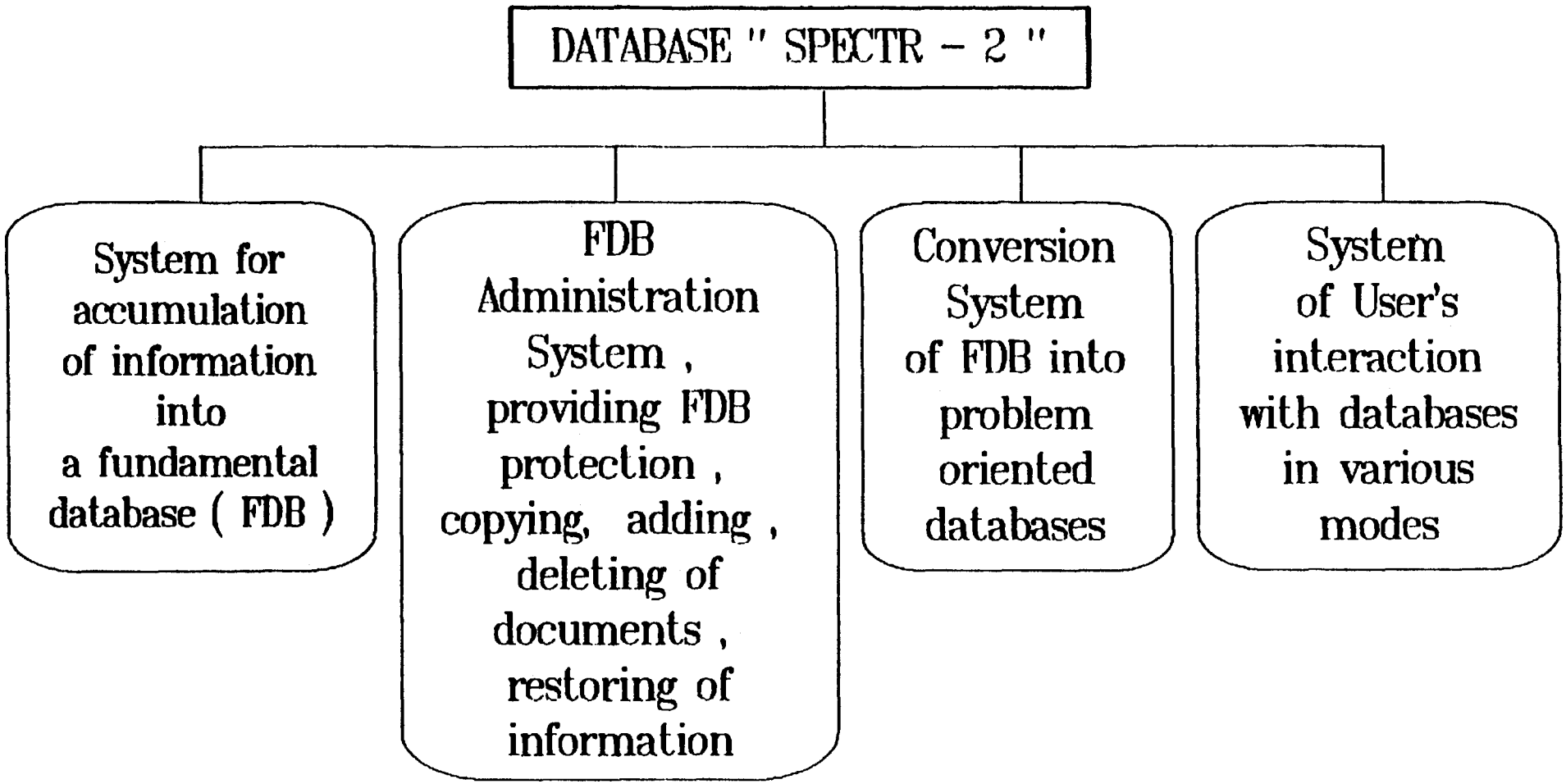

DATABASE " SPECTR - 2 "
System for accumulation of information into a fundamental database (FDB)
FDB Administration System , providing FDB protection , copying, adding , deleting of documents , restoring of information
Conversion System of FDB into problem oriented databases
System of User's interaction with databases in various modes

Fig. 3

The document structure in "Spectr-2" ADB is oriented into the use of "DIALOG-2" (West analogues "Stairs") as the information search system. The documents of the following types are supported in "Spectr-2" DB:1- "Ionization potential" ; 2- "Electronic Transitions"; 3- "Excitation cross-section";4- "Excitation rate" ; 5- "Information supplier" ; 6- "Bibliography" ; 7- "Commentaries".

The document of different type are interfaced at a level of similar terms. For exemple, if reference number in the "Bibliography" document coincides with the reference number of the "Electronic transition" documents, they are interfaced at the logical level.

Interaction of the Terminal User with "Spectr-2" DB . The terminal user is provided an opportunity to obtain information from "Spectr-2" ADB in a dialogue mode. The dialogue mode is realised in the electronic computer in the local TV access network by EC-7920 equpment and its analogues under OC MVT 6.1 operational system control and higher in the TV acces system. (see Fig. 3)

The searching prescript is compiled from terms or part of terms truncated from the right and logical operators between them. The result of fulfilling searching prescipts is the number list of documents containing information given in the conditions. This list may be processed by three methods to obtain the so called output forms: by means of report generators and the output of the resulting tables to the printer in interactive mode; by means of obtaining tables built on the results of the search in the packeting mode; by means of information output into the intermediate file for further processing and use in application programmes.

"Spectr-2' ADB Information accumulation. At present ADB "Spectr-2" provides data about spectral characteristics of ions of

isoelectronic sequences H-Ag (theoretical calculations, observation data, experimental results compilation). The total volume of information is about 200000 documents for which, because LS-communication diagrams are mostly spread and traditionally obvious, the classification by extreme LS-terms is used. The possibility to analyse statistical weights of the corresponding wave functions in the framework of multiconfidurational approximation is reserved for complex spectr.

The theoretical calculations of spectra and radiation transition probabilities in hydrogen-like ions were made by methods of Dirac relativistic theory with the subsequent account of quantum-electrodynamic effects and adjustments linked with the nuclear structure.

For helium isoelectronic series the theoretical calculations of atomic spectral characteristics were made by two alternative methods: the method of relativity theory of excitations by 1/z and within the framework of semi-empirical approach which uses experimental approximations of transition wavelengths along isoelectronic sequence.

The energy of levels in Li-like ions were calculated in the similar way, through obtained by the method of model potential in the relativity wersion was also used. The calculations of oscillator forces and radiation transition probabilities were curried out by the method of Fuse model potential which mode it possible to simplify mathematical computations radically due to the simple analitical form of wave functions. The calculations of level energy for Be-like ions were made both by the method of excitation theory by 1/z & Hartry-Fock approximation. In order to increase accurracy of computations combination of methods of self-consistent field and semi-empirical dependencies along Z were

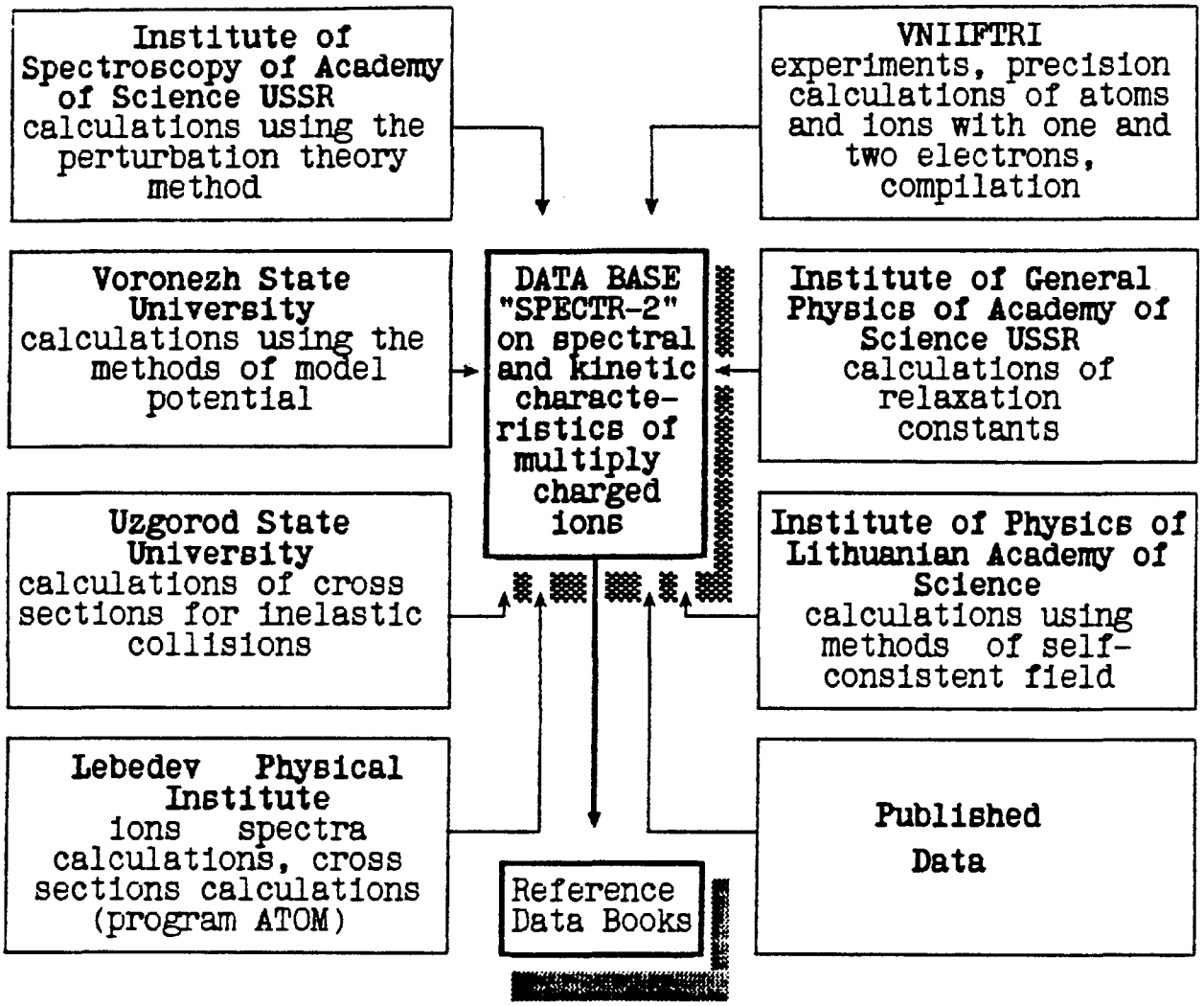


Fig. 4

used which helped to perform overall adjustment to study their matching with the experimental data.

The main volume of theoretical data concerning spectral characteristics of other isoelectronic sequences (O-, F-, Ne-,Na-like ions) was obtained by the relativistic method of self-consistent field (in Hartry-Fock-Pauli approximation) which allows to determine the values of atomic constants with the accuracy close to the experimental one.

Spectra calculations of H- to Na- like ions were made in the various institutes of the USSR (Spectroscopy Institute, USSR Academy of Sciences, Institute of Physics, USSR Academy of

Sciences, Institute of Physics, Lithuania SSR Academy of Sciences, Voronezh State University,NPO VNIIFTRI). Besides, for the above mentioned types of ions practically all presently known experimental data about the spectral lines in the area of $\lambda < 100$ Å A have been entered into the database. (Fig. 4)

"Spectr-2" ADB contains the results of spectrum studies for ions from Mg- to Ag- like isoelectronic sequences in the region $\lambda < 100$ A published prior to 1990.

Data structure of database "Spectr-2" input documents and of Dialog-2 system loaded fields .

In the following tables the detailed rules of requisites arrangement in segments for all types of DB "Spectr-2" documents are presented. These tables contain the information about requisites type (searchable - S, nonsearchable - N), storage-type in loaded form (F - format field, T - text field). For requisites with label 'E' only the power of value is searchable, while the mantissa is not a searchable item. For requisites marked with F1 only the first symbol forms the format field, it is necessary to perform summary inquiries about the availability of the particular types of information. Character '&' denotes indefinite length.

These tables contain segment names and format field names, which presents in the dialog session.

Column numbers in the tables means:

1 - segment level

2 - data length

3 - load type

Document "Ionization potential"

N Name of requisite	The place in the input document		
	1	2	3
1.Chemical symbol of element	001	2	SF
2.Atomic number	001	3	SF
3.Isoelectronic sequence	001	4	SF
4.Spectroscopic symbol	005	3	ST
5.Ground state configuration	005	&	ST
6.Ionization potential (eV)	006	18	ST
7.Accuracy of ion.pot.value	006	9	NT
8.Method	006	2	ST
9.Reference (to original literature source)	006	5	ST

Dooument type "Transition"

N	Name of requisite	The plaoe in the input dooument 1	2	3
1.	Chemioal symbol of element	001	2	SF
2.	Atomio number	001	3	SF
3.	Isoeleotronio sequenoe	001	4	SF
4.	-------- Configuration --------	020	&	ST
5.	Multiplioity	021	1	ST
6.	Orbital momentum	021	1	ST
7.	Total momentum	023	&	ST
8.	1 Energy level (cm^{-1})	050	18	NT F1
9.	Energy aoouraoy	050	9	NT
10.	Method	050	2	NT
11.	------- Referenoe --------	050	5	NT
12.	Configuration	040	&	ST
13.	Multiplioity	041	1	ST
14.	Orbital momentum	041	1	ST
15.	Total momentum	043	&	ST
16.	2 Energy level (cm^{-1})	051	18	NT F1
17.	Energy aoouraoy	051	9	NT
18.	Method	051	2	NT
19.	------- Referenoe --------	051	5	NT
20.	Transition of the optioal eleotron	060	&	ST
21.	Wavelength	061	18	SF
22.	Aoouraoy	061	9	NT
23.	Method	061	2	SF1
24.	Referenoe ----------	061	5	ST
25.	Transition Probability	066	18	NT
26.	Aoouraoy	066	9	NT
27.	Method	066	2	NT
28.	Referenoe ----------	066	5	NT
29.	Oscillator strength	071	18	NT
30.	Aoouraoy	071	9	NT
31.	Method	071	2	NT
32.	Referenoe ----------	071	5	NT
33.	Autoionization probability	076	18	NT
34.	Aoouraoy	076	9	NT
35.	Method	076	2	NT
36.	Referenoe ----------	076	5	NT

Document "Excitation cross section

N Name of requisite	The place in the input document		
	1	2	3
1.Chemical symbol of element	001	2	SF
2.Atomic number	001	3	SF
3.Isoelectronic sequence	001	4	SF
4.Configuration	020	&	ST
5.Multiplicity	021	1	ST
6.Orbital momentum	021	1	ST
7.Total momentum	023	&	ST
8.Configuration	040	&	ST
9.Multiplicity	041	1	ST
10.Orbital momentum	041	1	ST
11.Total momentum	043	&	ST
12.Cross section	200	1	SFT
13.Method	200	2	ST
14.Projectile particle	200	6	ST
15.Reference	200	5	ST
16.Data type (table of parameters)	200	4	ST
17.Argument array	201	60	NT
18.Function array	201	60	NT

Document "Excitation rate coefficient

N Name of requisite	The place in the input document		
	1	2	3
1.Chemical symbol of element	001	2	SF
2.Atomic number	001	3	SF
3.Isoelectronic sequence	001	4	SF
4.Configuration	020	&	ST
5.Multiplicity	021	1	ST
6.Orbital momentum	021	1	ST
7.Total momentum	023	&	ST
8.Configuration	040	&	ST
9.Multiplicity	041	1	ST
10.Orbital momentum	041	1	ST
11.Total momentum	043	&	ST
12.Excitation rate	300	1	SFT
13.Method	300	2	ST
14.Projectile particle	300	6	ST
15.Reference	300	5	ST
16.Data type (table of parameters)	300	4	ST
17.Argument array	301	60	NT
18.Function array	301	60	NT

REPORT ON IAEA A+M DATA UNIT ACTIVITIES FOR THE PERIOD SEPTEMBER 1989 - SEPTEMBER 1990

R.K. JANEV

1. Data Evaluation and Parametrization

1.1. Updating of Carbon and Oxygen databases and new parametrization

- Inclusion of new data information (since 1987) and data re-evaluation (particularly at low energies);
- Data fitting to new analytic fit expressions for σ_{CX} and σ_{ION} with appropriate asymptotics.

* General forms:

$$\tilde{\sigma}_{CX} = A_1 \left[\frac{\exp(-A_2/\tilde{E})}{1+A_3\tilde{E}^2+A_4\tilde{E}^{4.5}} + \frac{A_5 \exp(-A_6\tilde{E})}{\tilde{E}^{A_7}} + \frac{A_8 \exp(-A_9/\tilde{E})}{1+A_{10}\tilde{E}^{A_{11}}}\right]$$

$$\tilde{\sigma}_{CX} = \sigma_{CX}/q, \quad \tilde{E} = E/q^{1/2}, \quad E \text{ in keV/u},$$

$$\tilde{\sigma}_{ion} = B_1 \exp(-B_2/\tilde{E}) \ln(1+B_3\tilde{E})/(B_4+\tilde{E})$$

$$\tilde{\sigma}_{ion} = \sigma_{ion}/q, \quad \tilde{E} = E(keV/u)/q$$

* Most of the work has been done

1.2. Completion of the database for neutral H-beam penetration into fusion plasmas

- Existing database updated with recent (since 1988) information and extended to lower energies (particularly for heavy-particle excitation);
- Collision processes with He^{2+} ions singled out from other impurities;
- Ionization and charge exchange cross sections treated independently in the electron removal to allow for possible CXRS diagnostics;
- New scalings for n-n' and n → continuum transitions by electron impact adopted.

1.3. Database for particle interchange processes in edge plasmas

- Data compilation and evaluation work has been continued

1.4. Database for physical sputtering (normal incidence)

- Re-evaluation of existing data on physical sputtering by light (H, D, He, Li, Be)- and self-ions has been performed (jointly with Dr. E.W. Thomas) for materials of fusion interest;
- A uniform, three-parameter analytic fit to evaluated data has been established and fit parameter determined;
- Semi-empirical dependences of fitting parameters on masses and nuclear charges of colliding species have been established (≡ semi-empirical formula with predictive power);
- Shifted-Maxwellian averaging of sputtering yields underway.

1.5. Database for backscattering (normal incidence)
(work performed jointly with Drs. E.W. Thomas and W. Eckstein)

- Re-evaluation of existing (including very recent) backscattering data for light ions and self-ions from surfaces of fusion interest has been performed (normal incidence case).
- Analytic fit representation of evaluated data to one general expression, alowing for different projectile-target mass ratios.

1.6. Database for Li-beam penetration into plasmas
(joint work with H.P. Winter's group, TUW)

- Data compilation, evaluation and generation for all Li/Li^{*} - e, H^{+}, A^{q+} processes involved in Li-beam attenuation.

2. ALADDIN System Development and ALADDIN Data Formatting

2.1. ALADDIN system development
(More details in J.J. Smith's presentation)

- System software modification according to comments/suggestions at the last DCN meeting.
- Preparation of new ALADDIN Manual.

2.2. ALADDIN data formatting

- ALADDIN formatting of:
  * Physical sputtering data;
  * Ion backscattering data;
  * All A+M data compiled and/or evaluated by the IAEA A+M Data Unit;
  * PPPL Reports on H/He A+M data and Hydrocarbons.

3. Co-ordinated Research Programmes (CRPs)

3.1. CRP on "A+M data for fusion edge plasmas" (1988-1991)

- Work on data generation and evaluation continues.
- Preparation of Nucl. Fusion Supplement Vol. 2, devoted to A+M plasma edge processes and data.

3.2. CRP on "Plasma-interaction induced erosion of fusion reactor materials" (1990-1993)

- Programme has just started with 10 participating laboratories.
- Programme objective: to generate evaluated net erosion rates for prime candidate PFC materials.
- Programme closely related to ITER needs.

3.3. CRP on "Atomic data for medium- and high-Z impurities in fusion plasmas" (1991-1994)

- Programme recommended by the IAEA AGM on metallic impurities (May, 1990).
- Programme has just been initiated (proposed 15 participating laboratories).
- Programme has to be approved by the IAEA by the end of 1990.

4. Individual Research Contracts in Support to Data Activities
(granted only to developing countries)

1) "Molecular spectroscopy relevant to fusion edge plasma" (Dr. N. Konjevic).
2) "Cross section calculations for ionization of excited hydrogen and helium" (Dr. R. Rivarola).
3) "Studies of ion-impact ionization processes pertinent to fusion plasmas" (Dr. S. Mukherjee).
4) "Measurements of electron impact ionization cross sections" (Dr. N. Djuric).
5) "Application of improved bipartition model of ion transport to calculate ion reflection and radiation damage for fusion technology" (Dr. Luo Zhengming).
6) "Radiation effects on the first wall material of fusion reactors" (Dr. Yu Jinnan).
7) "Evaluation of A+M data for metallic impurities in plasmas" (Dr. Jia Baolin).

5. Meetings Organized During Reporting Period

1) SM: "Review of the status of A+M data for fusion edge plasma studies" (September 11-13, 1989; 25 participants).
2) CM: "8th A+M DCN Meeting" (September 14-15, 1989; 15 participants).
3) AGM: "A+M data for metallic impurities in fusion plasmas" (May 16-18, 1990; 18 participants).
4) CM: "Thermal response of plasma facing materials and components" (June 11-13, 1990; 10 participants).
5) CM: "9th Meeting of A+M data centres and ALADDIN network" (September 20-21, 1990).

6. Bibliographic Database

- Two issues of the Int. A+M data bibliographic bulletin (input mainly from ORNL CFADC).

7. Planned Activities

7.1. Data evaluations

- Continuation of ongoing and initiated programmes (all CRPs, completion of databases on C^{q+}, O^{q+}, H-beam, Li-beam, physical sputtering, backscattering, Fe^{q+} (?)).
- Initiation of databases for:
  * He-beams (ITER urgent need),
  * Be, B (JET, ITER),
  * H and He trapping/detrapping (tritium inventory, He exhaust),
  * Thermo-mechanical data for C-C PFC materials.

7.2. Meetings planned for 1991

Meeting title	Tentative dates
1) RCM: plasma-interaction induced erosion rates of fusion reactor materials	May 15-17, Vienna
2) TCM: "Fusion materials property data	June 10-12, Vienna
3) CM: "10th A+M DCN meeting	September 23-24, Vienna
4) AGM: Subject to be determined by the IFRC Subcommittee	September 25-27, Vienna
5) SM: on He-beam data (if approved)	

ALADDIN Related Contributions

THE ALADDIN ATOMIC PHYSICS DATABASE SYSTEM

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ABSTRACT

ALADDIN is an atomic physics database system which has been developed in order to provide a broadly-based standard medium for the exchange and management of atomic data. ALADDIN consists of a data format definition together with supporting software for both interactive searches as well as for access to the data by plasma modeling and other codes.

The ALADDIN system is designed to offer maximum flexibility in the choice of data representations and labeling schemes, so as to support a wide range of atomic physics data types and allow natural evolution and modification of the database as needs change. Associated dictionary files are included in the ALADDIN system for data documentation. The importance of supporting the widest possible user community was also central to the ALADDIN design, leading to the use of straightforward text files with concatentated data entries for the file structure, and the adoption of strict FORTRAN 77 code for the supporting software. This will allow ready access to the ALADDIN system on the widest range of scientific computers, and easy interfacing with FORTRAN modeling codes, user developed atomic physics codes and databases, etc. This supporting software consists of the ALADDIN interactive searching and data display code, together with the ALPACK subroutine package which provides ALADDIN datafile searching and data retrieval capabilities to user's codes.

ALADDIN has been adopted as the standard international atomic physics data exchange format for magnetic confinement fusion applications by the International Atomic Energy Agency (IAEA). Entry of critically evaluated atomic data sets into ALADDIN format is to be coordinated by the IAEA Atomic and Molecular Data Unit, which will also coordinate long-term development and distribution of updated software and documentation. The increasingly widespread adoption of the ALADDIN data format can be expected to greatly facilitate access to atomic data both within and outside of this original fusion application area.

INTRODUCTION

The basic motivation for development of the atomic physics data system to be described here was the need to facilitate the exchange and use of atomic and molecular data across a wide range of atomic physics researchers and those in other fields who are users of such data for various applications. The goal was thus to provide a basic, common language for atomic and molecular data exchange, creation of databases, and accessing atomic data by user applications. ALADDIN[1] (A Labeled Atomic Data Interface) was developed at the Princeton Plasma Physics Laboratory to address these needs, originally within the context of the atomic and molecular data needs of the magnetic confinement fusion energy (MFE) research community. The invited papers presented at the "Atomic Processes for Fusion" sessions at this conference illustrate some of the many applications of atomic data in MFE research. ALADDIN was adopted May 1988 by the International Atomic Energy Agency (IAEA) Atomic and Molecular Data Unit as a standard data format for MFE applications, and ALADDIN-based atomic data exchange is now becoming broadly established within the MFE community. Extensive data sets are now in place, and others are under continuing development as the user group expands and existing applications codes and databases are adapted to ALADDIN. ALADDIN is, however, potentially applicable in a similar role for use in many other research areas, and could be developed as a basis for mutually beneficial sharing and exchange of atomic, molecular, surface physics, other data amongst various application areas. Hopefully, this presentation will serve to encourage such application of the ALADDIN system to atomic physics related research activites outside of the fusion community.

In short, the ALADDIN objective is to provide a basic, broadly-based standard medium for the exchange and management of atomic data, which therefore must be straightforward to use, highly flexible, and widely transportable.

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"Atomic Processes in Plasmas", Gaithersburg, MD, USA 1989
AIP Conference Proceedings 206

WHAT EXACTLY IS ALADDIN ?

The ALADDIN system comprises several related components, consisting of a data format, supporting software, specific data labeling schemes, and finally, the data itself. Users can select and adapt various elements of the system as best suits their own needs.

The most fundamental ALADDIN component is a defined but extremely flexible data format for entering and labeling atomic data as entries in ASCII (text) data files.

Next, the ALADDIN system includes specific supporting FORTRAN-77 software to facilitate user access to ALADDIN data. The ALADDIN code provides interactive data search and access from a user's terminal, while the ALPACK subroutine package provides a "black box" subroutine interface to ALADDIN data files from a user's FORTRAN codes.

Any given practical implementation of ALADDIN relys on specific choices of ALADDIN data labeling schemes appropriate for these applications. These labeling schemes can combine standardized systems established by the IAEA and other data centers along with a user's own schemes to describe their application-specific data.

Finally, the ALADDIN system includes specific data available either directly in ALADDIN-based datafile compilations or from other databases and codes which can read and write ALADDIN format files for data exchange. Associated ALADDIN dictionary files provide documentation and user information via keyword reference from the data files.

A schematic overview of how the ALADDIN system can serve to communicate atomic data between various sources and applications is illustrated in Fig. 1.

BASIC TECHNICAL CONSIDERATIONS IN THE ALADDIN DESIGN

The basic ALADDIN data storage format employs ASCII data files consisting of concatenated, independent entries. Such sequential "text" data files are by far the most readily transmitted and read across all computer systems, using media such as floppy disks, tape, computer networks and electronic mail. Also, the user's favorite text editor can serve as a basic and familiar way of searching, reading, and editing data entries. These data files can also be simply sorted by data type and printed out, allowing easy publication and use of the data even by those without convenient access to computers. Each ALADDIN data entry contains searchable attribute labels, together with the data itself.

Following the same emphasis on portability, primary supporting ALADDIN software is written in strict FORTRAN 77. This is, in practice, still the principal programming language for scientific applications, and as such, it is widely available on a full range of systems from PC's to Crays. Conveniently, the FORTRAN 77 standard also offers some support for character string manipulation, which simplifies ALADDIN's label-based searching and data handling approach.

DATA FILES vs. SUBROUTINES

An important point incorporated in the ALADDIN design is the observation that information in data files is much more easily manipulated than information coded into software. ALADDIN therefore keeps as much information as possible in data files, with the software kept as universal and data-independent as possible. However, the structure of languages such as FORTRAN require that some procedural information associated with interpreting the data must be contained in lines of code compiled into each program that uses the data.

This procedural information can be seperated into two types. First, we have the data file read, data search, and data store procedures. The ALADDIN approach is to design a general data labeling and search retrieval method, insensitive to data types being read. This software procedure receives only key searching information, and returns data identifying information together with the data itself into generalized buffer arrays. Secondly, we have the procedure(s) necessary for returning data values at specific points from the stored data representation. Here, a subroutine library is provided to interpret each data representation (by using the mathematical form of the data fitting equation, for example), with the subroutine to be called selected based on a keyword label associated with the data itself.

To summarize, ALADDIN uses "self-identifying" data containing keyword references to associated procedures and documentation as much as possible. This philosophy is akin to what would be called an "object-oriented" approach in computer terminology.

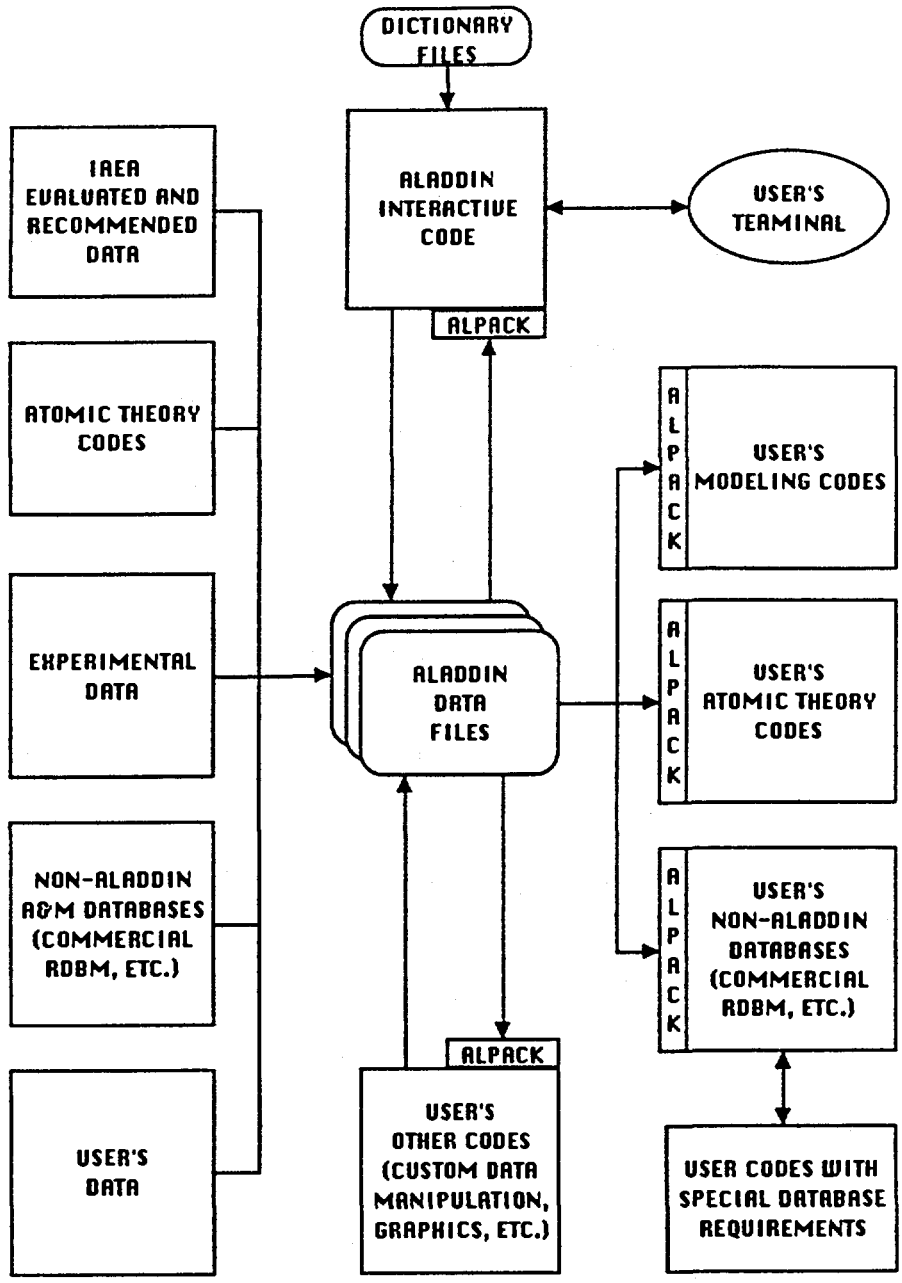


Fig. 1

NECESSARY COMPONENTS OF THE DATA ENTRIES

Atomic data to be stored can be looked at as a function of the form

$$F_{ijk...}(x, y ... | a, b, c ...)$$

where (i, j, k ...) are a set of (discrete) selection variables describing the data (atomic process type, element, charge state, etc.) and the functional form of F. This mathematical form uses one or more supplied fitting coefficients (or tabular data points) (a, b, c ...), which are used to return the desired data value (cross section, rate coefficient) corresponding to input of the (typically continuous) independent variables (x, y ...) (for example, energy, temperature).

ALADDIN represents the searchable attributes (i,j,k...) of each data entry by lists of arbitrary character string-based labels in the entry header. These "searchable labels" include the physics identifiers, data source and revision number, and other information, as well as identifying the procedure to call to read this entry's specific format and the procedure to call to calculate the data function F. An important additional application for these labels are as keywords referring to entries in the

"dictionary files" associated with the ALADDIN data files. These dictionary files provide whatever documentation is necessary to fully support the data entries themselves. Distinct from the information contained in these searchable labels for each entry are the "coefficients" (a, b, c...), defined by ALADDIN as non-searchable information which is to be passed as input to the function evaluation routine.

HIERARCHICAL AND BOOLEAN SEARCHABLE LABELS

As just described, the searchable labels serve to identify each ALADDIN entry. These labels are treated by ALADDIN as a list of arbitrary character strings, and can be placed in both hierarchical and boolean search structures to provide flexibility in designing specific labeling schemes.

Hierarchical labels are defined as a sequence of labels where the order of appearance is significant. Much information (especially physics labelling) naturally has this form. For example, a simple hierarchical label sequence for spectral line excitation rate coefficient data might be set up as follows:

SLEXR 26 24 255.2

where these labels describe the data type, element (Z = 26), charge state (XXIV), and wavelength (255.2 Å), respectively.

Boolean labels are used to represent independent attributes whose entry order does not have a fixed sequence, and which are tested individually in a search using the Boolean logical operators .AND. and .NOT.. Typical boolean label information would be the data source, fitting accuracy, a dictionary file keyword reference to documentation, etc. ALADDIN uses two reserved boolean label types for special functions. An "access label" with a $ prefix flags special procedures to read the coefficient field data, while the "evaluation label" denoted by a # prefix specifies the data fitting function and associated procedure call.

ALADDIN DATA FORMAT SPECIFICATION

Figure 2 illustrates the structure and components of an ALADDIN entry. The first label of any entry is the access label. Access labels always begin with the reserved special symbol $, with an access label consisting of a $ symbol alone denoting a standard single-precision floating point data list in the coefficient field. Following the access label is the list of ordered hierarchical labels, which are simply character strings delimited by intervening blanks. The hierarchical label field is terminated by the & symbol, whereupon follows the similarly blank-delimited boolean label field. The first boolean label is always taken to be the access ($) label, followed by the (optional) other entries in this boolean label field. The final boolean label is always the evaluation label beginning with a # symbol, which also serves to delimit the end of the entire searchable label header. The header field may extend across many lines, as necessary.

On the next line following the end of the searchable label header may appear one or more optional comment lines, begining with the ! character. These may contain any desired text, but extensive or . .petitive documentation is best provided in the dictionary files and referred to by keyword boolean labels rather than placed in these embedded comment lines.

On the next line following the searchable label header and optional comment lines begins the coefficient field. This field again may extend across an arbitrary number of lines, and contains the actual "data" in the entry. These coefficient field lines are initially handled by ALADDIN only as character strings, to provide complete freedom in the choice of data structures. As mentioned above, the default structure later assumed for this field is blank-delimited single-precision floating point numbers.

Figure 3 shows a simple test data file in ALADDIN format, including spectral line excitation data represented using the form due to Mewe and a simple function represented using the linearly interpolated TAB1D tabular data form[3]. The actual ALADDIN data file also allows for a comment section at the beginning of the file, as shown, before the first data entry denoted by occurence of the $ character. This figure hopefully makes clear how simple, in practice, it is to make up an ALADDIN labeling scheme and start using data in ALADDIN form. For further discussion, and standardized labeling schemes, please refer to the IAEA ALADDIN publications[2,3].

ALADDIN SUPPORTING SOFTWARE

ALADDIN supporting software is intended to provide the functionality essential to allow new users to rapidly incorporate ALADDIN into their work. At the present, this consists of a set of FORTRAN 77 routines, conceptually divided into two

ALADDIN DATA FORMAT

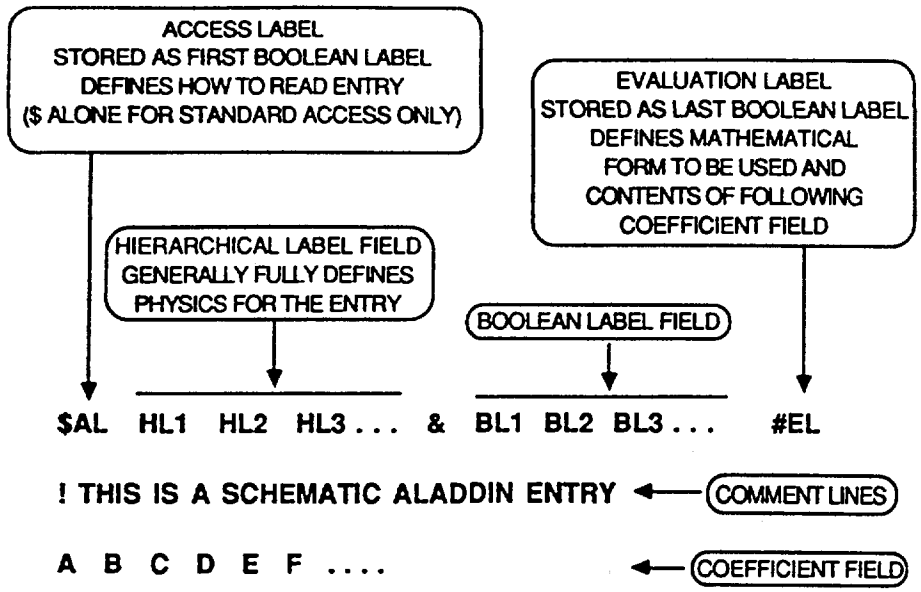


Fig. 2

SIMPLE ALADDIN DATA FILE EXAMPLE

```
THIS IS A TEST DATA FILE FOR ALADDIN, WITH #MEWE AND #TAB1D DATA
$ SLEXR  8 3  703.36  & RAH/PPPL #MEWE
703.36  0.0  0.18   1.0   0.6    0.0    0.0    0.28
$ SLEXR  8 4  790.36  & RAH/PPPL #MEWE
790.36  0.0  0.15   1.0   0.6    0.0    0.0    0.28
$ SLEXR  8 8  18.97  & RAH/PPPL #MEWE
18.97  0.0  0.4162  1.0    0.04   0.21   -0.04   0.28
$ SLEXR  8 8  102.5  & RAH/PPPL #MEWE
! THIS IS A COMMENT LINE IN THE FOURTH ENTRY
0.0  774.37  0.0791  0.1100  0.27   0.08   0.0    0.28
$ SLEXR  26 24  192.1  & FEXXIV RAH/PPPL #MEWE
192.1   0.0  0.0478  1.0    0.6848  0.9652  -0.4783  0.28
$ SLEXR  26 24  255.2  & FEXXIV RAH/PPPL #MEWE
255.2   0.0  0.0177  1.0    0.6648  0.9652  -0.4783  0.28
$ TEST  #TAB1D
0.0 0.0  100.0 100.0  200.0 100.0
```

Fig. 3

functional groups: the ALADDIN interactive code, and the ALPACK subroutine package.

The ALADDIN interactive code provides a basic interactive data searching, display, and manipulation capability from the user's terminal. It is a command-based program, which can be installed on a wide variety of hardware, requiring only a true FORTRAN-77 compatible compiler. The user specifies the hierarchical and boolean labels to be searched for in a given ALADDIN data file, and the ALADDIN interactive program will sequentially search through the data file until a matching data entry is found. The search strings include "wild cards" and other constructs to provide a flexible searching capability. Once found, data entries can be displayed to the terminal, and the data function (fitting function) can be evaluated at specified points (energies, temperatures, etc.) with the resulting data values (cross sections, rate coefficients, etc.) displayed to the screen or written to a file. On-line access to documentation describing not only the ALADDIN data files but also other ALADDIN nomenclature, fitting forms, references to the literature, etc., can also be accessed on-line from the ALADDIN interactive program by asking for keyword searches in

associated ALADDIN dictionary files. A list of the present ALADDIN interactive code command set indicates the code's basic, straightforward approach:

H, {C/R}	HELP (SHOW THIS COMMAND SUMMARY)
{LABEL}?	QUERY THE ALADDIN DICTIONARY ABOUT {LABEL}
SL, L	SEARCH LABELS (DEFINE NEW SEARCH LABELS)
S	SEARCH FOR NEXT MATCHING ENTRY
G##	GO TO ENTRY AT SPECIFIED SEQUENCE NUMBER
N	NEXT (GO TO NEXT SEQUENTIAL ENTRY NUMBER)
D{FEL!CS*}	DISPLAY TO TERMINAL ITEM(S) SPECIFIED BY SUFFIX CHARACTER(S): Files, Entry, Labels, !comments, Coefficients, Search labels, *all display fields
WR	WRITE CURRENT ENTRY TO OUTPUT ALADDIN FILE
EV	EVALUATE FITTED DATA POINTS FOR CURRENT ENTRY
R	REWIND INPUT ALADDIN DATA FILE
F	FILE (SELECT INPUT ALADDIN DATA FILE)
OF	OUTPUT FILE (SELECT WR COMMAND OUTPUT FILE)
EF	EV FILE (SELECT EV COMMAND OUTPUT DATA FILE)
QF	QUERY FILE (SELECT QUERY DICTIONARY FILE)
EX, EN	EXIT OR END ALADDIN

The ALPACK subroutine package provides a simple interface to ALADDIN data files for user's applications codes, as shown in Fig. 4. ALPACK reproduces the same basic search capability as the on-line ALADDIN interactive code, but now via subroutine calls from the user's code. Successive data entries are read in using ALREAD. The desired hierarchical and boolean search label sequences (again, with possible wild card constructs) are passed to the ALCOMP subroutine, which compares these with the entry header, flagging successful matches. The label and coefficient field information from the ALADDIN entry are then available in COMMON blocks for use by the calling code. The subroutine ALRECF provides conversion of standard (default) coefficient field data from character strings to real (floating point) values which are then passed to the appropriate evaluation subroutine.

It is not possible or desirable to present here a comprehensive user's manual describing the entire evolving ALADDIN system in detail. For this purpose, the reader is encouraged to consult the references at the end of this paper, and contact the IAEA Atomic and Molecular Data Unit, Vienna, Austria, which will be coordinating ALADDIN development and distribution of ALADDIN software and data files.

ROLE OF THE INTERNATIONAL ATOMIC ENERGY AGENCY (IAEA)

ALADDIN was adopted as the standard IAEA atomic and molecular data format for MFE applications at Consultant's meeting of the IAEA Atomic and Molecular Data Unit[2] in May, 1988. Continued IAEA coordination of ALADDIN development is planned so as to ensure the organized, effective growth of the ALADDIN system.

This coordinating role will occur at several levels. First, the IAEA Atomic and Molecular Data Unit will continue to provide international coordination of atomic physics efforts towards providing comprehensive, critically evaluated ALADDIN data sets, particularly for MFE applications. Already, a wide range of international MFE atomic data centers have adopted the ALADDIN system as a standardized format for communication of their atomic physics data. The IAEA also will act to provide standardized ALADDIN labeling schemes for a wide range of atomic, molecular, and surface physics data, as well as standardized ALADDIN software development, documentation and distribution[3].

SUMMARY

ALADDIN is designed to provide a basic, broadly-based standard system for the exchange and management of atomic data. To meet this goal of a universal data format, highest priority has been placed on a system which is straightforward to use, highly flexible, and widely transportable.

The ALADDIN system consists of several elements. Most fundamentally, ALADDIN defines a basic data format, based on ASCII data files, which allows a wide variety of data types to be flexibly accomodated within a common structure based on self-describing data entries, associated subroutine libraries and "dictionary" documentation files. Supporting software provides access to ALADDIN files both interactively and from user's codes.

ALADDIN has been adopted as the standard international atomic data format by the IAEA Atomic and Molecular Data Unit for MFE applications. The IAEA is

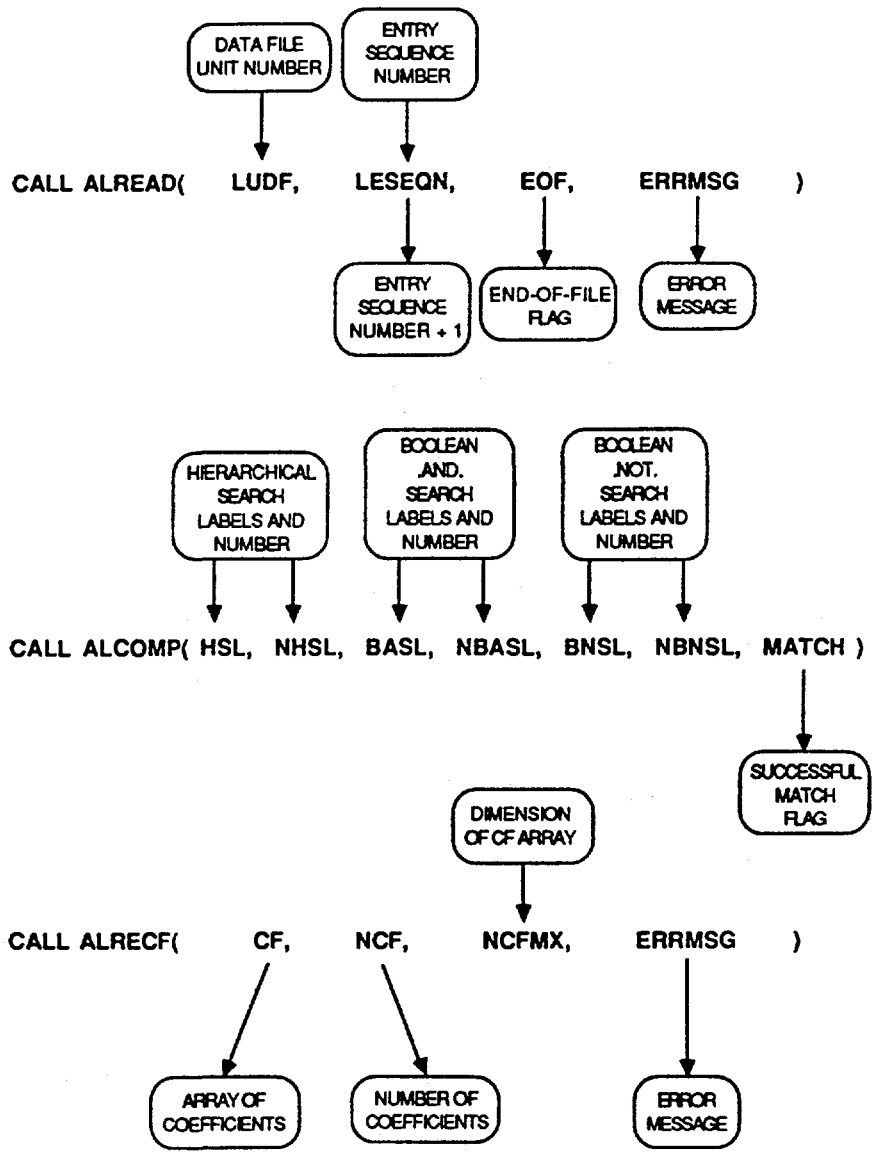


Fig. 4

providing continued coordination of ALADDIN labeling conventions, system development and the provision of recommended data. ALADDIN-based atomic physics data compilations and data exchange are now becoming broadly established in the MFE community, and can be profitably extended for use in other applications.

New ALADDIN users and contributors are strongly encouraged!

ACKNOWLEDGEMENTS

The rationale for the ALADDIN system arises from the need to deal with the large body of diverse atomic physics data required for MFE and other research programs. The existence and continued development of this body of data is, of course, due to the efforts of many theoretical and experimental atomic physicists. It is to be hoped that, in return for their efforts, ALADDIN will provide them with the satisfaction of even more widespread and fruitful application of the results of their research. The efforts of R. Janev and J. Smith at the IAEA have been and continue to be crucial to realizing the international coordination of MFE atomic physics data base development in general and ALADDIN in particular. Particular thanks for discussions, encouragement, and ALADDIN beta testing go to R. Phaneuf at ORNL.

This work was supported by U.S. DoE contract # DE-AC02-76-CHO-3073.

REFERENCES

(1) R.A. Hulse, "ALADDIN - A Labeled Atomic Data Interface for Fusion Applications", to be submitted for publication. (see also presentation in reference 2)
(2) "IAEA Consultant's Meeting on the Atomic Database and Fusion Applications Interface", May 9-13, 1988, Vienna, Austria, IAEA Summary Report INDC(NDS)-211/GA, Sept. 1988.
(3) "ALADDIN Manual, Version 1.0", IAEA Atomic and Molecular Data Unit report IAEA-NDS-AM-17, Vienna, Austria, June 1989.

CURRENT ACTIVITIES AT LOS ALAMOS

R. E. H. Clark and J. Abdallah, Jr.

Data Available in ALADDIN Format

Ti - All Ionization stages

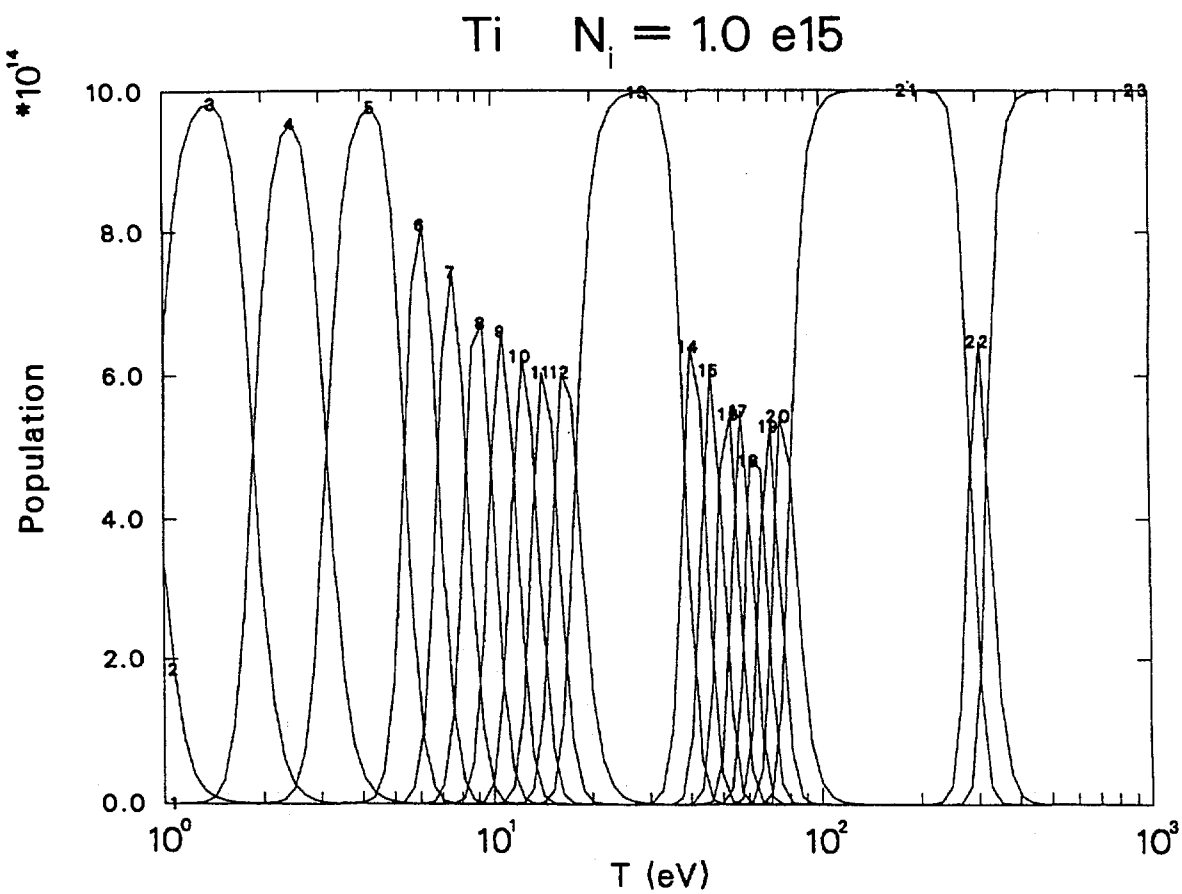
B III

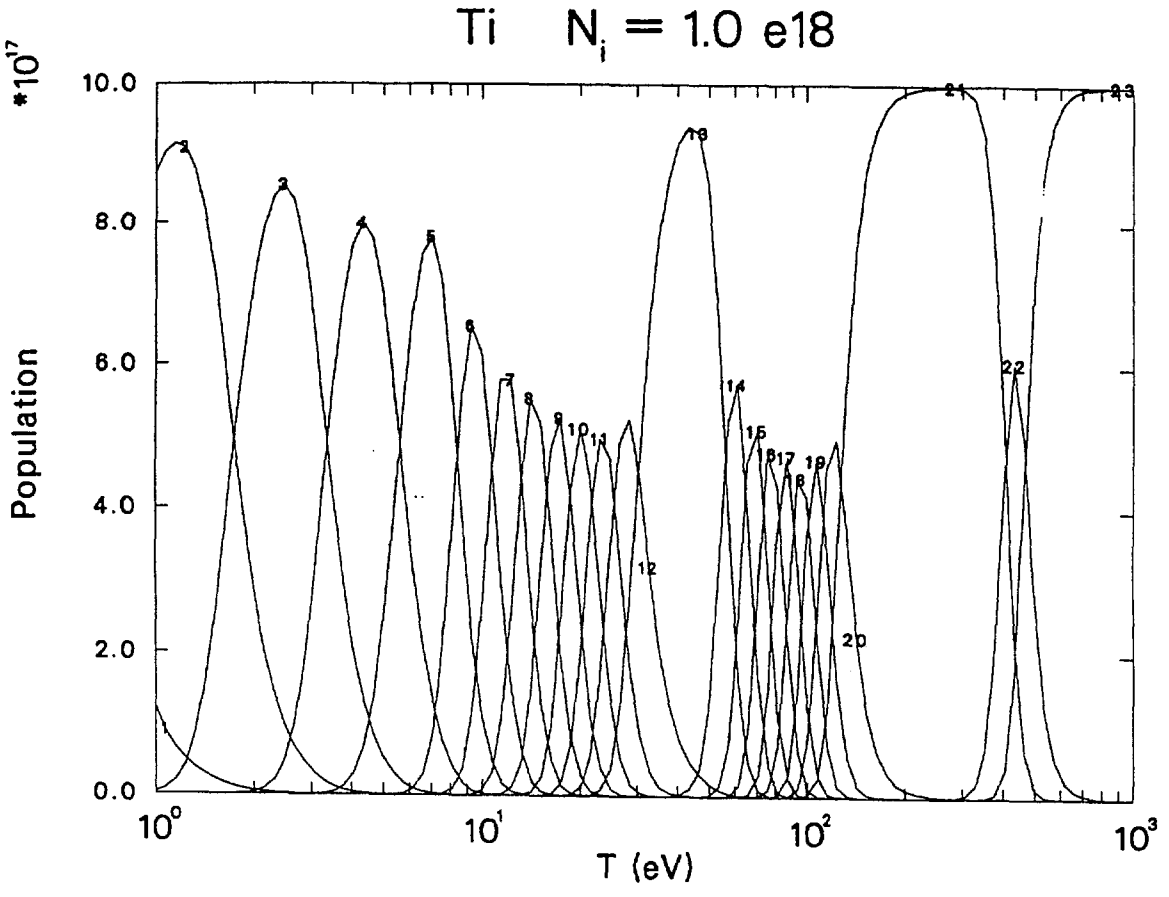
C III

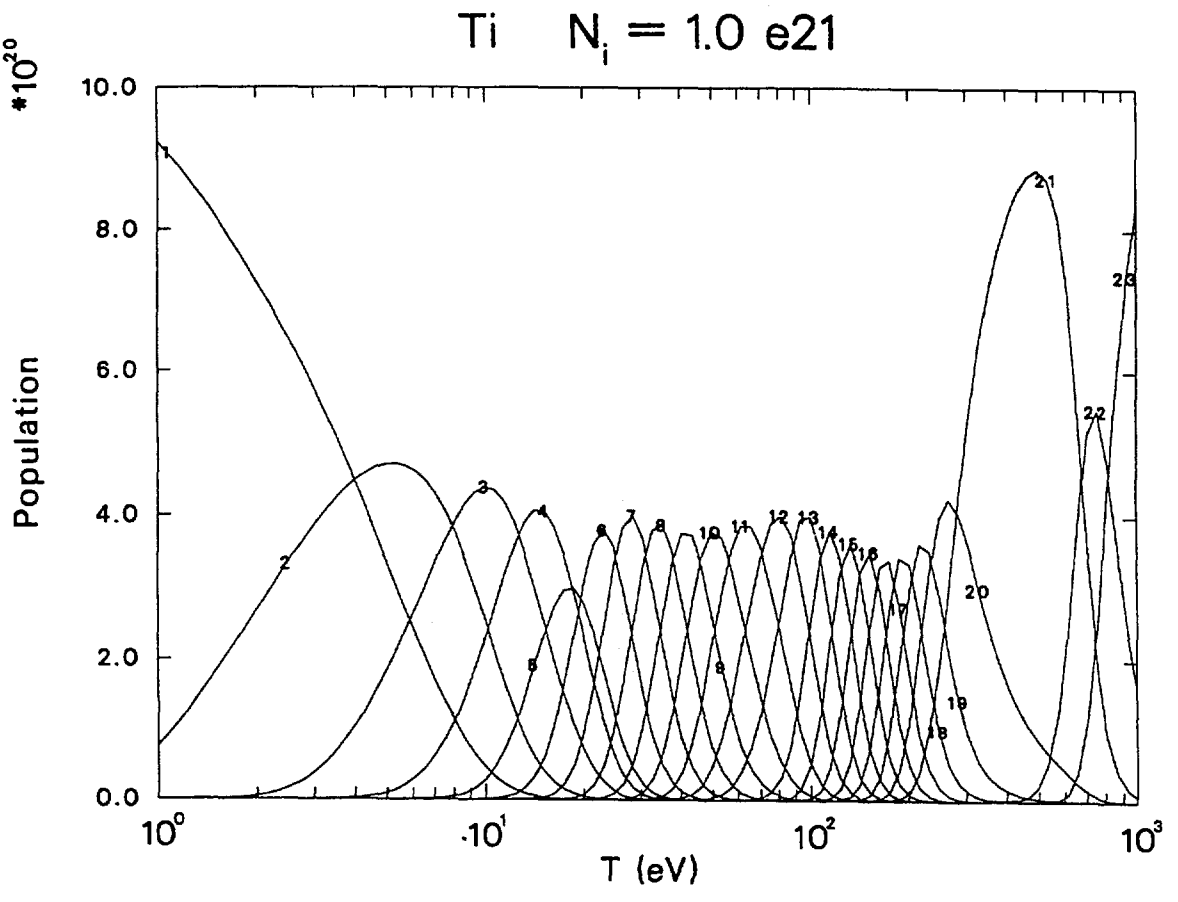
	n - n'	Number of Transitions
C III	2 - 4	52
	2 - 5	68
	3 - 3	221
	4 - 4	72
	4 - 5	252
B III	2 - 2	2
	3 - 3	8
	4 - 4	18
	5 - 5	32

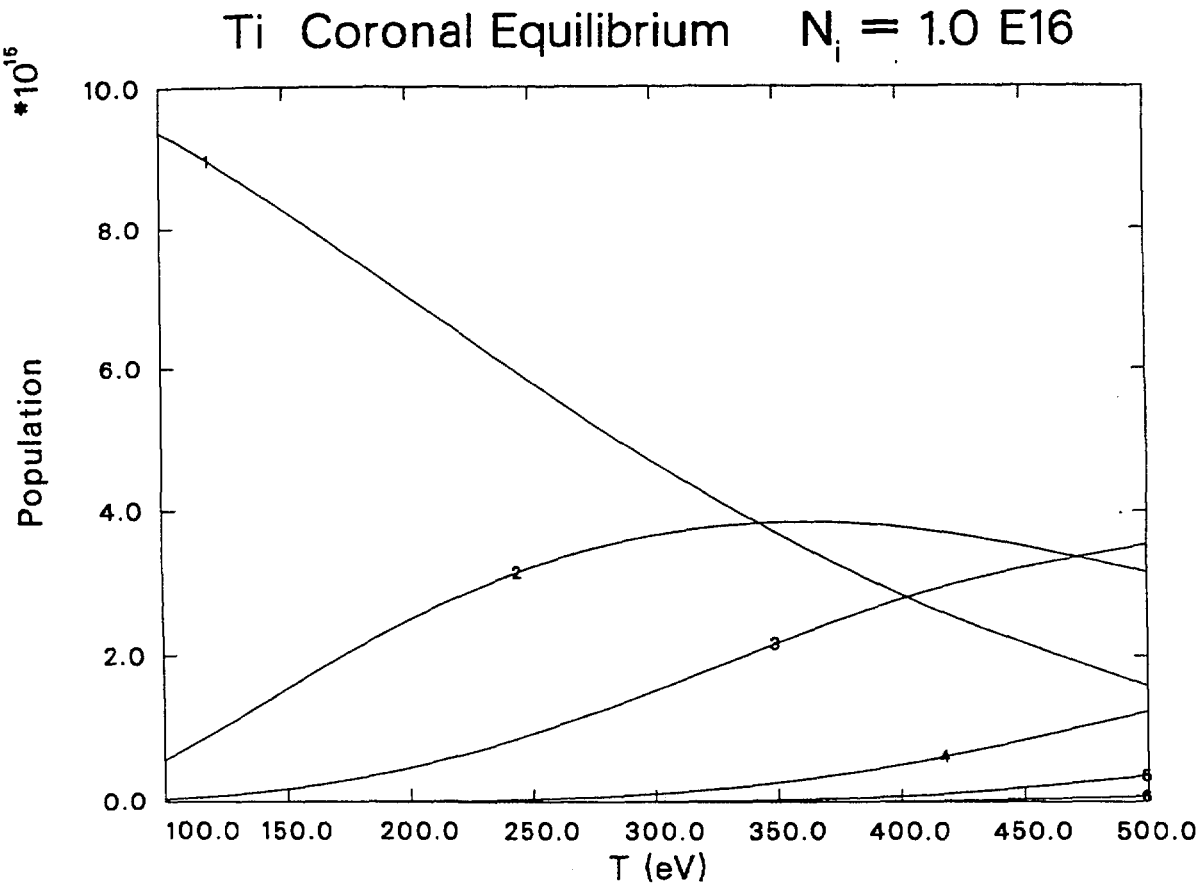
Table I. Number of configurations, collisional excitations, autoionization rates and oscillator strengths calculated for each ion stage.

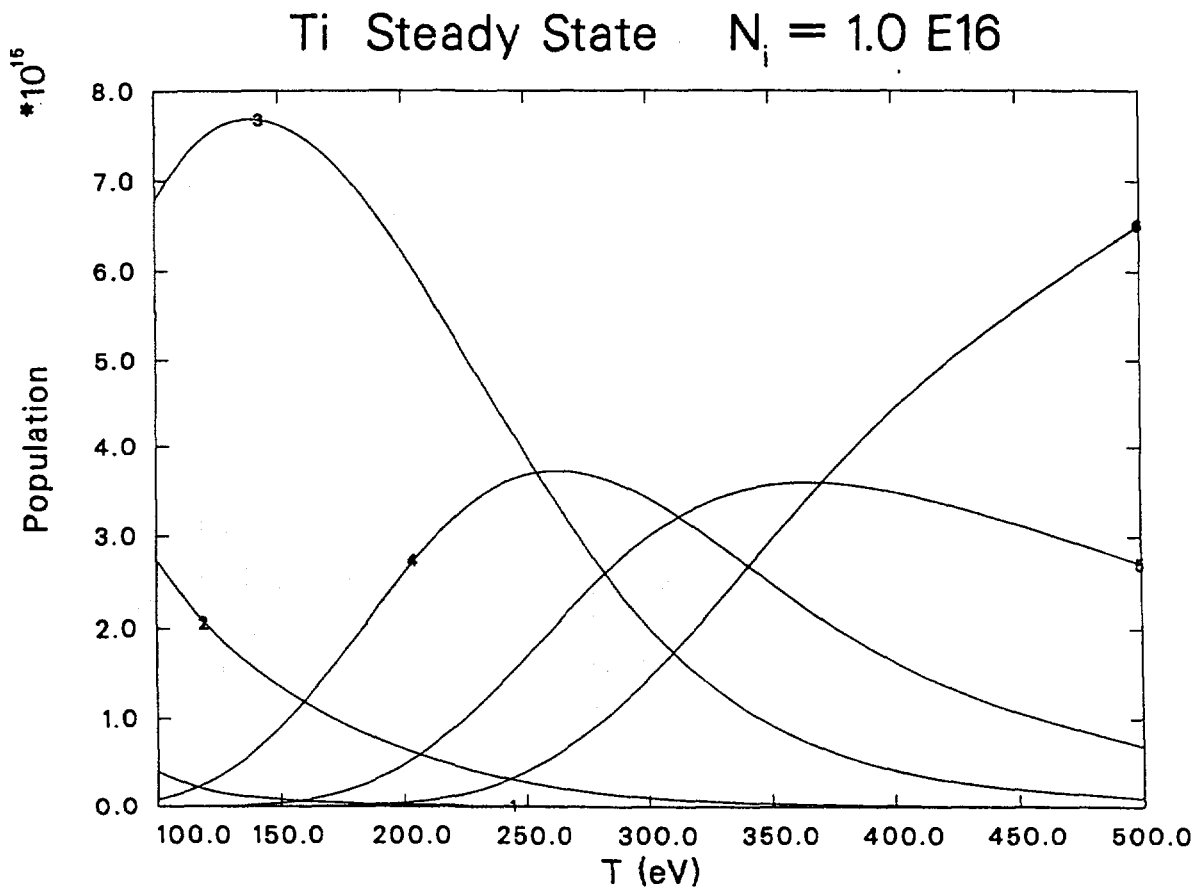
Ionization Stage	Number of Configurations	Number of Excitations	Number of Autoionizations	Number of gf
1	233	35	1609	1015
2	195	38	1054	834
3	825	59	10278	4950
4	780	59	8511	4698
5	546	50	5128	3141
6	590	54	5279	3546
7	594	54	5017	3575
8	594	54	4867	3575
9	594	54	4610	3575
10	539	54	3650	3180
11	309	44	1615	1602
12	246	47	1176	1262
13	427	36	2051	2460
14	453	38	2439	2715
15	455	38	2430	2730
16	455	38	2408	2730
17	455	38	2314	2730
18	377	38	1811	2190
19	209	26	808	1060
20	119	27	366	596
21	120	14	366	600
22	15	14	0	40

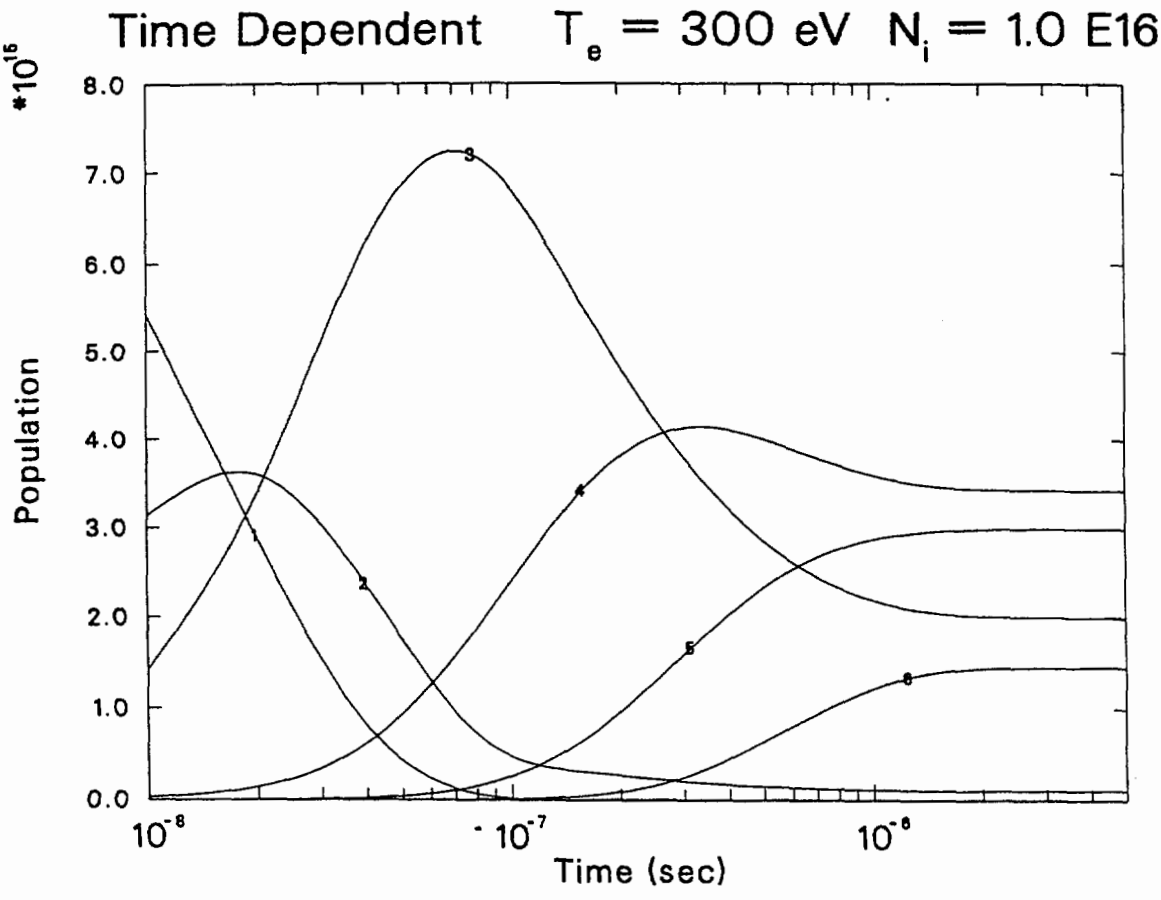


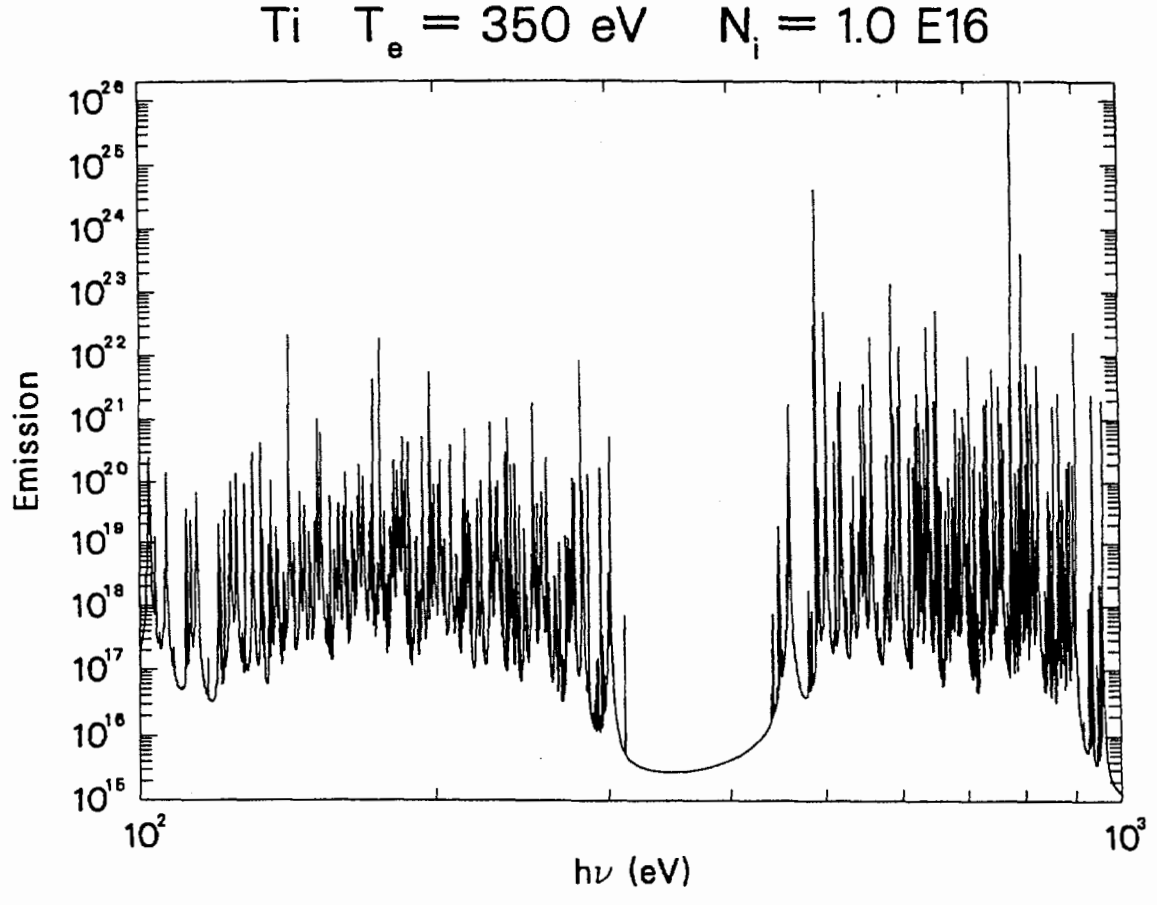

Ti N$_i$ = 1.0 e18
*10^{17}
Population
T (eV)


Ti N$_i$ = 1.0 e21
*10^{20}
Population
T (eV)

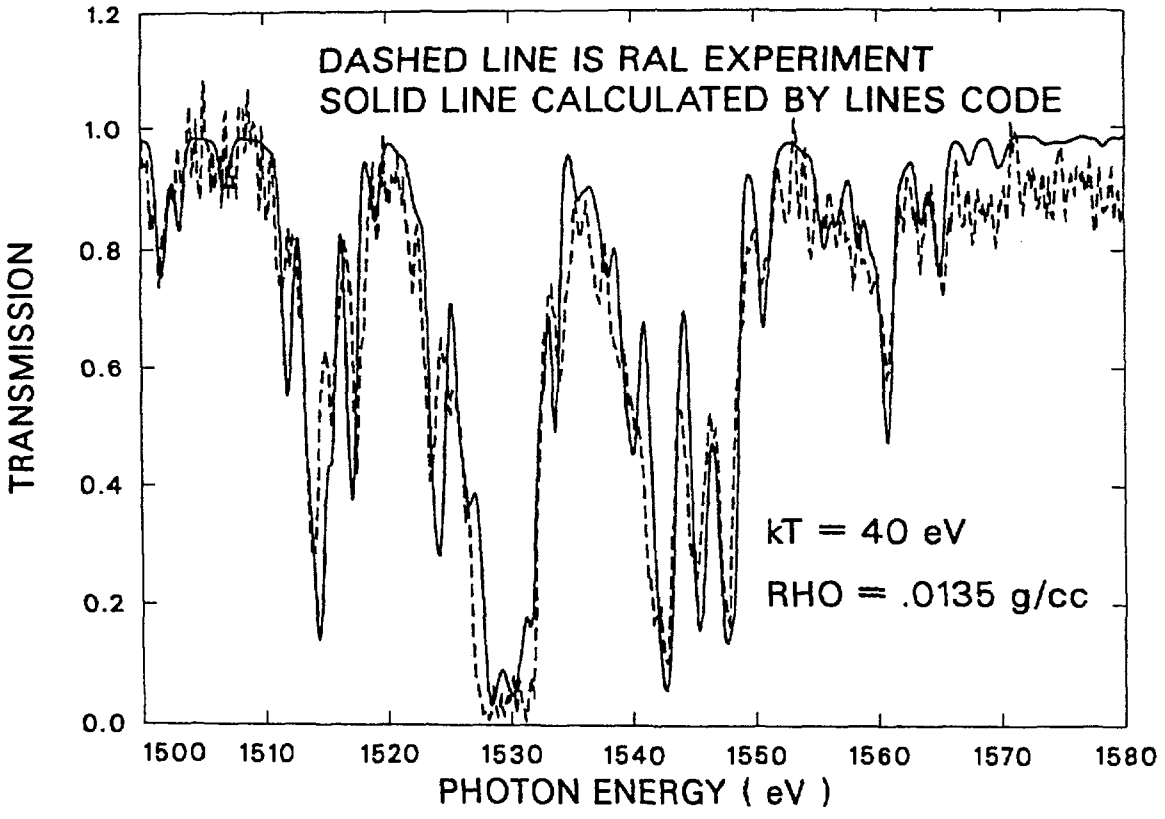

Ti Coronal Equilibrium N_i = 1.0 E16
*10^15
Population
10.0
8.0
6.0
4.0
2.0
0.0
100.0 150.0 200.0 250.0 300.0 350.0 400.0 450.0 500.0
T (eV)
1
2
3
4
5
6


Ti Steady State N_i = 1.0 E16
*10^15
Population
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
100.0 150.0 200.0 250.0 300.0 350.0 400.0 450.0 500.0
T (eV)
1
2
3
4
5
6


Time Dependent T_e = 300 eV N_i = 1.0 E16
*10^15
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Population
1
2
3
4
5
6
10^-8
10^-7
10^-6
Time (sec)


Ti T_e = 350 eV N_i = 1.0 E16
10^26
10^25
10^24
10^23
10^22
10^21
10^20
10^19
10^18
10^17
10^16
10^15
Emission
10^2
10^3
hν (eV)

ALUMINUM X-RAY TRANSMISSION



HIERARCHICAL LABELS

CONFIGS

TERMS

LEVELS

GF

PHOTION

AUTOION

BRAT

```
  Configuration #   1
Shell       Energy(eV)
1s2         8.5690000e+03
2s2         1.9459000e+03
Total configuration energy(eV) =  -2.2109530e+04

  Configuration #   2
Shell       Energy(eV)
1s2         8.5283000e+03
2p2         1.8733000e+03
Total configuration energy(eV) =  -2.1977051e+04

  Configuration #   3
Shell       Energy(eV)
1s2         8.5483000e+03
2s1         1.9491000e+03
2p1         1.8897000e+03
Total configuration energy(eV) =  -2.2053140e+04



Listing of LS-terms
 Index   Energy(eV) Configuration
   1   -6.5957e+00  ( 2s2   1S)  1S
   2    4.6538e+01  ( 2s1   2S)  2S  ( 2p1   2P)  3P
   3    8.5950e+01  ( 2s1   2S)  2S  ( 2p1   2P)  1P
   4    1.2323e+02  ( 2p2   3P)  3P
   5    1.4326e+02  ( 2p2   1D)  1D
   6    1.6844e+02  ( 2p2   1S)  1S
```

Listing of fine structure energy levels

Index	J	Energy(eV)	Configuration						
1	0.0	-6.5957e+00	(2s2	1S)	1S				
2	0.0	3.6572e+01	(2s1	2S)	2S	(2p1	2P)	3P
3	1.0	4.0541e+01	(2s1	2S)	2S	(2p1	2P)	3P
4	2.0	5.2129e+01	(2s1	2S)	2S	(2p1	2P)	3P
5	1.0	8.5950e+01	(2s1	2S)	2S	(2p1	2P)	1P
6	0.0	1.1200e+02	(2p2	3P)	3P			
7	1.0	1.2095e+02	(2p2	3P)	3P			
8	2.0	1.2684e+02	(2p2	3P)	3P			
9	2.0	1.4326e+02	(2p2	1D)	1D			
10	0.0	1.6844e+02	(2p2	1S)	1S			

Mixing for level with j, energy(eV) = 0.0 -6.5957e+00

Coefficient	Basis state		
9.8008e-01	(2s2	1S)	1S
2.3430e-02	(2p2	3P)	3P
1.9720e-01	(2p2	1S)	1S

Wavelength(nm)	Energy(eV)	gf	Index1	Index2
2.6304e+01	4.7136e+01	1.7674e-03	1	3
1.3397e+01	9.2546e+01	1.5445e-01	1	5
1.7349e+01	7.1464e+01	5.6051e-02	3	6
4.7587e+01	2.6055e+01	9.3264e-04	5	6
9.6940e+00	1.2790e+02	2.5377e-04	3	10
1.5030e+01	8.2490e+01	1.0497e-01	5	10
1.4694e+01	8.4376e+01	6.4364e-02	2	7
1.5420e+01	8.0407e+01	4.4769e-02	3	7
3.5427e+01	3.4998e+01	5.3662e-04	5	7
1.8016e+01	6.8819e+01	6.5621e-02	4	7
1.4367e+01	8.6296e+01	8.4551e-02	3	8
3.0324e+01	4.0887e+01	3.0209e-02	5	8
1.2070e+01	1.0272e+02	5.1795e-03	3	9
2.1633e+01	5.7314e+01	1.7186e-01	5	9
1.6596e+01	7.4708e+01	1.5655e-01	4	8
1.3605e+01	9.1135e+01	6.9726e-02	4	9

Enhancements for Version 1.1 of ALADDIN

J.J. Smith

At the last data center meeting a number of proposals were made for improvements to the first version, 1.0, of ALADDIN distributed by the A+M Data Unit. The scope of the improvements was defined in the presentation of Dr. Hulse, "Future Development of the ALADDIN system", which was presented at the last Data Centre Network meeting. The two basic areas for improvements are:

1. Functional Changes to ALADDIN

   These can be summarized as:

   a) Inclusion of searching procedure for numeric values and the introduction characters in search labels.
   b) The re-introduction of the "Ev" command to generate simple tables of values on linear or logarithmic grids from evaluation function. The current "Ev" command which generates linearly interpolable tables was to be redefined as a new "LT" command.
   c) Specification of non-standard access label "$D" for entries containing coefficients in double precision.
   d) Modification of the output format for table of values generated from the "Ev" and "LT" command.

2. Provision of Labelling Schemes and Dictionaries for Classification of Spectroscopic and Surface Interaction Data

   a) For large data sets or bases of spectroscopic data a scheme for classification and labelling has been defined by Dr. Clark, and this scheme provides for a consistent format for indexing the basic configurations, terms and levels which can then be reffered scheme has been used to store an extensive database for atomic structure and collisional data for photon and electron collision, including a complete database for e^- and hv collisions with all ionization stage of Ti.
   b) A labelling scheme for the classification of surface interaction data was presented at the last data centre meeting from proposals of Janev and Thomas. This format has been used to store and work with sputtering and reflection data in the IAEA A+M data unit.

Searching

- Add search on numerical value of a label in addition to character string match
  - necessary for searching continuous variables used as hierarchical labels, such as wavelengths, energies, etc.
  - new search will work on any hierarchical labels which are "clean" numbers without added characters, etc.
  - search "label" construct will test for a numeric match over a range between values a and b

    =a,b match hierarchical label value between values a and b

  - logical defaults for common special cases

    =a equal to a
    =,b less than or equal to b
    =a, greater than or equal to a

  - non-numeric labels will just give "no match", not an error
- Add substring single character wild card (ABCD?FGH)

Define access label $D to flag double precision coefficients as a special coefficient data field

- Use ALDPCF instead of ALRECF to convert the coefficient field
- Values read into new double precision coefficient array DCF rather usual single precision array CF
- Fitting function routines for double precision fits should use double precision only for coefficients
  - no physical quantity known well enough to require double precision
- Modify ALEV1D to have both CF and DCF arrays, use of DCF flagged by $D
- $D also acts as flag also to allow printout format to be altered for double precision values
  - remove FEXTN flag added to IAEA v1.0

```
C                ********************************
C                * ALTAB AND SUPPORTING ROUTINES *
C                ********************************
C  ..... ..........................................................
C-----    BLOCK FOR EVALUATION FUNCTIONS WITH NON-BLANK (EXCLUDING '$D')
C-----                      ACCESS LABELS.
C
C     FOR ALL EVALUATION FUNCTIONS WITH NON STANDARD ACCESS LABELS
C     (EXCLUDING THE SPECIAL '$D' ACCESS LABEL), THE CALL TO THE ROUTINE
C     FOR HANDLING THE INTERACTIVE DIALOG MUST BE INCLUDED IN THE
C
      IF (BL(NBL) .EQ. '#'.AND. BL(1) .EQ. '$TABSPY') THEN
        CALL RTABSPY
      ELSE
C
C-----      BLOCK FOR EVALUATION FUNCTIONS WITH BLANK AND '$D'
C-----                      ACCESS LABELS.
C
C     FOR ALL EVALUATION FUNCTIONS WITH BLANK ACCESS LABELS (SINGLE
C     PRECISION COEFFICIENTS) OR '$D' ACCESS LABEL (DOUBLE PRECISION
C     COEFFICIENTS) READ THE APROPRIATE COEFFICIENTS INTO ARARAY CF
C     OR DCF.
C
C       RETREIVE NUMERIC COEFFICIENTS FOR THIS FUNCTION THE COEFFICIENTS
C       ARE SINGLE PRECISON NUMBERS
C
        IF(BL(1) .EQ. '$') THEN
          CALL ALRECF(CF, NCF, NCFMX, ERRMSG)
          NDCF = 0
        ELSE IF(BL(1) .EQ. '$D') THEN
          CALL ALDPCF(DCF, NDCF, NCFMX, ERRMSG)
          NCF = 0
C
          ELSE
C
C          CATCH-ALL ENTRIES WITH NON-BLANK OR NON-'$D' ACCESS LABELS
C
           WRITE(LUTOUT,
     &       '(/'' ERROR - ACESS LABEL MUST BE BLANK OR ''$D'' '')')
           RETURN
          ENDIF
C
        IF (ERRMSG .NE.  ' ') THEN
          WRITE(LUTOUT, '(/1X,A)') ERRMSG
          RETURN
        ENDIF

C       RETREIVE NUMERIC COEFFICIENTS FOR THE FUNCTION. THE COEFFICIENTS
C       ARE SINGLE PRECISON NUMBERS
C
         IF(BL(NBL) .EQ. '#MEWE') THEN
          CALL RMEWE
C------
         ELSE IF(BL(NBL) .EQ. '#BELI') THEN
          CALL RBELI
C------
         ELSE IF(BL(NBL) .EQ. '#CHEB') THEN
          CALL RCHEB
    ..............................................
    ..............................................
C------
        ELSE IF(BL(NBL) .EQ. '#TAB1D') THEN
          CALL RTAB1D
C------
```

Example of Subroutine to Control the Handling of an Interactive Dialog for Evaluation Function ALCHEB.

```
C
C#####################################################################
C
      SUBROUTINE RCHEB
C
      EXTERNAL ALCHEB
C
      INCLUDE 'ALPCOM.FOR'
C
      INCLUDE 'ALCOM.FOR'
C
      LOGICAL ALCIEQ
      EXTERNAL ALCIEQ
      DIMENSION XRANGE(10)
C
      WRITE(LUTOUT, '(/'' ORNL:CFADC CHEBYSHEV POLYNOMIAL FIT'')' )
C
C      CHECK NUMBER OF SINGLE PRECISION COEFFICIENTS
C
      IF(NCF .NE. 11) THEN
        WRITE(LUTOUT, '(/'' INCORRECT NUMBER OF COEFFICIENTS )'')')
        RETURN
      ENDIF
      WRITE(LUTOUT, '(/'' (INPUT VALID RANGE FROM'',
     &     1PE10.2, '' TO'', 1PE10.2, '')'')' ) CF(10), CF(11)
C
C      INCLUDE CODING TO CHOICE BETWEEN TABLE OUTPUT TYPES
C
      IF(ALCIEQ(CMND(1:2),'EV')) THEN
        CALL ALEV1D(ALCHEB)
      ELSE
        CALL ALREVD(PERUNC,XRANGE(1),XRANGE(2))
        IF (PERUNC .EQ. 0.0) RETURN
        NRANGE=1
C
        CALL ALTB1D(PERUNC,ALCHEB,NRANGE,XRANGE)
C
      ENDIF
C
      RETURN
```

```
      SUBROUTINE ALCHEB(PET, PCF, KNCF, PDCF, KNDCF, PFIT, KERMSG)
C
C     THIS IS AN ORNL:CFADC SUBROUTINE TO CALCULATE CROSS SECTIONS IN
C     (cm[2]) VERSUS ENERGY IN (EV/AMU) OR RATE COEFFICIENTS IN
C     (cm[3]/s) VERSUS MAXWELLIAN TEMPERATURE IN (eV) FROM CHEBYSHEV
C     POLYNOMIAL FITTING COEFFICIENTS
C
C     THESE FITS ARE VALID ONLY BETWEEN THE LIMITS EMIN AND EMAX,
C     WHICH ARE COEFFICIENTS PCF(10) AND PCF(11) IN THE ENTRY DATA FIELD
C
C     PET = COLLISION ENERGY IN eV/amu OR MAXWELLIAN TEMPERATURE IN eV
C
C     KERMSG = BLANK IF NO ERRORS
C
C     PFIT = CROSS SECTION IN cm[2] OR RATE COEFFICIENT IN cm[3]/s
C
C     WRITTEN BY H. HUNTER, CFADC OAK RIDGE NATIONAL LABORATORY
C-----------------------------------------------------------------------
C     SINGLE PRECISION COEFFICIENTS MUST BE SUPPLIED IN ARRAY PCF
C=======================================================================
C
      REAL PET, PCF, PFIT
      REAL EMIN, EMAX, CHEB, EMINL, EMAXL, ENL, XNORM
      REAL TWOX, PREV, PREV2
C
      DOUBLE PRECISION PDCF
      DIMENSION PCF(KNCF), PDCF(KNDCF)
C
      CHARACTER*(*) KERMSG
C
      EMIN = PCF(10)
      EMAX = PCF(11)
      IF(PET .GE. EMIN .AND. PET .LE. EMAX) THEN
        KERMSG = ' '
      ELSE
        KERMSG = 'OUTSIDE RANGE OF FIT IN ALCHEB'
        RETURN
      ENDIF
C
C     CALCULATE POLYNOMIAL USING RECURSION RELATION
C
      K = 9
      CHEB = PCF(K)
      EMINL = LOG(EMIN)
      EMAXL = LOG(EMAX)
      ENL= LOG(PET)
      K = K-1
      XNORM = (ENL-EMINL-(EMAXL-ENL)) / (EMAXL-EMINL)
      TWOX = 2.0 *  XNORM
      PREV2 = 0.0
   10 PREV = CHEB
      IF(K .NE. 1) THEN
        CHEB = PCF(K) + TWOX*PREV - PREV2
        PREV2 = PREV
        K = K-1
        GO TO 10
      ENDIF
      CHEB = 0.5*PCF(1) + XNORM*PREV - PREV2
      PFIT = EXP(CHEB)
  100 RETURN
      END
```

Reinstate original "EV"-style linear / log data points for quick access to data values

- Provides needed fast, simple output of data values at fixed number of points
- Modify file output format slightly or ease of use by other codes
  - ! flags comment lines
  - # flags new line giving number of lines and columns for input "DO" loop
  - * flags line with column headers
  - use evaluation label as data column header
  - setup header for easy copy/paste for Macintosh
- Example of modified format

```
Test ev command output file
!
# 10  2
*          INPUT              #MEWE

 1     1.000000E+00       8.158804E-09
 2     1.111111E+00       7.890224E-09
 3     1.222222E+00       7.652079E-09
 4     1.333333E+00       7.438783E-09
 5     1.444444E+00       7.246118E-09
 6     1.555556E+00       7.070816E-09
 7     1.666667E+00       6.910307E-09
 8     1.777778E+00       6.762531E-09
 9     1.888889E+00       6.625819E-09
10     2.000000E+00       6.498793E-09
```

Table 1. Classes of *PSI collisions

(defined by type of the projectile and state of the surface)

1. e + surface
2. e + adsorbate + surface
3. atom + surface
4. atom + adsorbate + surface
5. Molecule + surface
6. Molecule + adsorbate + surface
7. Photon + surface
8. Photon + adsorbate + surface

In this notation atom (molecule) represents atom (molecule) or atomic (molecular) ion.

Table 2. Categories of PSI processes

(defined by fate of projectile or kind of observed particle)

1. Particle adsorption (sticking) penetration
2. Penetration (Range, Energy Loss)
3. Particle trapping, retention and release (detrapping)
4. Particle desorption (including thermal)
5. Particle backscattering (reflection)
6. Secondary electron emission (particle induced)
7. Sputtering (including physical, physics-chemical, chemical, and enhanced sublimation)
8. Composite PSI processes

* PSI = particle-surface interaction

B. PROCESS LABELS

Table 3. Categorization and Labelling of Particle-Surface Collision Processes

	1.	Class of collision
(*)	2.	Type of collision
(*)	3.a	Chemical symbol of projectile
(*)	3.b	Charge state of projectile
(* *)	3.c	Quantum state of projectile
(*)	4.a	Chemical symbol of target
(*)	4.b	Aggregation state of target
(*)	5.a	Chemical symbol of substrate
(*)	5.b	Aggregation state of substrate
		---------- (collision)
(*)	6.a	Chemical symbol of observed species
(# *)	6.b	Charge state of observed species
(* *)	6.c	Quantum state of observed species
(*)	6.d	Aggregation state of observed species
(*)	7.a	Chemical symbol of target
(*)	7.b	Aggregation state of target

Notes: (1) Labels marked * are mandatory.
(2) Aggregation state is either:
(a) Surface (or solid) - surf.
(b) Adsorbed - ads.
(c) Trapped - trap.
(3) Labels for charged (# *) and quantum states (* *) are added when necessary to specify a particular reaction channel. These should follow the scheme for atomic collision data.
(4) In many cases the charge and quantum state of the observed species may not be known (as for example in total sputtering).
(5) Sections 4 and 5 are both required only if the problem involves one species adsorbed on another. In most cases there is only a single target situation and 5 is omitted.
(6) The post collision situation lists first, as item 6, the observed species, which is not necessarily the projectile. This will differ from the atomic data case.
(7) The final entry 7 is listed only for completeness and is the target material (or substrate underlying an adsorbate). It should be the same as item 4 is an adsorbate). In general item 7 is undefined in the specification of data and is redundant.

(8) Entry 3 is always the incident particle when is a free atom, ion or electron. The entry 6 is always the observed species and this is normally also a free atom, ion or electron.

Table 4. Dictionary of Collision Processes

No.	Process	Abbreviation	Symbolic Notation
	Group A. Binary Processes Leading to Reflection of the Incident Species		
A.1.	Reflection of atoms - total	RAT	A+B(surf)→A+B(surf)
A.2.	Reflection of atoms - specific	RAE	A+B(surf)→A^*+B(surf)
A.3.	Reflection of atoms - specific	RAC	A+B(surf)→A^{k+}+B(surf)
A.4.	Dissociation of molecules and reflection	RMD	AB+C(surf)→A+B+C(surf)
A.5.	Reflection of atoms - energy distribution	RAENER	A+B(surf)→A+B(surf)
A.6.	Reflection of electrons - total	RET	e+B(surf)→e+B(surf)
A.7.	Reflection of electrons - energy distribution	REENER	e+B(surf)→e+B(surf)
	Group B. Binary Processes Leading to Ejection of the Target Species		
B.1.	Sputtering by atoms - total	SAT	A+B(surf)→B+B(surf)
B.2.	Sputtering by atoms leading to specific excited states	SAE	A+B(surf)→B^*+B(surf)
B.3.	Sputtering by atoms leading to specific charge states	SAC	A+B(surf)→B^{k+}+B(surf)
B.4.	Sputtering by atoms - energy distribution	SAENER	A+B(surf)→B+B(surf)
B.5.	Sputtering by electrons	SE	e+B(surf)→B+B(surf)
B.6.	Electron ejection by photons	EEP	hν+B(surf)→e+B(surf)
B.7.	Secondary electron ejection by atoms	SEA	A+B(surf)αe+B(surf)
B.8.	Secondary electron ejection by atoms energy distribution	SEAENER	A+B(surf)→e+B(surf)

4.1.3 Atomic Structure, Radiative Processes and Autoionization Processes

Atomic structure, radiative processes, and autoionization processes are needed in plasma modeling. All of this information is readily incorporated into the ALADDIN system. The hierarchical labeling is summarized in Table 6. The general scheme of labeling is similar to that described above. The inclusion of an integer index for each configuration, LS-term, and fine-structure energy level can be used in place of the full set of quantum numbers both in the radiative processes and in the collisional processes.

TABLE 6

ATOMIC STRUCTURE, RADIATIVE PROCESSES, AND AUTOIONIZATION PROCESSES

No.	Process	Hierarchical Label
S.1	Configuration average energies	CONFIGS
S.2	LS-term energies	TERMS
S.3	Fine Structure Level Energies	LEVELS
R.1	Bound-Bound Radiative Transitions	GF
R.2	Bound-Free Radiative Transitions	PHOTION
AI.1	Autoionization Rates	AUTOION
AI.2	Branching Ratios	BRAT

Table I. Number of configurations, collisional excitations, autoionization states and oscillator strengths calculated for each ion stage.

Ionization Stage	Number of Configurations	Number of Excitations	Number of Autoionizations	Number of gf
1	233	35	1609	1015
2	195	38	1054	834
3	825	59	10278	4950
4	780	59	8511	4698
5	546	50	5128	3141
6	594	54	5279	3546
7	594	54	5017	3575
8	594	54	4867	3575
9	594	54	4610	3575
10	539	54	3650	3180
11	309	44	1615	1602
12	246	47	1176	1262
13	427	36	2051	2460
14	453	38	2439	2715
15	455	38	2430	2730
16	455	38	2408	2730
17	455	38	2314	2730
18	377	38	1811	2190
19	209	26	808	1060
20	119	27	366	596
21	120	14	366	600
22	15	14	0	40

III. Evaluated Atomic Databases

A. A+M Collisional Databases

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

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, H_2 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 37830, USA (1987).

5. "Atomic and Molecular Data for Fusion, Part II - Recommended Cross Sections and Rates for Electron Ionisation 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).

6. "Recommended Data for Excitation Rate Coefficients of Helim Atoms and Helim-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, H_2, He and Li Atoms and Ions with Atoms and Molecules, Vol. 1. C.F. Barnett, (Editor). Report ORNL-6086/V1, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, 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).

Note: The above numerical data files are formatted in the ALADDIN database management system. The evaluated data and the ALADDIN system software and mannual are available on request, free of charge, from the IAEA Atomic and Molecular Data Unit. The data files can be provided on high or low density floppy diskettes or magnetic tape. The IAEA is also connected to the EARN-Bitnet network and requests for data can be sent to RNDS@IAEA1.

B. 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, Nagoya, Japan (1987).

2. "Energy Dependence of the Yields of Ion-Induced Sputtering of Montatomic 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, Nagoya, Japan (1988).

ITER PHYSICS R+D PROGRAMME 1991/92 AND BEYOND (UP TO 1995)

TASKS REQUIRING A+M AND PSI DATA INFORMATION

1. R+D AREA: POWER AND PARTICLE EXHAUST PHYSICS*

T A S K S

1) PH 1.1. Experimental exploration in hydrogenic background plasmas, characteristics of the scrape-off-layer (SOL), divertor plasma and divertor target loads, validation and development of models

(1) Investigations involving A+M and/or PSI data information:

- Plasma power flow into SOL and in edge/divertor regions
- Detailed power balance
- Impurity and neutral particle transport (and sources)
- Hydrogen and impurity recycling
- Plasma edge diagnostics (H_α and others)
- Development/validation of SOL/plasma edge modelling codes

(2) Required A+M/PSI data on:

- All elastic and inelastic A+M processes between edge plasma constituents
- All impurity generation PSI processes (including secondary electron emission)

(3) A+M/PSI data needs for PH 1.1 covered by existing IAEA programmes:

- CRP on A+M data for fusion edge plasmas (1988-1990; continuation to 1991/92 required)
- CRP on plasma induced erosion rates of PFC (1990-1993)
- Several individual research contracts
- (Data evaluation within DCN)

(4) A+M/PSI data needs not covered (sufficiently or at all) by current IAEA programmes:

- Energy/angular distribution of reaction products (both for A+M and PSI data; partial coverage)
- Elastic and momentum transfer data (not covered)
- Hydrogen retention: trapping/detrapping data (partially covered)
- Secondary election emission (not covered)

(5) Fusion Labs contributing to PH 1.1 (modelling and diagnostic aspects only):

EC (+Canada): ASDEX-UP (J. Neuhauser), TEXTOR (U. Samm) CCFM/TdeV (B. Stanfield), AEA Fusion/COMPASS (P. Johnson)

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* High Priority

Japan: JAERI (M. Azumi), JAERI/JT-60U (M. Nagami), JAERI/JFT-2M (M. Mori), NISF/JIPP-T-IIU (K. Toi), NIFS Okayama Univ. (S.-I. Itoh), Kyoto Univ. (T. Ohbiki), Nagoya Univ./NAGDIS, HYBTOK-II (S. Takamura), Univ. Tsukuba/GAMMA 10 (K. Yatsu)

USSR: KURCHATOV/T-10 (V. Vershkov), KURCHATOV/SPRUT-4 (V. Pistunovich), IOFFE/FT-1 (V. D'yachenko), IOFFE/TUMAN-3 (M. Gryaznevich)

USA: GA, LLNL/DIII-D (M. Mahdavi/D. Hill), LANL (K. Werley), MIT/Alc. C-MOD (B. Lipschultz), GA, LLNL/DIII-D (G. Porter), PPL, UCLA/PBX (M. Okabayashi), PPPL/TFTR (D. Manos), Univ. Texas/TEXT-U (C. Ritz)

2) PH 1.2. Impurity radiation and transport in the bulk, SOL and divertor plasma (including: viability of powerfully radiating plasma edge)

(1) Investigations involving A+M/PSI data information:

- Impurity transport in core, SOL and divertor plasmas
- Impurity radiation losses (radial and poloidal distributions, edge plasma radiation)
- Wall impurity influxes
- Search for methods for impurity radiation enhancement in the edge only (with no fuel dilution effects and violation of density limit): Z-optimization of injected impurities
- Validation/development of 1.5-D and 2-D modelling codes

(2) Required A+M/PSI data on:

- All processes involved in ionization balance and impurity transport (including multistep processes in the edge region)
- All radiative processes (with required energy level information)
- Impurity generating PSI processes

(3) A+M/PSI data needs for PH 1.2 covered by existing IAEA programmes:

- CRP on A+M data for plasma edge (1988-90; need for continuation)
- CRP on erosion rates (only partly) (1990-1993)
- CRP on metallic impurities (1990-1993) (proposed for approval)
- (DCN data compilation and evaluation activities)

(4) A+M/PSI data needs not covered by current IAEA programmes

- A+M data for Be and B
- Collisional data for Z ~ 10 elements
- Data on radiative power losses
- Particle-impact (impurity) desorption data

(5) Fusion labs contributing to PH 1.2. (A+M/PSI aspects):

EC (+Canada): IPP/ASDEX-UP (G. Fussmann), NFR/(JET+TEXTOR) (B. Emmoth), KFA Jülich/TEXTOR (U. Samm), CCFM/TdeV (B. Gregory), AEA Fusion/JET, COMPASS (N. Peacock)

Japan: JAERI (M. Azumi), JAERI/JFT-2M (M. Mori), NIFS, Okayama Univ. (S.-I. Itoh), Kyoto Univ./HELIOTRON (T. Ohbiki), Kyushyu Univ./TRIAM-1M (S. Itoh)

USSR: KURCHATOV/SPRUT-4, LENTA-M (V. Pistunovich), KURCHATOV/T-10 (V. Vershkov)

USA: GA, LLNL/DIII-D (S. Lippman), (PH 1.2a: T. Petrie), MIT/Alc. C-MOD (E. Marmar), ORNL/ATF (R. Isler), PPPL/PBX (R. Kaita), PPPL/TFTR (B. Stratton), Univ. Texas/TEXT-U (W. Rowan)

3) PH 1.3. Exhaust of helium and hydrogenic species

(1) Investigations involving A+M data information:

- Transport of He^{2+} and He^{+} in the core and SOL regions
- Transport of He^{2+}, He^{+} and He^{o} in divertor region
- Determination of He^{o}/H^{o} in divertor region
- He recycling

(2) Required A+M/PSI data on:

- All collision processes of He^{2+}, He^{+} and He^{o} with other plasma constituents in the core, scrape-off and divertor regions
- Helium retention/release in/from wall and plate materials

(3) A+M/PSI data needs for PH 1.3 covered by current IAEA programmes:

- CRP on A+M data for edge plasmas (mainly He^{o})
- (ORNL Redbook vol. 1, 1990)

(4) A+M/PSI data needs still not covered by IAEA programmes:

- Collision data of He^{2+}, He^{+} with impurities (high energies)
- Electron and proton collisions with excited He (low energies)
- He^{q+}(q=0-2) collisions with surfaces and trapping/detrapping processes

(5) Fusion Labs contributing to PH 1.3. (A+M/PSI aspects only)

EC (+Canada):	IPP/ASDEX-UP (H. Vernickel), KFA Jülich, ORNL, UCLA, NIFS/TEXTOR (D. Hillis, K. Finken), CCFM/TdeV (B. Gregory)
Japan:	JAERI/JFT-2M (M. Mori), NIFS, Okayama Univ. (S.-I. Itoh)
USSR:	IOFFE, KURCHATOV/T-10, T-15, TUMAN-3 (V. Sergeev), IOFFE/TUMAN-3 (A. Korotkov), KURCHATOV/T-10, T-15 (E. Berezovskii, V. Pistunovich)
USA:	MIT/Alc. C-MOD (B. Lipschultz), PPPL/PBX (R. Kaita), PPPL/TFTR (E. Synakowski), Univ. Texas/TEXT-U (W. Rowan)

4) PH 1.4. Active control and optimization of divertor and startup limiter conditions

(1) Investigations involving A+M/PSI data:

- Control of impurity influxes from plates/limiter
- Optimization of divertor plasma parameters (density, temperature) and hydrogen recycling
- Control of volume power exhaust in divertor region (gas and impurity injection)
- Wall pumping ad divertor neutral density enhancement
- Fuelling near flow reversal point and effects on impurity and helium transport
- Divertor performance modelling

(2) A+M/PSI data required:

- All inelastic A+M processes in a divertor plasma (required in impurity and neutral transport codes)
- Data for specific (injected) impurities, (radiation power losses)

- PSI processes involved in H, He wall pumping (retention/release times)
- Temperature dependence of impurity generation PSI processes

(3) A+M/PSI data needs covered by current IAEA programmes:

- CRP on A+M data for plasma edge (1988-1990; continuation for 1991/92 required)
- CRP on erosion rates of PFC (partly only)

(4) A+M/PSI data needs not adequately covered by IAEA programmes:

- Trapping/detrapping PSI processes (for H and He)
- Ion-atom momentum transfer (for impurity transport codes)
- Data for specific impurities (as yet unspecified)

(5) Fusion Labs contributing to PH 1.4.

EC (+Canada): IPP/ASDEX-UP (J. Neuhauser), IPP/W7-AS (A. Weller), KFA Jülich, UCLA, NIFS/TEXTOR (R. Conn, K. Dippel, A. Miyahara, CCFM/TdeV (P. Conture)
Japan: JAERI (M. Azumi), JAERI/JFT-2M (M. Mori), Nagoya Univ/NAGDIS, CSTN-III, HYBTOK-II (S. Takamura)
USA: GA, JAERI, LLNL, ORNL, SNL, UCLA, JET/DIII-D (M. Schafter), LANL (K. Schoenberg), LLNL/DIII-D (G. Porter), MIT/AlcD-MOD (B. Lipschultz), PPPL/PBX (H. Kugel)

5) PH 1.5. Characterization and test of plasma-facing components (PFC)

(1) Investigations involving PSI and PMI data:

- Characterization of net erosion rates of candidate PFC materials (in particular: carbon-fiber-composites (CFC), B-, Si-, Ti- doped CFC, Be and its compounds, high-Z materials (Nb, Mo, W)), including temperature dependence, ion dose dependence, neutron irradiation dose dependence
- Hydrogen isotope retention in PFC materials, including location and mode of bonding
- Thermo-mechanical properties of PFC materials under normal and off-normal operation conditions (elastic and stress moduli, thermal conductivities, fatigue lifetimes, etc)
- Temperature and radiation dose dependence of thermo-mechanical properties of PFC materials

(2) PSI/PMI data needs covered by present IAEA programmes:

- CRP on erosion rates of PFC materials (1990-1993)
- Compilation and evaluation of thermo-mechanical data for CFC, C-C and doped C-C (starting 1991)
- Two individual research contracts on radiation damage of structural materials

(3) PSI/PMI data needs not covered by present IAEA programmes:

- Hydrogen isotope retention (in particular: tritium inventory)
- Systematic radiation damage data for PFC materials
- Thermo-mechanical data for non-C-C candidate materials

(4) Fusion Labs contributing to PH 1.5.

EC (+Canada): IPP/ASDEX-UP+W7-AS (J. Roth), KFA Jülich, ORNL, NIFS, UCLA/TEXTOR (J. Winter), CCFM/TdeV (B. Terreault)
Japan: NISF/CHS (K. Matsuoka), Kyushyu Univ./TRIAM-1M (S. Itoh), Nagoya Univ./NAGDIS, CSTN-III, HYBTOK-II (S. Takamura), Univ. Tsukuba/GAMMA 10 (K. Yatsu), ELT/TPE-1RM15 (K. Sugisaki)
USSR: KURCHATOV/SPRVT-4, LENTA-M (V. Pistunovich), IOFFE/TUMAN-3 (S. Lebedev), KURCHATOV/T-15 (V. Khrabov, A. Vertiporokh), FIAE (Troitsk) SIA "ENERGY"/T-14, T-3M-2 (S. Mirnov)
USA: GA, SNLL, UCLA, LLNL, ANL/DIII-D (C. Wong), GA/DIII-D (G. Jackson), MIT/Alc. C-MOD (E. Marmar/B. Lipschultz), PPPL/PBX (H. Kugel), PPPL/TFTR (M. Ulrickson)

2. R+D AREA: 4: OPTIMIZATION OF OPERATION SCENARIO AND LONG-PULSE OPERATION

1) Task PH 4.1. Long-pulse operation experience

Sub-task: PH 4.1e: Neutral beam current drive (NBCD)

(1) Investigations involving A+M data:

- Investigation of neoclassical effects on NBCD
- Investigation of current drive efficiency in the region of critical beam velocities (onset of Alfvén instabilities)
- Dependence of beam stopping cross section on the impurity mix, electron temperature and density

(2) A+M physics involved

- All electron, proton and impurity ion collision processes with hydrogen in the region from ~ 1 keV/u (*) to 2 MeV/u and involving hydrogenic excited states up to n=7

(3) Available data

- Database available for energies above 20 keV/u, with:
  * scaled proton excitation data (for $n \geqq 7$)
  * scaled proton electron removal data (for $n \geqq 2$)
  * scaled impurity-ion electron removal data (for $n \geqq 2$, $q \geqq 3$)
  * empirical formulae for n-n' transitions

(4) Data needed down to E/q ~ 1 keV/u for:

- proton and impurity-ion excitation of H (for $n \leqq 7$)
- proton and impurity ionization of $H^*(n)$
- proton and impurity charge exchange on $H^*(n)$
- more reliable formulae for n-n' transitions (in heavy particle collisions)

(*) Such low energies are required to accurately take into account the stopping due to beam-self ion collisions

2) PH 4.5.
======= Fuelling physics: Pellet ablation model

(1) Investigations involving A+M/PSI data:

- pellet ablation processes
- effects of thermal and suprathermal electrons and fast ions on pellet ablation
- velocity dependence of pellet penetration depth
- pellet ablation modelling
- pellet ablation diagnostics

(2) A+M/PSI data required:

- PSI processes due to plasma particle and impurity bombardment (energy deposition, erosion)
- A+M processes involving plasma particle-eroded pellet material interaction
- A+M processes involved in pellet ablation soft X-ray diagnostics

(3) A+M/PSI data produced by current IAEA programmes:

(4) A+M/PSI data needs not covered by current IAEA programmes

- PSI processes with solid hydrogen (under electron, proton and impurity impact) leading to erosion and evaporation
- plasma particle and impurity impact processes with H and H_2 at energies corresponding to T $\propto$ 10-20 keV

3. R+D AREA: DIAGNOSTICS

(1) Diagnostics for physics phase involving A+M data

Plasma Parameter	Diagnostic Method	Comment
- Ion/electron temperature	Neutral particle analysis	For edge plasma
	CXRS	Needs diagnostic NB
- D/T density	Neutral particle analysis	For edge plasma
	Visible spectroscopy	For edge plasma
- Impurity content	VUV, visible spectroscopy	Edge plasma, SOL
	X-ray spectroscopy	Core plasma
	CXRS (?)	Heating beam (?)
- Confined α-particles	CXRS	Needs diagnostic beam (He^0)
	Neutral particle analysis	Needs diagnostic beam (He^0)

- He concentration	CXRS	Needs diagnostic beam
	Neutral particle analysis	Needs diagnostic beam
- Divertor plasma parameters	Visible spectroscopy	Needs radiation resistent optics
- Erosion rates	Visible spectroscopy	
- q(r) (current density)	Motional stark effect	Needs diagnostic beams

(2) A+M physics required

- H-beam attenuation processes for beams of E ~ 100-200 keV/u
- He^0-beam attenuation processes for beams of E ~ 0.5-2 MeV/u and E ~ 30-100 keV/u

(3) Data availability

- Database not complete, particularly with respect to processes involving excited states

(4) Particularly important data needs

- Radiation damage of diagnostic components

  * neutron, γ, X-ray radiation damage
  * charged particle radiation damage
  * He-acummulation problem

  } → A+M/PSI involved

Appendix 6

Status of the Fusion A+M DCN Manpower (in P-Y)

Data Centre	Professional Staff		Technical Staff			Data Production Capabilities	
	Scientific Permanent	Consultants	Computer Support	Technical Assistance	Clerical Staff	Theory	Experiment
1. NIST (a) At. Energy Levels	1.0	0.3	0.4	0.8	0.1	-	2.0
2. NIST (b) At. Trans. Probabilities	1.0	-	0.2	0.2	0.2	1.5	0.5
3. ORNL CFADC	0.4	0.2	0.5	-	0.5	0.8	2.5
4. QUB Belfast	1.0	0.6	0.5	0.3	-	2.0	-
5. NIFS Nagoya	2.0	0.5	0.5	0.5	0.2	-	-
6. JAERI AMDU	0.6	0.1	0.1	0.2	-	0.5	0.5
7. GAPHYOR Orsay	2.0	0.5	1.5	-	-	2.0	-
8. KURCHATOV INST. AMDU Moscow	1.5	0.8	0.5	-	-	3.0	7.0

9. CRAAMD IAPC Beijing	4.0	3.0	3.0	2.0	1.0	3.0	8.0
10. CNDC-AMDU Beijing	2.0	-	-	-	-	-	-
11. NDC-AMDU Obninsk	1.0	1.0	1.0	1.0	0.5	2.0	2.0
12. ENEA NDC-AMDU Bologna	0.6	-	0.2	-	-	-	-
13. JILA Boulder	1.5	0.5	-	-	-	-	-
14. VNIIFTRI Mendeleevo	2.6	-	2.0	1.0	1.0	1.5	1.0
15. IAEA AMDU	1.5	0.2	0.5	-	1.0	-	-
TOTAL DCN	22.7	7.7	10.9	6.0	4.5	16.3	23.5