International Atomic Energy Agency

INDC(NDS)-259/N7

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

# IAEA ADVISORY GROUP MEETING ON

# "TECHNICAL ASPECTS OF ATOMIC AND MOLECULAR DATA PROCESSING AND EXCHANGE"

(10th Meeting of A+M Data Centres and ALADDIN Network)

Vienna, 23 and 24 September 1991

SUMMARY REPORT

Prepared by R.K. Janev

February 1992

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

INDC(NDS)-259/N7

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## SUMMARY REPORT

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## Abstract

This Summary Report contains the proceedings and conclusions of the IAEA Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (10th Meeting of A+M Data Centres and ALADDIN Network) convened on September 23 and 24, 1991, in Vienna. The progress reports of the national A+M data centres are also appended to this Report.

Reproduced by the IAEA in Austria
February 1992

92-00844

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## 1. INTRODUCTION

On September 23 and 24, 1991, the IAEA Atomic and Molecular (A+M) Data Unit convened at the IAEA Headquarters in Vienna an Advisory Group Meeting on "Technical Aspects of Atomic and Molecular Data Processing and Exchange" (10th Meeting of A+M Data Centres and ALADDIN Network) to review the progress made during the period September 1990 - September 1991 by the national data centres in the area of compilation, evaluation and generation of atomic and molecular data for fusion and discuss the status and developments in the methodology of data processing and exchange by using the ALADDIN system. The Meeting also discussed the priorities in the data compilation and evaluation programmes of the A+M Data Centre Network for the next year (and beyond) in the context of ITER design and operating tokamaks A+M data needs.

The Meeting was attended by 12 participants representing the national A+M data centres, one observer and 4 staff members of the IAEA A+M Data Unit and Nuclear Data Section (see Appendix 1). Only the Belfast University A+M Data Centre was not represented at the Meeting.

## 2. MEETING PROCEEDINGS

The Meeting was opened by Mr. J.J. Schmidt, Head of the Nuclear Data Section, with some recollections from the past and recent developments of A+M Data Centre Network and the IAEA A+M data activities. The work of the Meeting then proceeded in the following sessions (see Appendix 2: Meeting Agenda):

Session 1: Current activities and near-future plans of A+M data centres;
Session 2: Status of ALADDIN, data processing and exchange;
Session 3: Priorities in A+M data compilation and evaluation;
Session 4: Meeting conclusions and recommendations.

During the first session of the Meeting, representatives of national A+M data centres and the IAEA A+M Data Unit presented progress reports on the data compilation, evaluation and generation activities in the period September 1990 - September 1991, and regarding their plans for the next year. The summaries of these progress reports are reproduced in Appendix 3. In the area of compilation and evaluation of spectroscopic data for fusion relevant elements impressive results were reported from the NIST (W.L. Wiese), VNIIFTRI (A.Ya. Faenov) and JAERI (T. Shirai) data centres. Extensive collisional data compilation and evaluation efforts were reported from the NIFS (H. Tawara), ORNL (D. Schultz), ENEA (E. Menapace), JAERI (T. Shirai), CRAAMD (Han Guoxing) IAE, Beijing (Yao Jinzhang) and IAEA (R.K. Janev). Data compilations and evaluations in the areas of particle-surface interactions and material properties data for fusion have also been reported from several data centres (IAEA, IAE (Beijing), NIFS). Data genaration for fusion have been reported from the GAPHYOR (K. Katsonis), ORNL (D. Schultz), Kurchatov Institute (V.A. Abramov), CRAAMD (Han Guoxing), ENEA (E. Menapace), NIFS (H. Tawara), Obninsk (V. Piksaikin) and VNIIFTRI (A.Ya. Faenov) data centres. Bibliographic data compilations during the reporting period have been done by ORNL, NIST, GAPHYOR (J.L. Delcroix) and Kurchatov Institute data centres.

The session on data processing and exchange started with reports from the data centres on their experiences with implementing ALADDIN in their data storage and data management practices. The appropriatness of ALADDIN for such purposes was reafirmed by all of the data centres. Suggestions for ALADDIN system up-grading in the area of spectroscopic data were put forward by the VNIIFTRI representative, but the Meeting adhered to its earlier position for keeping the present format of ALADDIN "frozen" for certain period of time. Nevertheless, the new format for handling the spectroscopic data within ALADDIN, proposed by the NIST data centre, was found attractive and consistent with the broadly accepted labelling conventions of the NIST book series on spectroscopic data. The Meeting, therefore, encouraged the NIST effort to convert their recommended spectroscopic databases into the newly proposed spectroscopic ALADDIN format.

The head of the IAEA A+M Data Unit reported on the recent developments of ALADDIN to incorporate material properties data into the system. V. Osorio and J.J. Smith, ex-staff members of the Nuclear Data Section, reported on the work done towards extending certain of the ALADDIN features related mainly to its organizational shell and access to data capabilities. A one hour practical demonstration of the new ALADDIN features was organized by V. Osorio.

In the session on A+M data compilation, evaluation and generation priorities, the head of the IAEA A+M Data Unit provided information on the most urgent data needs related to the current and planned experiments on the operating large tokamaks (JET, JT60-U, TFTR, Tore Supra, DIII-D, ASDEX, etc) and to the design of next step fusion devices (ITER, NET, FER, BPX, etc). The most important among these priorities are those connected with the interpretation of the Be(B)-experiments on JET (Textor), diagnostics and modelling of impurity influxes in JET, TFTR, ASDEX and other operating tokamaks, establishment of the He-beam based alpha particle diagnostics on JET and for ITER, modelling of the impurity radiation losses in the edge plasmas of present and next-step fusion machines, modelling of transport, retention and exhaust of helium from divertor plasmas, establishment of databases related to the erosion and thermo-mechanical properties of candidate materials for plasma facing components, etc. The establishment of databases for high-Z impurities (W and Mo) and some diagnostic relevant elements (Li, Ne, Ar, Ga) has also to be considered as a priority.

In the last session of the Meeting the participants discussed questions related to the enhancement of the co-operation within the data centre network and with the fusion laboratories. It has been noted that direct co-operation already exist between several data centres (ORNL-NIST, NIST-JAERI, ENEA-JAERI, ORNL-NIFS, NIST-NIFS, CRAAMD-NIFS) which significantly improves the efficiency of the work of the Network. The IAEA A+M Data Unit has also established direct collaborative relations with most of the data centres (ORNL, NIFS, GAPHYOR, Kurchatov Institute, CRAAMD) mainly in the ares of data evaluation and data generation. Direct co-operations between the data centres and major fusion laboratories (ORNL-PPPL, ORNL CFADC-ORNL Fusion Division, NIST-PPPL/DIII-D, NIFS-Japanese fusion labs, JAERI A+M Data Unit-JAERI fusion labs, GAPHYOR-Tore Supra, Kurchatov Inst. A+M Data Unit-Kurchatov Inst. Fusion Lab) has also been intensified recently, and this process should further be encouraged. In this context, the ORNL data center intends to establish computer provisions for direct access to their ALADDIN databases from any of the US fusion laboratories using the US fusion programme computer network (NERSC).

## 3. CONCLUSIONS AND RECOMMENDATIONS

The Meeting discussions during the last two sessions have led to the following conclusions and recommendations:

### A. Status of data compilation and evaluation activities

1) The current level of data compilation activity successfully follows the growth of fusion community needs for various types of data. The data compilation is done within the regular programmes of most of the data centres, within the existing IAEA research co-ordination programmes, and during the preparation stages of IAEA organized experts' meetings on specific data areas. Data compilation activity is still being pursued in some of the fusion laboratories for satisfying the need in certain specific modelling or diagnostic studies.
2) The level of data evaluation activity can be considered as satisfactory only having in mind the existing manpower and budgetary constraints of the co-operating data centres. The growth of fusion programme needs for evaluated data, particularly with the current progress in the design of next-step fusion devices, requires a much more vigorous effort in this direction. The IAEA A+M Data Unit makes attempts to improve the situation by excersizing various supplementary assistance forms (special service agreements with individual consultants, convening small experts' group meetings, fostering data evaluation collaboration among the data centres) and using some of the regular specialists' meetings also for data evaluation purposes, but the size of this effort appears insufficient to solve the problem.
3) Enhancement of data evaluation activity is essential if the needs of the fusion programme for recommended A+M data are to be met. Extended joint work of small experts' group is a efficient form for data evaluation, and should be given adequate attention and budgetary support. The IAEA A+M Data Unit is in a position to excersize its co-ordinating role also in the data evaluation process, but its technical basis (especially in terms of appropriate manpower) must adequately be improved.

## B. Priorities in data compilation, evaluation and generation

1) General priorities in compilation, evaluation and generation of atomic and plasma-material interaction data for fusion, as established at the last meeting of IFRC Subcommittee on Atomic and Molecular Data for Fusion (September 1990) remain unchanged (see IAEA Report INDC(NDS)-244/M9). However, in view of the current actions of the IAEA A+M Data Unit on completing the databases for He and Li atoms, and for Be and B ions (see IAEA Reports INDC(NDS)-253 and INDC(NDS)-254, respectively) any provision from the data centres of new collisional data on these elements would be highly useful.
2) Data compilation, evaluation and generation work on medium- and high-Z impurities should also be enhanced in view of the needs explicitly expressed in the design process of next-step fusion devices (ITER, NET, FER and BPX). Part of this activity is covered by an ongoing IAEA co-ordinated research programme, but support from the data centres, especially with respect to the data compilation aspect, would be helpful. A similar attention should be also devoted to the collisional A+M edge plasma processes, particularly those involving molecular species, with establishing appropriate links between this activity and the corresponding IAEA co-ordinated research programme.
3) The compilation of plasma-material interaction data by the data centres having the appropriate expertise in this field is to be further enhanced, particularly for the processes leading to material erosion.
4) Data generation within the data centres is highly encouraged as a way to fill the gaps in existing databases or improve the accuracy of some of the data.

## C. Data processing and exchange (ALADDIN)

1) With inclusion of the new labelling schemes in ALADDIN to incorporate particle-surface and material properties data and with the recent development of the ALADDIN package, the preparation of a new ALADDIN Manual seems to be necessary further step. The question of the format for spectroscopic data in the new ALADDIN version should be resolved on

the basis of the progress made by NIST in conversion of their data in the proposed alternative format. The preparation of the new ALADDIN Manual should be one of the immediate priorities of IAEA A+M Data Unit.

2) The present rate of data exchange between data centres and fusion laboratories can be considered as satisfactory. Direct recommended data distribution from national data centres to fusion users is encouraged. The attempt of ORNL data centre to create a user-accessible ALADDIN database on the U.S. NERSC supercomputer network is an example which should be followed by other centres whenever possible. The IAEA A+M Data Unit should explore its technical possibilities for up-grading its data distribution system to a similar level.

3) In view of the considerable body of various types of recommended data that presently exists, an effort should be made by both the IAEA A+M Data Unit and the national data centres to create packages of databases for direct use in certain fusion application codes. The IAEA A+M Data Unit has already created such packages for calculation of carbon and oxygen radiative losses and plasma colling rates, and the establishment of a package for hydrogen recycling in divertors (in co-operation with the Kurchatov Institute) is now in progress. Creation of similar packages for hydrogen (including its molecular form) radiation at the edge and for helium exhaust has a high priority.

Appendix 1

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

**23 and 24 September 1991, IAEA Headquarters, Vienna, Austria**

### LIST OF PARTICIPANTS

| | |
|---|---|
| Dr. V.A. Abramov | Institut Atomnoi Energii I.V. Kurchatova, Ploshchad I.V. Kurchatova, Moscow D-182, 1231182, U.S.S.R. |
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IAEA

| | |
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| Dr. J.J. Schmidt | Nuclear Data Section, IAEA, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, Austria |
| Mr. J.J. Smith | Data Development Section, IAEA, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, Austria |
| Mr. V. Osorio | Physics Section, IAEA, Wagramerstrasse 5, P.O. Box 100, A-1400 Vienna, Austria |

Appendix 2

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

**23 and 24 September 1991, IAEA Headquarters, Vienna, Austria**

## MEETING AGENDA

MONDAY, September 23

| | | |
|---|---|---|
| 09:30 - 09:45 | - Opening<br>- Adoption of Agenda | (Room: C07-IV) |
| Session 1: | Current activities and near-future plans of A+M Data Centres | |
| Chairman: | Abramov | |
| 09:45 - 11:00 | Reports from Data Centres:<br>Wiese (NIST), Faenov (VNIIFTRI), Shirai (JAERI) | |
| 11:00 - 11:15 | Coffee break | |
| 11:15 - 12:30 | Reports from Data Centres:<br>Tawara (NIFS), Schultz (ORNL) | |
| 12:30 - 14:00 | Lunch | |
| Session 1: | Cont'd | |
| Chairman: | Wiese | |
| 14:00 - 15:45 | Reports from Data Centres:<br>Delcroix/Katsonis (GAPHYOR), Menapace (ENEA), Abramov (Kurchatov Institute) | |
| 15:45 - 16:00 | Coffee break | |
| 16:00 - 18:00 | Reports from Data Centres:<br>Han Guoxing (CRAAMD), Yao Jinzhang (IAE, Beijing), Piksaikin (Obninsk), Janev (IAEA) | |

TUESDAY, September 24

| | |
|---|---|
| Session 2: | Status of ALADDIN, data processing and exchange |
| Chairman: | Delcroix |
| 09:00 - 10:30 | ALLADIN implementation and developments: Comments from Data Centres (all participants) |
| 10:30 - 10:45 | Coffee_break_ |
| 10:45 - 11:00 | ALADDIN developments at the IAEA (J.J. Smith/V. Osorio) |
| 11:00 - 12:00 | Demonstration of new ALADDIN features (A-2329) |
| 12:00 - 14:00 | Lunch |
| Session 3: | Priorities in A+M data compilation and evaluation |
| Chairman: | Janev |
| 14:00 - 15:15 | Discussion on priorities in A+M data compilation, evaluation and exchange |
| 15:15 - 15:30 | Coffee_break_ |
| Session 4: | Meeting conclusions and recommendations |
| Chairman: | Janev |
| 15:30 - 17:00 | Formulation and adoption of meeting conclusions |

Appendix 3

# PROGRESS REPORTS OF THE NATIONAL A+M DATA CENTRES AND THE IAEA A+M DATA UNIT

# REPORT ON IAEA A+M DATA UNIT ACTIVITIES: SEPT. 1990 - SEPT. 1991

R.K. JANEV

## 1. DATABASE MAINTENANCE AND DEVELOPMENT

### 1.1 A+M Databases

1) H-collisional database: continued up-dating
2) Li-beam database: ALADDIN formatting, σ-parametrization
3) He-beam database: establishment initiated
4) Be, B-databases: establishment initiated
5) $C^{6+}$, $O^{8+}$+H SSEC database: nearly completed

### 1.2 PMI Databases

1) Light-ion reflection database: completed; ALADDIN formatted
2) Physical sputtering database: nearly completed
3) PMI database for pyrolytic graphites: initiated

### 1.3 Special Purpose Databases

1) Impurity cooling rates: C, O - initiated
2) H-recycling database: initiated; "standard" kinetic scheme established

## 2. ALADDIN SYSTEM DEVELOPMENT

2.1 Labelling system and dictionaries established for material properties data

2.2 ALADDIN Data Formatting:

- All new in-house evaluated data and database up-dates have been ALADDIN formatted

2.3 System's Environment Modifications:

(To be reported by J.J. Smith and V. Osorio in 2nd session)

3. CO-ORDINATION OF RESEARCH PROGRAMS

1) CRP on "A+M data for fusion edge plasmas" (1988-1991):
- concluded;
- continuation for 1992-93 requested;

2) CRP on "Plasma-interaction induced erosion of fusion reactor materials" (1990-1993):
- 1st RCM convened, results analyzed;

3) CRP on "A+M data for medium- and high-Z plasma impurities" (1991-1994):
- established, with 11 participants;

4. MEETINGS ORGANIZED

1) CM on "Evaluation of thermo-mechanical properties data for carbon-based PFMs" (December 1990):
- database for pyrolytic graphites;
- ALADDIN Dictionary and Labelling Schemes.

2) RCM on "Plasma-interaction induced erosion of fusion reactor materials" (May 1991):
- first CRP results reported;
- plans for next-year work adopted.

3) CM on "Atomic data for He-beam alpha particle diagnostics" (June 1991):
- comprehensive database identified and recommended (including multistep processes);
- additional data generation in progress.

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Individual research contracts: 7
A+M: 5
PMI: 2

4) CM on "Atomic data for Be and B" (June 1991):
   - data status analyzed;
   - electron-impact collision data for ground state ions recommended;
   - database for heavy-particle collision processes assembled and critically evaluated.

* 5) AGM on "A+M data for fusion plasma impurities" (Sept. 25-27, 1991):
   - improve existing database on metallic impurities;
   - specify priorities for the CRP on medium- and high-Z impurities.

## 5. PUBLICATIONS PREPARED

1) "Proceedings of the AGM on A+M data for metallic impurities in fusion plasmas"

   Physica Scripta vol. T37 (1991)

2) "Atomic and Plasma-Material Interaction Data for Fusion", vol. 1 (1991) (to appear)

   (A Supplement to the Nucl. Fusion journal)

   - contains PMI data and reviews

* 3) Vol. 2 (1992) of the same series: nearly completed
   - contains A+M data for the plasma edge

4) Bibliographic A+M Data Bulletin
   - one issue

## 6. ACTIVITIES PLANNED FOR 1992

### 6.1 Database development and data publication

1) To complete establishment of datbase on:
   - H-beam penetration
   - He-beam penetration
   - Li-beam penetration
   - Be, B (basic processes)
   - $C^{q+}$, $O^{q+}$ (with new analytic fits)

2) To publish the above databases in "book format".

## 6.2 Meetings in 1992

| Title | | Dates / Place |
|---|---|---|
| 1) 2nd RCM on: | "Plasma-interaction induced erosion" | May / Vienna |
| 2) AGM: | 11th A+M DCN Meeting | 15,16 June / Vienna |
| 3) RCM on: | "A+M data for fusion edge plasmas" (if CRP approved) | 17-19 June / Vienna |
| 4) CM on: | t.b.d. | tbd / Vienna |
| 5) TCM on: | "A+M data for fusion reactor technology" | 12-16 October Cadarache, France |
| 6) TCM: | 7th IFRC A+M Subcommittee Meeting | Cadarache 17,18 Oct. or 19,20 October |

## Activities of the Data Centers on Atomic Spectroscopy at the National Institute of Standards and Technology During the 1990/1991/ Period

W. L. Wiese

| | Director | Workforce |
|---|---|---|
| 1. Atomic Energy Levels and Wavelengths | W. C. Martin | 2 Professionals |
| 2. Atomic Transition Probabilities | W. L. Wiese | 1¼ Professionals |
| 3. Spectral Line Shapes and Shifts | W. L. Wiese | Occasional Guest Scientists, Contractors |

### Work areas for data compilations (chemical elements):

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

## In-House Database Development at NIST

1. Bibliographic databases (compilation and classification of literature references):

All recent literature references (for atomic energy levels since 1985; for atomic transition probabilities since 1980) are entered into a database utilizing ORACLE software and HP 9000 computer (Special Assistance by the NIST Standard Reference Data (SRD) program for database design).

2. Numerical Data:

A general spectroscopic database has been implemented by OSRD personnel. This database contains wavelengths, energy levels and transition probabilities in a unified format. Critically evaluated data on Fe-group elements (energy levels and transition probabilities) have been loaded into the database. Also, energy levels for Na, Mg, Al, Si, P, S, Cu, Kr, Mo and rare earth elements and wavelengths for Mg and Al have been entered. Again, ORACLE software has been used.

New data compilations during 1990/91:

J. Sugar and A. Musgrove, Energy Levels of Krypton, Kr I through Kr XXXVI, J. Phys. Chem. Ref. Data 20, 859-915 (1991).

T. Shirai, T. Nakagaki, Y. Nakai, J. Sugar, K. Ishii and K. Mori, Spectral Data and Grotrian Diagrams for Highly Ionized Copper, Cu X - Cu XXIX, J. Phys. Chem. Ref. Data 20, 1-81 (1991).

V. Kaufman and W. C. Martin, Wavelengths and Energy Level Classifications of Magnesium Spectra for all Stages of Ionization (Mg I through Mg XII), J. Phys. Chem. Ref. Data 20, 83-152 (1991).

V. Kaufman and W. C. Martin, Wavelengths and Energy Level Classifications for the Spectra of Aluminum (Al I through Al XIII), J. Phys. Chem. Ref. Data 20, 775-858 (1991).

N. Konjević and W. L. Wiese, Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms (A Critical Review of Selected Data for the Period 1983 through 1988), J. Phys. Chem. Ref. Data 19, 1307 (1990).

# CONTROLLED FUSION ATOMIC DATA CENTER

Oak Ridge National Laboratory
Activity/Progress/Plans
October 1990 - September 1991

R.A. Phaneuf and D.R. Schultz

1. *Bibliographic Data Base:*
*The on-line bibliographic data base has been kept up to date, and now contains 23,550 categorized and indexed references from 120 journals, covering the period from 1978 to the present. 1050 new references were added during the past year. Literature searches are performed monthly by 4 ORNL fusion atomic physics staff members and by 5 expert consultants under contract to the Data Center. Updates of the bibliography are sent twice yearly on diskette to the IAEA, NIFS and JAERI Data Centers. A version of the CFADC personal-computer-based on-line search and retrieval system is also installed at Justus Liebig University in Giessen, Germany, where updates of the dBase III+ database files are sent annually. The CFADC answers specific requests for data and bibliographic searches at a rate of two per week.*

2. *Data Compilation and Evaluation:*
*In collaboration with R.K. Janev of the IAEA and H. Tawara of NIFS, data were collected and evaluated for state-selective electron capture in collisions of $C^{q+}$ and $O^{q+}$ ions with H, $H_2$ and He. Cross sections were recommended for 87 $C^{6+}$ + H and $O^{8+}$ + H reaction channels, and a preliminary ALADDIN database was created based on spline fits to the data. A manuscript containing graphical represesentations of the data was prepared for submission to Atomic Data and Nuclear Data Tables. Analytical fits will be made to the recommended cross sections, and an ALADDIN database will be created for distribution. The recommended database will be expanded to include the other reactants as more data become available.*

3. *Atomic Data Base for Be and B Ions:*
*The database for collisions of Be and B ions with H, $H_2$ and He was reviewed and evaluated as part of an IAEA Consultants' meeting, and a Working Group Report was prepared by the CFADC.*

4. *ALADDIN Database:*
*The CFADC has continued to distribute the ALADDIN database program and ORNL "Redbook" data files via diskette and electronic mail. A user-accessible ALADDIN database will be created on the U.S. NERSC supercomputer network.*

5. *CAMOS Survey of AMO Experimentalists in the U.S.:*
*A survey of experimental atomic, molecular and optical (AMO) scientists in the U.S. was carried out by the Committee on Atomic, Molecular and Optical Sciences (CAMOS) of the National Research Council. The data from this survey is being analyzed by the CFADC, and a summary report will be prepared.*

# Atomic and Molecular Data Unit
# Japan Atomic Energy Research Institute
# Progress Report 1990-1991

Toshizo Shirai

A four-year program to make the third edition of Evaluated Atomic and Molecular Data Library (JEAMDL-3) for fusion was initiated at 1988. This program has been pursued in collaboration with the Research Committee on Atomic and Molecular Data.

## 1. Recent Activities and Work in Progress

Analytic expressions fitted to Barnett's recommended data have been given for the total electron capture cross-sections by H, $H^+$, and $H_2^+$ in collisions with atoms, molecules and ions in an collaboration with R. Phaneuf of ORNL. Analytic expressions use the functional form proposed by Green and McNeal [J. Geophys. Res. 76, 133 (1971)] and some modified forms to allow extrapolation outside the energy range of the recommended data. The results for electron capture by H, $H^+$, and $H_2^+$ are given in Appendix.

Critical evaluation and compilation has almost been completed of spectroscopic data for highly ionized ions, V VI-V XXIII and Cr V-Cr XXIV, in joint work with J. Sugar and W.L. Wiese of NIST. A similar work is now in progress for Mn VII-Mn XXV.

These works were supported by the U.S.-Japan Fusion Cooperation program.

A collaboration was initiated with Y. Zou of IAPCM on the calculation of differential excitation cross section of ions by electron impact in the close-coupling approximation. As the first case, the 1s-2s and 2p excitations of hydrogenlike ions from $He^+$ to $C^{5+}$ were examined.

## 2. Recent Publications

<u>Collision Cross Section Data</u>

1. Nuclear Fusion, Supplement, Vol.2 (1991) in press: "Extended

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

2. Phys. Rev. A (1991) in press: "Algebraic-eikonal approach to the electron-molecule-collision process: Vibrational excitation and quadrupole interaction," A. Mengoni and T. Shirai.

Spectroscopic Data

3. J. Phys. Chem. Ref. Data 20, 1 (1991): "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.

4. J. Phys. Chem. Ref. Data, submitted: "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

5. JAERI-M 91-050 (1991): "Report of the 1990 workshop on plasma-materials interactions for fusion research," edited by S. Nagai and K. Ozawa (in Japanese).

## 3. Activity Plans for 1991 to 1992

Further work will be performed to make analytic expressions for the collision cross-sections of H, $H_2$, He, and Li atoms and ions with atoms and molecules of Barnett [ORNL-6086/V1, (1990)].

Critical evaluation and compilation of spectroscopic data will be extended to the Kr ions. The Ti compilation of Mori et al. [Atom. Data Nucl. Data Tables, 34, 79 (1986)] will be revised with new experimental data presently available.

# ACTIVITY REPORT at DPC/NIFS 1990/91

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## Activities in 1990-91

Our present activities are focused on A&M data compilation and evaluation relevant to plasma diagnostics and modelling in the center and edge regions.

1) Atomic and molecular data for hydrocarbon molecules relevant to edge plasmas modelling have been evaluated and the final results are going to be published in Nuclear Fusion Supplement soon. Some new data of total scattering of electrons from hydrocarbon molecules have also been obtained experimentally. For the first time a clear isomer effect has been observed in propene and cyclopropane which has also confirmed theoretically by McKoy et al.

2) Because of the recent interest to low-Z material coatings inside fusion plasma devices, the electron transfer data for $Be^{q+}$ and $B^{q+}$ ions in colliding with H, $H_2$ and He targets have been compiled and reported. It is found that not only experimental data but also theoretical data are too limited to evaluate except for those of $Be^{4+}$ and $B^{5+}$ ions colliding with H atoms and pointed out that more systematic investigations for these elements are urgently required theoretically as well as experimentally.

3) In order to give some useful data for estimating the penetration of particles into plasmas, the stopping cross sections for hydrogen and helium beams have been calculated, based upon a wave-packet model recently developed, and a series of tables for various target atoms have been given in NIFS-DATA report.

4) Systematic comparisons has been performed of rate coefficients for electron ionization of H to Ni ions in all their ionization stages, obtained from empirical formulas by Lotz, Arnaud-Rothenflug, Bell et al. and Pindzola et al. A series of the figures of the comparison have recently been published

in our NIFS-DATA report.

5) Recently a systematic review has been made on basic problems related with polarization phenomena in plasmas and applications of polarization of photons emitted to plasma diagnostics. A report is under preparation for publication in NIFS-DATA.

**ALADDIN activities**

Our evaluated A&M data-base system, ERIC, is being developed. This system incorporates the Aladdin in calculating the observed spectra from plasmas and plasma modelling. Presently this is still under various tests prior to the routine use.

Internal Reports

1) U.I.Safronova, T.Kato, K.Masai, L.A.Vainshtein and A.S.Shlyapzeva, NIFS-DATA-8 (1990)
Excitation collision strengths and rate coefficients for O V, Si XI, Fe XXIII and MO XXXIX by electron impact ($1s^22s^2$ - $1s^22s2p$, $1s^22p^2$ transitions)

2) T.Kaneko, NIFS-DATA-9 (1990)
Partial and total electronic stopping cross sections of atoms and solids for protons

3) K.Shima, N.Kuno, M.Yamanouchi and H.Tawara, NIFS-DATA-10 (1991)
Fractions of ions of Z=4-92 (0.02-6 MeV/u) and Z=4-20 (up to 40 MeV/u) emerging from a carbon foil

4) T.Kaneko, T.Nishihara, T.Taguchi, K.Nakagawa, M.Murakami, M.Hosono, S.Matsushita, K.Hayase, M.Moriya, Y.Matsukuma, K.Miura and H.Tawara, NIFS-Data-11 (1991)
Partial and total electronic stopping cross sections of atoms for a singly charged helium ions ; part I

5) H.Tawara, NIFS-DATA-12 (1991)
Total and partial cross sections of electron transfer processes for $Be^{q+}$ and $B^{q+}$ ions in collisions with H, $H_2$ and He gas targets - status in 1991

6) T.Kaneko, M.Nishikori, N.Yamato, T.Fukushima, T.Fujikawa, S.Fujita, K.Miki, Y.Mitsunobu, K.Yasuhara, H.Yoshida and H.Tawara, NIFS-DATA-13 (1991)
Partial and total electronic stopping cross sections of atoms for a singly charged helium ions ; part II

7) T.Kato, K.Masai and M.Arnaud, NIFS-DATA-14 (1991)
Comparison of ionization cross sections and rate coefficients of ions from hydrogen through nickel

**Related published papers**

1) T.Kato, J.Lang and K.E.Berrington, At. Data & Nucl. Data Tables 44 (1990) 133
Intensity ratios of emission lines from O V ions for temperature and density diagnostics, and recommended excitation rate coefficients

2) H.Nishimura and H.Tawara, J. Phys: B 24 (1991) L363
Some aspects of total scattering cross sections of electrons for simple hydrocarbon molecules

3) H.Tawara, H.Nishimura, Y.Itikawa, H.Tanaka, and Y.Nakamura, Nucl. Fusion (accepted)
Electron-impact processes with hydro-carbon molecules

4) P.Hvelplund, S.K.Bjφrnelund, H.Knudsen and H.Tawara, Phys. Scripta (1991) (accepted)
Electron capture in collisions between medium velocity multiply charged ions and H and $H_2$

**On-going and future activities**

1) Data compilation related impurities such $H_2O$, CO and $CO_2$ molecules by electron impact
2) Data compilation of excitation cross sections and rate coefficients of He atoms under electron impact.
3) Data compilation of electron transfer cross sections of intermediate (MeV) energy, heavy ions
4) Data compilation of energy distributions of sputtered atoms by ion impact

# Activity Report 1990 / 1991

Jinzhang YAO

(Institute of Atomic Energy, P.O.Box 275–41, Beijing, P.R. China)

A group of Atomic and Molecular Data was established at Chinese Nuclear Data Center, Institute of Atomic Energy since 1987. Data collection, compilation and evaluation work is in progress for atomic and molecular collision data, plasma surface interaction as well as thermal–mechanical properties for materials of fusion interest involved first wall, wall armor, limiters and divertor plates etc. in a TAKAMAK device.
Collaborations with Drs LUO Zhengming, ZHANG Di, WANG Neng–ming and LI Yexiang, Institute of Nuclear Science and Technology, Sichuan University; YU Jinnan, SHAN Changqi, Laboratory of Reactor Material and ZENG Xiantang, Group of Atomic Physics for experimental research, Institute of Atomic Energy have been made in data compilation and evaluation.

A. Atomic Collision Data

1) Electron impact ionization cross sections for atoms and ions with high Z
   YAO Jinzhang, YANG Qing, Communication of Nuclear Data Progress No.3, 54 (1990)
2) The Collision of Hydrogen Atom with Proton
   Wang Nengming, Chinese Journal of Atomic and Molecular Physics Vol. 8, No.1, 1772 (1991)
3) The $3d^8 4s - 3d^8 4p$ Transitions In Br IX
   Xiantang ZENG et al., Physica Scripta Vol. 42, 223 (1991)
4) Identification of The Transition Arrays $3d^7 4s - 3d^7 4p$ in BrX and $3d^6 4s - 3d^6 4p$ in BrXI
   X.T.ZENG, C.Jupen, P.Bengtsson, L.Engstrom, M.Westerlind and I.Martinson, Physica Scripta Vol. 43, 166 (1991)

B. Plasma Surface Interaction

1) PANDA–P A New Microcomputer Program for Ion Transport in Solids

LUO Zhengming, BAI Rongsheng and WANG Shiming, Nuclear Instr.& Methods in Physics Research B48 (1990)435

2) A New Parameter For Describing The Reflection Coefficient of Light Ions: Scaled Transport Cross Section

LUO Zhengming, Nucl. Instr. & Methods In Physics Research B48 (1990)444

3) Application of Improved Bipartition Model of Ion Transport to Calculate Ion Reflection and Radiation Damage for Fusion Techology

Luo zhengming et al., Research Contract with IAEA

4) Compilation of Desorption Cross for Collision of Stainless Steel Surface with $H^+$, $H_2^+$ And $H_3^+$

ZHANG Di, Internal Report

C. Research on Plasma Facing Materials

1) The Behavior of Diffusion And Permeation of Tritium Through 316L Stainless Steel

SHAN Chengqi, WU Aiju, CHEN Qingwang, Journal of Nuclear Mataerials Vol.179–181 (1991) 322

2) The Aspects of Diffusion And Permeation of Tritium Through TiC And TiN+TiC Blankets of 316L Stainless Steel

SHAN Changqi, WU Aiju et al., (to be published)

3) The Microstructure of The First Wall Constructural Materials Used in Fusion – Fission Hybrid Reactor

SHENG Zhongqi, XIAO Hong, PENG Feng, TI Zhongxin Private Communication

4) Radiation Effects on The First Wall Material of Fusion Technology

YU Jinnan et al., Research Contract with IAEA

# GAPHYOR DATA CENTRE
# Progress Report 1990-1991

J-L DELCROIX, K. KATSONIS

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

## 1. SOME STATISTICS.

As of the 15th of September 1991, 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 .

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

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

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

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

| SECTION 1 Structure | | SECTION 2 Photon.Coll.. | | SECTION 3 Electron. Coll | | SECTION 4 Atom.,Mol.Coll. | | SECTION 5 Macro.Prop | |
|---|---|---|---|---|---|---|---|---|---|
| EN | 71816 | AN | 1858 | SN | 1132 | SN | 1139 | PV | 1148 |
| CP | 271 | SN | 495 | SC | 469 | SP | 103 | FT | 1685 |
| DP | 3426 | SC | 315 | EL | 1752 | SC | 643 | VR | 154 |
| NP | 881 | EL | 208 | EX | 5118 | EL | 804 | ZT | 133 |
| PE | 2725 | FF | 84 | ER | 574 | EN | 2002 | CO | 135 |
| VR | 32166 | EX | 1722 | DX | 189 | EX | 2638 | DN | 656 |
| TR | 12813 | ER | 412 | XX | 464 | ER | 1195 | VI | 753 |
| IN | 1057 | DX | 104 | DO | 46 | DX | 8011 | CT | 818 |
| DT | 229 | XX | 65 | IN | 5035 | XX | 2317 | TD | 312 |
| DS | 1777 | DO | 89 | RC | 213 | DO | 295 | PE | 270 |
| XX | 79 | IN | 6416 | RR | 174 | TE | 2159 | EN | 2661 |
| EA | 1041 | DT | 536 | RE | 115 | IN | 7500 | DM | 58 |
| | | DS | 3517 | RO | 68 | TI | 29 | RN | 935 |
| | | P2 | cancelled | RD | 560 | DT | 984 | FE | 359 |
| | | P3 | cancelled | RS | 605 | LN | cancelled | CE | 160 |
| | | P4 | cancelled | AT | 1655 | LP | cancelled | ME | 625 |
| | | PN | cancelled | DT | 59 | MP | cancelled | DE | 177 |
| | | NL | 149 | DS | 893 | 20 | cancelled | PI | 490 |
| | | PR | 300 | BS | 223 | 10 | 4198 | AT | 452 |
| | | | | PR | 100 | 0- | 264 | DT | 70 |
| | | | | | | 1- | 7 | PC | 67 |
| | | | | | | IM | 352 | FI | 31 |
| | | | | | | RI | 464 | MI | 887 |
| | | | | | | XD | 659 | DI | 185 |
| | | | | | | CX | 3720 | DA | 41 |
| | | | | | | C1 | 1302 | RC | 162 |
| | | | | | | CA | 285 | RR | cancelled |
| | | | | | | S1 | 636 | RE | cancelled |
| | | | | | | SR | 135 | RO | cancelled |
| | | | | | | IR | 14965 | RD | cancelled |
| | | | | | | IH | 967 | RS | cancelled |
| | | | | | | IA | 88 | RI | cancelled |
| | | | | | | ID | 681 | LA | 928 |
| | | | | | | AS | 4371 | MD | 96 |
| | | | | | | AH | 205 | ST | 1121 |
| | | | | | | DS | 2949 | | |
| | | | | | | DH | 146 | | |
| | | | | | | KE | 701 | | |
| | | | | | | PR | 3548 | | |
| Σ | 128281 | Σ | 15821 | Σ | 19444 | Σ | 70462 | Σ | 15569 |

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

c) At a recent meeting we described the methods now used in GAPHYOR for covering four "new" fields :

Internal shell structure

Neutral or ionized clusters
Interaction of Atoms and Molecules with Solids
Isoelectronic series

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

**Table 3: Number of entries in "new" fields (18-09-91)**

| | Iso-electronic Series | Internal Shell Structures | Clusters | Gas Surface Interactions |
|---|---|---|---|---|
| | Info = I | Info = : | Info = 8 | Info = / ou - |
| 1 élément | 1778 | 440 | 529 | 285 |
| 2 éléments | 71 | 78 | 133 | 2313 |
| 3 éléments | 1 | 2 | 432 | 1096 |
| 4 éléments | 0 | 0 | 145 | 411 |
| Σ | 1850 | 520 | 1239 | 4105 |

# 2 CHANGES IN CLASSIFICATION SCHEME

## 2.1 Multiphoton processes

In the past we used the values P2,P3,P4,PN of process descriptor PR to code the multiphoton processes . We have decided to code now directly the number of acting photons in the initial state "molecules". This allows us to use for the process descriptor the usual values, like IN for ionization, EX for excitation, etc... For exemple the four photons ionization of Xenon is now written as :

$h\nu^4$ , Xe /IN/ e , $Xe^+$

which is more explicit that the older coding:

$h\nu$ , Xe /P4/ e , $Xe^+$

Consequently the values P2,P3,P4,PN have been cancelled in our list of values of the descriptor PR as shown in Table 2.

## 2.2 Charge transfer and associated processes

We have introduced a better description of charge transfer, ionization and related processes in collisions between heavy particles , using the following values of the descriptor PR :

Processes creating one or more new free electron:

IN Ionization
TI Transfer ionization
DT Detachment

Electron transfer processes completely resolved:

10 10 Charge transfer
0- 0- Charge transfer
1- 1- Charge transfer
IM Mutual ionization
RI Ion-ion recombination
XD Dissiociative charge transfer
CX Other charge transfers

Composite processes (mixture of processes above)

C1 One-electron capture
CA n-electrons capture
S1 One-electron stripping
SR n-electrons stripping

Consequently the values LN,LP,MP,20 have been cancelled in our list of values of the descriptor PR as shown in Table 2. We have also cancelled the value RI in section 5 (see discussion in sub-section below) .

## 2.3 Electron-ion recombination processes

In the early years of plasma physics most of the known information about electron-ion recombination processes was related to the "global" recombination coefficients ( rate of decay of electron density ). This information was put in section 5 of GAPHYOR ( with the value RC of descriptor PR )

More recently the detailed analysis of recombination led to calculation and measurement of specific rates for a given mechanism. For these we use the following values of PR :

RR Radiative e-i recombination
RE Three-body e-e-i recombination
RO Three-body e-e-o recombination
RD Dielectronic e-i recombination
RS Dissiociative e-i recombination

We put this kind of information in section 3 ( electronic collisions ). But as a result of history we were until recently using the five specific values above also in section 5 (macroscopic properties) . We have decided to stop this rather unsatisfying procedure. Consequently the values RR,RE,RO,RD,RS have been cancelled in our list of values of the descriptor PR in section 5 as shown in Table 2 .

# 3 DIRECT ENTRY AND UPDATING SITUATION

We have described last year a recent development : 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 on a disket, which is then entered into the main system .This new working method , which is beeing adopted by an increased number of our fiteen experts, has many advantages :

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

As a result, the speed of up-dating of GAPHYOR is shown in Table 4 . It is convenient to specify this by a coefficient that we call the "updating rate" UP.

The notations in this Table are, for each searched journal :

$\Sigma$ = Total number of entries

F89 = Number of entries (Publication year = 89)

F90 = Number of entries (Publication year = 90)

F91 = Number of entries (Publication year = 91)

NY = Number of effective years (80-89 period of publication)

Av 80-89 = Annual average number of entries (80-89)
UP89 = Updating rate 89 = 100*F89/Av 80-89
F12=Number of entries for the last 12 monthes (stopping at month -6)
UP12 = Updating rate for the last 12 monthes (stopping at month -6)
= 100*F12/Av 80-89
Rank = Rank of journals by total number of entries

The normal value of the updating rate is 100. The differences between the actual value of this rate and the normal value are the object of the following comments in the last column of Table 4 :

| | |
|---|---|
| ***D | Direct entry, excellent situation and short delay |
| *** | Excellent situation |
| ** | Good situation |
| * | Fair situation |
| N | A new expert has been recently elected to improve the situation |
| N? | GAPHYOR is looking for a new expert |
| CONF | Conference |
| THES | Theses |
| END | Terminated Journal ( new name, ...) |
| NEW | New Journal |

One can see that the updating situation has improved since two years. Situation is excellent for journals where we use direct entry ( 2 monthes delay only for Phys.Rev.A ). There are still a few cases (see cells shown as 0? , like CHPL, JP/B, CHPH, JFII,PSC, russian journals) where some improvement is needed. .We are presently working on these journals .

**Table 4 : UPDATING RATES of GAPHYOR ( 15-09-91 )**

| Rank | CODE | Journals | Σ | F89 | F90 | F91 | F<80 | NY | Av 80-89 | UP89 | F12 | UP12 | Rem. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | JCP | J.Chem.Phys. | 45510 | 2711 | 3269 | 907 | 17022 | 10 | 2431 | 112 | 3359 | 138 | ***D |
| 2 | PR/A | Phys.Rev. A | 15011 | 1667 | 1647 | 1174 | 6183 | 10 | 601 | 278 | 2409 | 401 | ***D |
| 3 | JPC | J.Phys.Chem. | 13868 | 1683 | 1819 | 0 | 1962 | 10 | 1009 | 167 | 1364 | 135 | *** |
| 4 | CHPL | Chem.Phys.Letters | 12512 | 0? | 634 | 0 | 5676 | 10 | 620 | 0 | 476 | 77 | *** |
| 5 | JP/B | J.Phys. B | 11440 | 0? | 0? | 0 | 5981 | 10 | 546 | 0 | 0 | 0 | N |
| 6 | JRD | J.Ph.Ch.Ref.Data | 9676 | 395 | 285 | 73 | 3258 | 10 | 606 | 65 | 287 | 47 | ** |
| 7 | ADND | At.Data,Nucl.Tab. | 7516 | 1042 | 978 | 433 | 989 | 10 | 512 | 204 | 1167 | 228 | ***D |
| 8 | EACC | Ph.El.At.Co.(cont) | 6619 | | | | 2104 | 10 | 452 | | | | CONF |
| 9 | JACS | J.Am.Chem.Soc. | 6366 | 132 | 890 | 0 | 4364 | 10 | 111 | 119 | 668 | 600 | ***D |
| 10 | JMSC | J.Mol.Str.(Th-Ch) | 5853 | 890 | 645 | 107 | 0 | 8 | 680 | 131 | 591 | 87 | ***D |
| 11 | IJMS | I.J.Mass Spectr. | 5622 | 349 | 522 | 0 | 2232 | 10 | 287 | 122 | 392 | 137 | *** |
| 12 | JMSP | J.Mol.Spectr. | 5250 | 254 | 314 | 0 | 1668 | 10 | 327 | 78 | 236 | 72 | *** |
| 13 | CHPH | Chem.Phys. | 4676 | 0? | 494 | 0 | 1760 | 10 | 242 | 0 | 371 | 153 | ***D |
| 14 | MOL | Mol.Phys. | 3572 | 193 | 145 | 0 | 1411 | 10 | 202 | 96 | 109 | 54 | *** |
| 15 | THCA | Theor.Chem.Acta | 3443 | 68 | 137 | 0 | 1364 | 10 | 194 | 35 | 103 | 53 | *** |
| 16 | JFII | J.Ch.Soc.Farad.tr.II | 3371 | 183 | 0? | 0 | 1662 | 10 | 171 | 107 | 0 | 0 | N |
| 17 | JMSR | J.Mol.Struct. | 3069 | 345 | 350 | 33 | 777 | 10 | 191 | 181 | 296 | 155 | ***D |
| 18 | PSC | Physica Scripta | 2901 | 366 | 0? | 0 | 738 | 10 | 216 | 169 | 0 | 0 | N |
| 19 | IJCK | Int.J.Chem.Kinet. | 2848 | 282 | 378 | 124 | 140 | 10 | 221 | 128 | 408 | 185 | ***D |
| 20 | IJQC | Int.J.Quant.Chem. | 2413 | 35 | 0? | 0 | 693 | 10 | 172 | 20 | 0 | 0 | N |
| 21 | ZP/D | Z.Phys.D | 2310 | 726 | 279 | 298 | 0 | 4 | 495 | 147 | 507 | 102 | ***D |
| 22 | JQS | J.Quant.Sp.Rad.tr. | 2166 | 146 | 111 | 0 | 1190 | 10 | 87 | 169 | 83 | 96 | ***D |
| 23 | GECO | Gas.Electr.Conf. | 2139 | 0 | 170 | 0 | 698 | 10 | 127 | 0 | 128 | 100 | *** |
| 24 | JOSA | J.Opt.Soc.Am. | 2100 | 124 | 106 | 0 | 1056 | 10 | 94 | 132 | 80 | 85 | ***D |
| 25 | CJCH | Can.J.Chem. | 2026 | 28 | 0? | 0 | 811 | 10 | 122 | 23 | 0 | 0 | N |
| 26 | ZFKH | Zh.Fiz.Khim. | 1996 | 93 | 80 | 0 | 563 | 10 | 135 | 69 | 60 | 44 | ** |
| 27 | THES | Theses | 1950 | 11 | 1 | 0 | 1181 | 10 | 77 | 14 | 1 | 1 | THES |
| 28 | IPPJ | Pl.Ph.Rpt.(Nagoya) | 1938 | 17 | | | 624 | 10 | 131 | 13 | | | END |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 29 | CJP | Can.J.Phys. | 1784 | 43 | 72 | 0 | 991 | 10 | 72 | 60 | 54 | 75 | *** |
| 30 | OAS | Opt.and Spectr. | 1647 | 0? | 0? | 0 | 1365 | 10 | 28 | 0 | 0 | 0 | N? |
| 31 | PRL | Phys.Rev. Letters | 1557 | 179 | 0? | 53 | 889 | 10 | 62 | 291 | 53 | 86 | ***D |
| 32 | BBUN | Ber.Bunsen Ph.Ch. | 1343 | 72 | 96 | 0 | 477 | 10 | 77 | 94 | 72 | 94 | *** |
| 33 | INOR | Inorg.Chem. | 1340 | 131 | 162 | 43 | 313 | 10 | 82 | 159 | 165 | 200 | ***D |
| 34 | PL/A | Phys.Lett. A | 1326 | 0? | 0? | 0 | 939 | 10 | 39 | 0 | 0 | 0 | N |
| 35 | JESP | J.Electr.Spectr. | 1283 | 43 | 28 | 0 | 633 | 10 | 62 | 69 | 21 | 34 | ** |
| 36 | BCSJ | Bull.Chem.Soc.Jap. | 1225 | 26 | 22 | 0 | 630 | 10 | 57 | 45 | 17 | 29 | ** |
| 37 | JFI | J.Ch.Soc.Farad.tr.I | 1130 | 45 | 0? | 0 | 641 | 10 | 49 | 92 | 0 | 0 | |
| 38 | ZN/A | Z.Naturforschung A | 1070 | 0? | 0? | 0 | 797 | 10 | 27 | 0 | 0 | 0 | |
| 39 | APJ | Astrophys.J. | 1064 | 68 | 42 | 0 | 622 | 10 | 40 | 170 | 32 | 79 | *** |
| 40 | JCPB | J.Ch.ph.Ch.bio. | 1052 | 115 | 88 | 0 | 275 | 10 | 69 | 167 | 66 | 96 | *** |
| 41 | APL | Appl.Phys.Letters | 1027 | 0? | 0? | 0 | 664 | 10 | 36 | 0 | 0 | 0 | |
| 42 | EACI | Ph.El.At.Co.(inv) | 977 | | | | 153 | 10 | 82 | 0 | 0 | 0 | CONF |
| 43 | JDP | J.de Phys. | 951 | 16 | 33 | 0 | 476 | 10 | 44 | 36 | 25 | 56 | *** |
| 44 | AAMP | Adv.At.Mol.Phys. | 928 | | | | 202 | 10 | 73 | 0 | 0 | 0 | ADV |
| 45 | KNCT | Kinet.and Catalys. | 923 | 83 | 6 | 0 | 315 | 10 | 60 | 138 | 5 | 7 | * |
| 46 | ARPC | Ann.Rev.Ph.Chem. | 916 | | | | 141 | 10 | 78 | 0 | 0 | 0 | ADV |
| 47 | JPHT | J.Photochem. | 863 | 54 | 17 | 0 | 404 | 10 | 44 | 122 | 13 | 29 | ** |
| 48 | IJQS | I.J.Quant.Ch.Symp. | 853 | 0? | 0? | 0 | 208 | 10 | 65 | 0 | 0 | 0 | CONF |
| 49 | ZP/A | Z.Phys. A | 803 | | | | 591 | 10 | 21 | | | | END |
| 50 | JAPH | J.Appl.Phys. | 799 | 12 | 1 | 0 | 287 | 10 | 51 | 23 | 1 | 1 | N |
| 51 | PH/A | Physica A | 798 | 0? | 0? | 0 | 672 | 10 | 13 | 0 | 0 | 0 | N |
| 52 | OPTC | Opt.Communic. | 794 | 0? | 0? | 0 | 436 | 10 | 36 | 0 | 0 | 0 | N |
| 53 | JDPC | J.de Phys.Colloques | 772 | 435 | | | 198 | 10 | 57 | 758 | | | END |
| 54 | JETP | Sov.Ph.J.E.T.P. | 748 | 0? | 0? | 0 | 712 | 10 | 4 | 0 | 0 | 0 | N |
| 55 | JPJ | J.Phys.Soc.Jap. | 707 | 0? | 0? | 0 | 481 | 10 | 23 | 0 | 0 | 0 | N |
| 56 | IJPP | Ind.J.Pure Appl.Ph. | 698 | 0? | 0? | 0 | 298 | 10 | 40 | 0 | 0 | 0 | N |
| 57 | TCCH | Top.Current Chem. | 698 | 175 | | | 67 | 10 | 63 | 277 | 0 | 0 | ADV |
| 58 | IJPB | Ind.J.Phys. B | 664 | 0? | 0? | 0 | 179 | 10 | 49 | 0 | 0 | 0 | N |
| 59 | ORNL | Oak Ridge N.L.Rpt. | 645 | 12 | 189 | 0 | 228 | 10 | 23 | 53 | 142 | 622 | ***D |
| 60 | FRDD | Farad.Disc.Ch.Soc. | 640 | 16 | 3 | 0 | 279 | 10 | 36 | 45 | 2 | 6 | * |
| 61 | USPN | Usp.Fiz.Nauk | 637 | 0? | 0? | 0 | 474 | 10 | 16 | 0 | 0 | 0 | N? |
| 62 | SPCA | Spectroch.Acta A | 596 | 31 | 69 | 0 | 303 | 10 | 22 | 138 | 52 | 231 | *** |
| 63 | OASK | Optik. i Spektr. | 482 | 0? | 0? | 0 | 31 | 10 | 45 | 0 | 0 | 0 | N |
| 64 | NIFD | Nagoya (Data Rpt) | 466 | | 441 | 25 | 0 | 0 | 0 | | 356 | 0 | NEW |
| 65 | JP/D | J.Phys. D | 441 | 16 | 0 | 0 | 207 | 10 | 23 | 68 | 0 | 0 | N |
| 66 | ZSKH | Zh. Strukt. Khim. | 433 | 0? | 0? | 0 | 263 | 10 | 17 | 0 | 0 | 0 | N? |
| 67 | PRLA | Proc.Roy.Soc. A | 418 | 0? | 0? | 0 | 398 | 10 | 2 | 0 | 0 | 0 | N |
| 68 | HTSU | High Temp. | 334 | 0? | 0? | 0 | 189 | 10 | 15 | 0 | 0 | 0 | N? |
| 69 | PH/B | Physica B+C | 334 | 0? | 0? | 0 | 184 | 10 | 15 | 0 | 0 | 0 | N |
| 70 | APPA | Acta Phys. Pol. A | 322 | 0? | 0? | 0 | 169 | 10 | 15 | 0 | 0 | 0 | N? |
| 71 | CR/B | Compt.R.Ac.Sc.B | 316 | 0? | 0? | 0 | 284 | 10 | 3 | 0 | 0 | 0 | N |
| 72 | SPLT | Spectrosc. Letters | 296 | 0? | 0? | 0 | 204 | 10 | 9 | 0 | 0 | 0 | N |
| 73 | ASAR | Astron.,Astroph. | 286 | 0? | 0? | 0 | 217 | 10 | 7 | 0 | 0 | 0 | N |
| 74 | JILA | J.I.L.A. Repts. | 266 | 0? | 0? | 0 | 21 | 10 | 25 | 0 | 0 | 0 | N |
| 75 | BEPL | Beitr.Plasma Phys. | 265 | 0? | 0? | 0 | 13 | 10 | 25 | 0 | 0 | 0 | N |
| 76 | LTFS | Litov.Fis.Sbor. | 264 | 0? | 0? | 0 | 193 | 10 | 7 | 0 | 0 | 0 | N? |
| 77 | PIGC | Phen.ion.gas.(cont) | 262 | | | | 262 | 10 | | | | | CONF |
| 78 | JGPR | J.Geophys.Res. | 257 | 0? | 0? | 0 | 164 | 10 | 9 | 0 | 0 | 0 | N |
| 79 | PLCH | Plas.Ch.(Symp.) | 248 | | | | 12 | 10 | 24 | 0 | 0 | 0 | CONF |
| 81 | ATPH | Int.Conf.At.Phys. | 228 | | | | 193 | 10 | 4 | 0 | 0 | 0 | CONF |
| 82 | SPTP | Sov.Ph.Tech.Ph. | 223 | 0? | 0? | 0 | 190 | 10 | 3 | 0 | 0 | 0 | N? |
| 83 | APOP | Appl.Optics | 209 | 0? | 0? | 0 | 114 | 10 | 10 | 0 | 0 | 0 | N |
| 84 | PCPP | Plas.Ch.Plas.Proc. | 173 | 0? | 0? | 0 | 0 | 9 | 20 | 0 | 0 | 0 | N |
| 85 | ZTF | Th. Tekh. Fiz. | 164 | 0? | 0? | 0 | 91 | 10 | 7 | 0 | 0 | 0 | N? |
| 86 | APJS | Astroph.J.Supp. | 161 | 0? | 0? | 0 | 135 | 10 | 2 | 0 | 5 | 225 | *** |
| 87 | TEKH | Theor. Exper. Kh. | 149 | 0? | 0? | 0 | 110 | 10 | 4 | 0 | 0 | 0 | N? |
| 88 | EUPL | Europhys.Letters | 148 | 22 | 21 | 0 | 0 | 4 | 36 | 61 | 16 | 43 | ** |
| 89 | ZNKH | Zh. Neorg. Khim. | 142 | 0? | 0? | 0 | 49 | 10 | 9 | 0 | 0 | 0 | N? |
| 90 | MNRS | M.Not.Roy.Astr.S. | 135 | 0? | 0? | 0 | 82 | 10 | 5 | 0 | 0 | 0 | N? |
| 91 | IVZF | Izv.Vys. Ush. Phys. | 134 | 0? | 0? | 0 | 103 | 10 | 3 | 0 | 0 | 0 | N? |
| 92 | SUSR | Surf.Sc. Repts | 134 | 0? | 0? | 0 | 0 | 8 | 18 | 0 | 0 | 0 | N? |
| 93 | ZETL | ZETP. Letters | 100 | 0? | 0? | 0 | 79 | 10 | 2 | 0 | 0 | 0 | N? |
| 94 | NJDC | Nouveau J.de Chim. | 98 | 0? | 0? | 0 | 45 | 9 | 6 | 0 | 0 | 0 | N? |
| 95 | DOKN | Dok.Ak.Nauk SSSR | 97 | 0? | 0? | 0 | 80 | 10 | 2 | 0 | 0 | 0 | N? |
| 96 | KVYE | Kym. Vys. Energ. | 89 | 0? | 0? | 0 | 61 | 10 | 3 | 0 | 0 | 0 | N? |
| 97 | JNBS | J.Res.Nat.Bur.St. | 83 | 1 | 0 | 0 | 62 | 10 | 2 | 48 | 0 | 0 | N? |
| 98 | CZJB | Czek. J. Phys. B | 26 | 0? | 0? | 0 | 20 | 10 | 1 | 0 | 0 | 0 | N? |
| 99 | IVZK | Izv.Vys.Ush.Khim. | 25 | 0? | 0? | 0 | 23 | 10 | 0 | 0 | 0 | 0 | N? |
| 100 | OSPK | Opt.y Sp.Sbor.Stat. | 13 | 0? | 0? | 0 | 0 | 10 | 1 | | | | N? |
| | | Totals | 229640 | 13335 | 14550 | 3270 | 86695 | | 13036 | 5491 | 14183 | 4864 | *** |

## 4. Numerical Data Base

It was reported in previous meetings that a numerical data base has been created on the basis of the commercial data base manager R:base System. The support has been further improved using the last version of R:base (5.01) which allows fully relational handling and compatibility with other commercial packages as DBase, for Intel i80x86-based personal computers and workstations. The advantage of this scheme is flexibility and the possibility to directly include an existing bibliographic and factual part, consisting of the information contained in GAPHYOR for the publication and the reaction corresponding to each entry. Also, the relational support allows a simple and very handy use of the data base. Nevertheless, in the light of prior discussions in the frame of this Network meetings, it appears that such DBM are recommended for special purposes i.e. implementation of inhomogeneous data collections for industrial application, illustration of bibliographic collections, manipulation of huge data collections etc. In any case, systematic collection of a wide spectrum of numerical data on the basis of relational DBM is outside the scope of the GAPHYOR team due to its very restricted manpower.

The solution for the numerical data ordering for concrete applications can only be found in the construction of smaller homogeneous collections on the basis of object-oriented schemes which can potentially palliate the lack of a dedicated expert system. For the needs of the A+M data for fusion, ALADDIN has been now widely used by the data centers and collaborating Laboratories and it is hoped that its systematic use will improve the standardization and exchange of such data. With the increasing compatibility of the commercial DBM packages the problem of bridges between the various proprietary numerical data collections kept locally and ALADDIN will be easily resolved.

In Orsay we have calculated and evaluated a considerable amount of atomic data which is continuously increasing. These data will be eventually implemented in ALADDIN, whenever the available manpower will allow the realization of the processes of verification and of input. As has been previously reported, the ALADDIN program provided by the IAEA has been successfully compiled with the most common Fortran compilers ( SVS, NDP ) and in various systems.

The collected data are coming from calculations often included in the frame of coordinated research programs (CRP) initiated by the IAEA A+M Data Unit and are resulting from application of the classical trajectory Monte Carlo (CTMC) method (see report to the forthcoming 'Atomic and Molecular Data for Fusion Plasma Impurities' CRP meeting) in the 1 to 5000 keV/amu energy range for collisions of low-, medium-, and high-Z ions, with H and He targets. For the moment being, cross sections for C, Ne, Al, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, and I ions have been compiled. These data are relevant to magnetic and inertial fusion applications.

# Activities in the A+M data in 1990-91 at Nuclear Data Centre (NDC) of Physics and Power Engineering Institute, Obninsk, USSR

V. Piksaikin, V. Malinovsky

## Introduction

The program of investigations of atomic processes and compillation of appropriate atomic and molecular data for nuclear excited plasmas is now in progress at the Physics and Power Engineering Institute.

## Compillation and evaluation of double-differential ionization cross sections

Compillation and evaluation of the experimental data work is in progress at the NDC on differential cross sections for ejection of electrons from isolated atoms and molecules by protons and heavy ions impact in the energy range from tens keV to several MeV/a.m.u. Cross sections differential in energy and angle of ejected electron were considered.

The singly differential cross sections for Ar were fitted by analytical formulae based on theoretical consideration of atomic ionization process. In fitting procedure a linear least square method (LSM) is used. This method allows to use in evaluation the results of several authors, makes it possible to include both random and systematic errors and finally to obtain recommended data.

For few parameters used in fitting procedure good agreement was obtained between the experimental results and fitting curves. As an example in Fig.1. the experimental results of singly differential ( in electron energy ) ionization cross section for proton-argon collisions and fitting LSM curve are shown for proton energy of 0.5 MeV.

## Experimental research

### 1. Measurements of doubly-differential cross sections for electron ejection in ion-atom collisions

Under the program an experimental set-up for measurement of energy and angular distributions of electrons ejected in collisions of ions with atoms and molecules of gases was put into operation.

The set-up comprises ion beam collimation system, target (gas cell) providing single ion-atom (or molecule) collision, electron-energy analyzer, vacuum system, system of registration of scattered at different angles ions that provides possibility to measure electron spectra in coincidence with scattered ions, i.e. for fixed impact parameter.

The doubly-differential electron ejection cross sections in argon by proton impact from 0.6 to 1.5 MeV were measured.

### 2. Measurement of X-ray production cross sections.

Technique for measurement of the characteristic X-rays production cross sections for excitation of inner shells of atoms by protons and helium ions with energies from 0.5 to 2.2 MeV was developed at the Institute.

Set-up is installed on the beam line of the Van-de-Graaf electrostatic accelerator and includes scattering chamber, Faraday cup for measuring incident ion current, detector of ions scattered by target atoms and characteristic X-rays spectrometer.

X-ray production cross sections were measured for L-emission of Au atoms by proton impact in the energy range 0.8-2.2 MeV.

### 3. Measurement of doubly differential ionization cross

section for fission fragments - He collisions [1].

The doubly differential ionizations cross sections have been measured for fission fragments -He collisions. The electron ejection angles were $30^{o}, 45^{o}, 60^{o}, 90^{o}$ and electron energy was 10eV to 1.5keV. Gas target was the atom beam and $^{252}Cf$ layer was used as a source of fission fragments. The electron spectra were measured by using time-of-flight technique. The experimental results are compared with theory calculations.

The total ionization cross sections measured is in good agreement with theory consideration.

On the basis of the obtained experimental results the ionization energy loss of fission fragments in the He gas were calculated.

In Fig.2 doubly-differential ionization cross sections for fission fragments - He gas collisions are shown.

In Fig.3 singly differential ionization cross section for light and heavy fission fragments - He gas collisions is shown.

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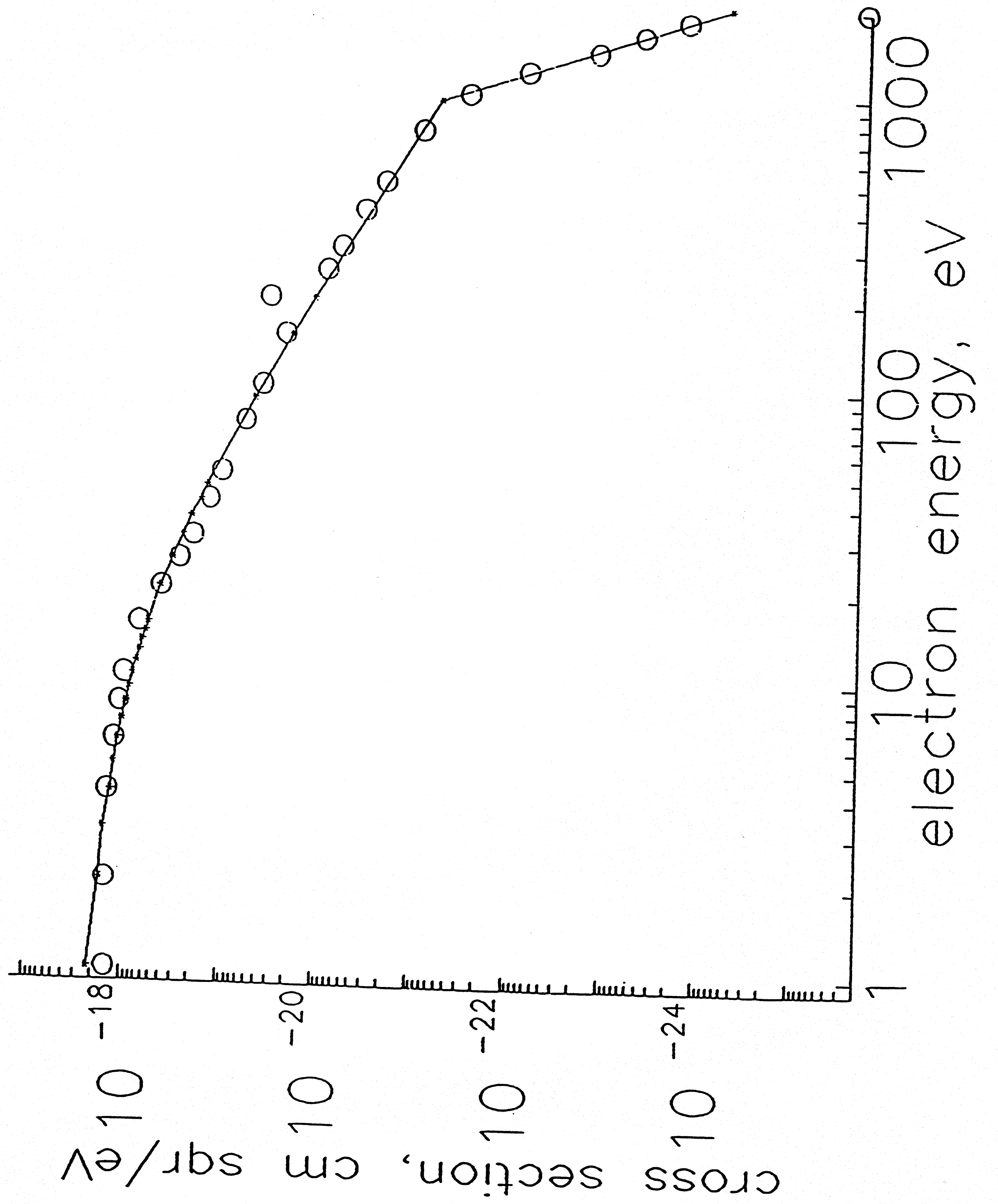
cross section, cm sqr/eV
$10^{-18}$
$10^{-20}$
$10^{-22}$
$10^{-24}$
electron energy, eV
1
10
100
1000

Fig. 1

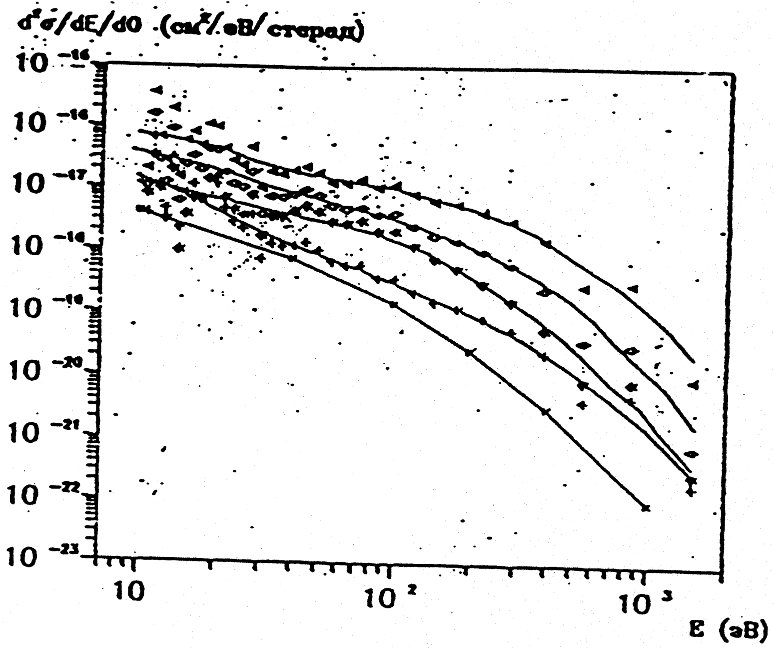
d²σ/dE/dΩ (см²/эВ/стерад)
10 ⁻¹⁵
10 ⁻¹⁶
10 ⁻¹⁷
10 ⁻¹⁸
10 ⁻¹⁹
10 ⁻²⁰
10 ⁻²¹
10 ⁻²²
10 ⁻²³
10
10 ²
10 ³
E (эВ)

Fig. 2.

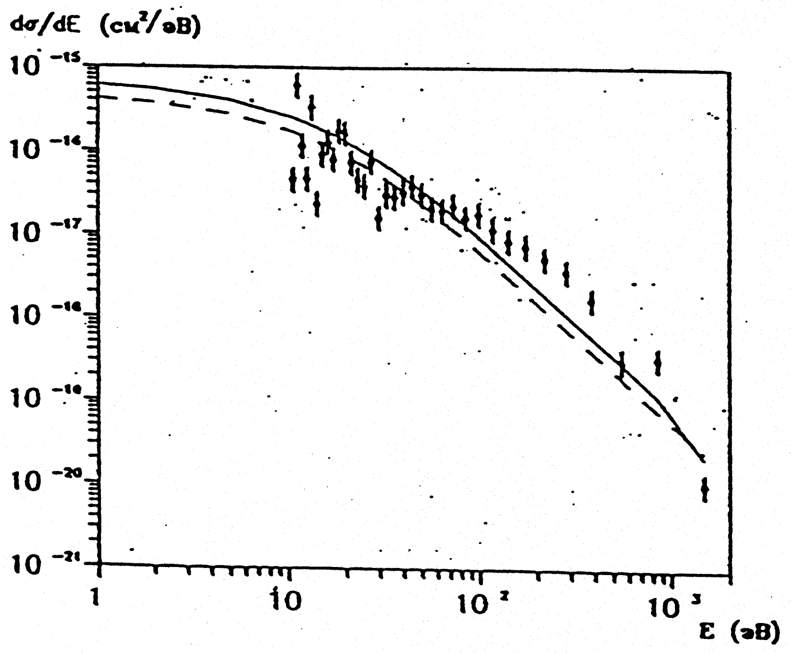
dσ/dE (см²/эВ)
10 ⁻¹⁵
10 ⁻¹⁶
10 ⁻¹⁷
10 ⁻¹⁸
10 ⁻¹⁹
10 ⁻²⁰
10 ⁻²¹
1
10
10 ²
10 ³
E (эВ)

Fig. 3

# Progress report for 1990-1991 at CRAAMD

Han Guoxing, Sun Yongsheng

IAPCM

P.O.Box 8009, Beijing, China

September, 1991

# OUTLINE

1. Data compilation and evaluation

2. Experiment

3. Theoretical calculation

Appendix 1.

Enclosed: CRAAMD-AM-7
-8
-9
-10

During the past year, we have fulfilled the following three tasks:

1. Data compilation and evaluation.

The work about the collection of electron-ion excitation for He-, Li-, Ne-, Mg-like ions have been completed. The collected data have been organized into library (or database), which includes original data (database A) and evaluated data or fitted coefficients (database B). The details of the compiled data are shown in Table I and Table II, and the details of the evaluation for electron impact excitation of Ne-like... can be seen in the bulletins "CRAAMD-A+M-7 and 8".

Table I: The library of references for electron impact exoitation
(up to Aug. 15, 1991)

| Name of datafile | Contents | Number of entres | Number of bytes |
|---|---|---|---|
| Ion.ph.A~ | | | 53,668 |
| Ion.potent.A~ | | | 168,532 |
| He-like.A | H.L.Zhang, D.H.Sampson<br>The Astrophys.J Supp.Series<br>63 487(1987) 8 < Z < 74, transitions<br>nlj-n'l'j', n,n'=1,2 | 840 | 643,365 |
| | F.P.Keenan, S.M.Mccann, A.E.Kingston<br>Physica_Scripta 35 432(1987) 1s2-nlj<br>n=2,3 Z=9-25 | 180 | |
| He-like.A₁ | K.A.Berrington, A.E.Kingston<br>J.Phys.B 20 6631(1987)He, nl-n'l'<br>n=1,2,3 n'=2,3 | 49 | 400,574 |
| | F.P.Keenan, S.M.Mccann, A.E.Kingston<br>Physica Scripta 35 432(1987) | 120 | |
| | H.L.Zhang, D.H.Sampson<br>The Astrophys. J.Supp.Series 63 487(1987) | 400 | |
| | A.K.Pradhan, D.W.Norcross, D.G.Hummer<br>The Astrophys.J 246 1031(1981) | 70 | |
| | N.R.Badnell J.Phys.B 218 955(1985) | 100 | |
| Li-like.A~ | H.L.Zhang ADNDT 44 31(1990)<br>Z=8-92 2lj-nlj n=3,4,5<br>66 Transitions RDW Method | 5,610 | 2,524,507 |

Table I (continued)

| | | | |
|---|---|---|---|
| Li-like.$A_1$* | H.L.Zhang ADNDT 44 31(1990)<br>Z=8-92 2l-nl n=3.4.5<br>25 Transitions RDW Method | 2.025 | 956.257 |
| Ne-like.H.A~ | P.L.Hagelstain ADNDT 37 121(1987)<br>Fe Se Y Mo Ag 666 Transitions<br>RDW Method | 3.330 | 224.988 |
| Ne-like.Z.A~ | H.L.Zhang ADNDT 43 1(1989)<br>Z=22-92 88 Transitions<br>RDW Method | 6.248 | 895.216 |
| Mg-like.A~ | A.K.Pradhan ADNDT 40 335(1988)<br>S Ar Ca Cr Fe Ni 120 Transitions<br>DW Method | 720 | 94.597 |
| He-like.B | From "He-like.A" | 1.020 | 327.270 |
| He-like.$B_1$ | From "He-like.$A_1$" | 739 | 204.049 |
| Li-like.B~ | From "Li-like.A" | 5.610 | 1.211.767 |
| Li-like.B1~ | H.L.Zhang ADNDT 44 31(1990)<br>z=8-92 2l-nl n=3.4.5<br>25 Transitions RDW Method | 2.025 | 459.000 |
| Ne-like.H.B~ | From "Ne-like.H.A" | 3.330 | 1.126.330 |
| Ne-like.Z.B~ | From "Ne-like.Z.A" | 6,248 | 2,116,794 |
| Mg-like.B~ | From "mg-like.A" | 720 | 237.180 |
| Ion.e.B | | | 140.656 |

Note: * in the Tape

Table II: Data organized into database in 1991

He-like ions

| Datafile | Contents | Entry number | Byte number |
|---|---|---|---|

## Table II (continued)

| | | | |
|---|---|---|---|
| He-like A | $1^1S-2^{(2S+1)}L_J$ <br> $2^{(2S+1)}L_J-2^{(2S'+1)}L'_{J'}$ <br> for Z=7-46 <br> $1^1S-3^{(2S+1)}L_J$ <br> for Z=9-25 | 1.020. | 643.365 |
| He-like B: | Fitted coefficients of He-like A | 1.020. | 327.270 |
| He-like $A_1$ | $1^1S-2^{(2S+1)}L$ <br> $2^{(2S+1)}L-2^{(2S'+1)}L'$ <br> for Z=2-46 <br> $1^1S-3^{(2S+1)}L$ <br> $2^{(2S+1)}L-2^{(2S'+1)}L'$ <br> for Z=2-46 <br> $1^1S-3^{(2S+1)}L$ <br> for Z=9-25 | 739. | 400.574 |
| He-like $B_1$: | Fitted Coefficients of He-like $A_1$ | 739. | 204.049 |
| Li-like A: | 2lj-nlj <br> n=3, 4, 5 <br> for Z=8-92 | 5.610. | 2.524.507 |
| Li-like B: | Fitted coefficients of Li-like A | 5.610. | 1.211.767 |
| Li-like $A_1$: | 2l-nl <br> n=3, 4, 5 <br> for Z=8-92 | 2.025. | 956.257 |
| Li-like $B_1$: | Fitted coefficients of Li-like $A_1$ | 2.025. | 459.000 |

## 2. Experiment.

(1) The emission spectra have been measured in collison between eleotron and He, Ne, Ar, Xe, H2 N2 systems. The wavelength range is 200-800 nm, the energy range of electrons is 200 eV-700 eV.

The task was done by Institute of Physics, Chinese Academy of Science, which is a member of CRAAMD. It has already been published at the XVII ICPEAC, Brisbane, Australia, July 10-16, 1991. The main results can be seen in Appendix 1.

(2) Total cross sections for electron scattering from Ne, Ar, $N_2$ have been measured in the impact energy range:

350-1200 eV, for Ne and Ar

250-1400 eV, for $N_2$.

The task was done by another member of CRAAMD, the University of Science and Technology of China, Hefei, Anhui Province. The main results are listed in Table III, IV, and V respectively. These results with an accuracy of 3.5% have been compared with available experimental, semi-empirical, and theoretical total cross sections.

Table III: Total cross section (in $a_0^2$)
for electron-Ne scattering

| | Exp. | | | | semi-empiric | | Theo. | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| E (ev) | This work | W[1] | G[2] | Z[3] | K[4] | H[5] | DWSBA[6] | QH[7] | MEP[8] | SEPDA[9] |
| 350 | 6.33 | 6.23 | | | | | | | | |
| 361 | | | | 5.82 | | | | | | |
| 400 | 5.50 | 5.76 | | 5.57 | 5.5 | 5.51 | 6.35 | 6.29 | 5.40 | 5.56 |
| 450 | 5.23 | 5.36 | | | | | | | | |
| 500 | 4.88 | 5.02 | | 4.93 | 4.8 | 4.77 | 5.47 | 5.45 | | |
| 550 | 4.77 | 4.67 | | | | | | | | |
| 576 | | | | 4.54 | | | | | | |
| 600 | 4.31 | 4.42 | | | 4.3 | | | | | |
| 650 | 4.13 | 4.20 | | | | | | | | |
| 700 | 3.89 | 4.03 | 4.16 | 3.85 | 3.9 | 3.88 | 4.37 | 4.40 | 3.84 | 3.87 |
| 750 | 3.82 | 3.88 | | | | | | | | 3.68 |
| 784 | | | | 3.68 | | | | | | |
| 800 | 3.71 | | 3.86 | | | | | | | |
| 850 | 3.50 | | | | | | | | | |
| 900 | 3.34 | | 3.47 | 3.36 | | | | | | |
| 950 | 3.24 | | | | | | | | | |

Table III (continued)

| | | | |
|---|---|---|---|
| 1100 | 3.04 | | |
| 1156 | | | 2.82 |
| 1200 | 2.86 | 2.80 | |

Table IV: Total cross section(in $a_0^2$) for electron-Ar scattering

| E (ev) | this work | W[1] | Z[2] | K[4] | N[10] | G[2] | H[6] | J[11] I | J[11] II |
|---|---|---|---|---|---|---|---|---|---|
| | exp. | | | | | | semi-empiric | theo. | |
| 350 | 16.4 | 16.09 | | | | | | | |
| 400 | 15.2 | 14.81 | 14.5 | 13.7 | | | 14.27 | 15.8 | 15.4 |
| 450 | 14.5 | 13.92 | | | | | | | |
| 500 | 13.8 | 13.08 | 12.8 | 11.8 | 13.9 | | 12.51 | 13.7 | 13.4 |
| 550 | 12.9 | 12.35 | | | | | | | |
| 600 | 12.1 | 11.71 | | 10.5 | 12.4 | | | | |
| 650 | 11.6 | 11.15 | | | | | | | |
| 700 | 11.2 | 10.62 | 10.4 | 9.5 | 11.5 | 10.92 | | 11.0 | |
| 750 | 10.6 | 10.13 | | | | | | | |
| 800 | 10.0 | | | 9.0 | 10.8 | 10.18 | | 10.1 | 10.0 |
| 850 | 9.51 | | | | | | | | |
| 900 | 9.43 | | 8.61 | | 10.1 | 9.29 | | | |
| 950 | 8.62 | | | | | | | | |
| 1000 | 8.41 | | 8.11 | | 9.50 | 8.61 | 7.86 | 8.64 | 8.65 |
| 1100 | 8.13 | | | | 8.54 | | | | |
| 1200 | 7.88 | | | | 7.68 | 7.29 | | | |

Table V: Total cross section(in $a_0^2$) for electron-$N_2$ scattering

| E (ev) | this work | D[12] | G[13] | B[14] | H[6] |
|---|---|---|---|---|---|
| 250 | 18.47 | | | 20.22 | |
| 258 | | 20.83 | | | |
| 300 | 17.89 | | | 18.14 | 17.34 |
| 324 | | 18.22 | | | |
| 350 | 16.08 | | | 16.53 | |
| 400 | 14.66 | 15.78 | | 15.25 | 14.54 |
| 450 | 13.75 | | | 14.15 | |

Table V (continued)

| | | | | | |
|---|---|---|---|---|---|
| 484 | | 13.65 | | | |
| 500 | 12.33 | | | 13.19 | 12.36 |
| 550 | 11.80 | | | 12.26 | |
| 576 | | 12.12 | | | |
| 600 | 10.92 | | 11.6 | 11.39 | 11.07 |
| 650 | 10.60 | | | 10.60 | |
| 676 | | 10.68 | | | |
| 700 | 10.18 | | 10.2 | 9.89 | 10.11 |
| 750 | 9.65 | | | 9.36 | |
| 784 | | 9.36 | | | |
| 800 | 9.26 | | | | |
| 850 | 8.73 | | 8.80 | | |
| 900 | 8.20 | 8.32 | | | |
| 950 | 7.81 | | | | |
| 1000 | 7.46 | | 7.62 | | |
| 1024 | | 7.57 | | | |
| 1100 | 7.24 | | | | |
| 1156 | | 6.82 | | | |
| 1200 | 6.93 | | 6.69 | | |
| 1296 | | 6.14 | | | |
| 1300 | 6.50 | | | | |
| 1400 | 5.94 | | | | |

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(3) X-ray attenuation coefficients and photoelectric cross sections of Sn have been measured. Using a new type x-ray source produced by proton excitation of

elementary or compound targets and Si(Li) detector system, mass attenuation coefficients of tin have been determined for the energy range from 3.3 to 28.1 keV. The experimental uncertainties of attenuation coefficients have been reduced to ±1% for intenser isolated characteristic x-rays. The total photoelectric cross sections have been obtained by subtracting scattering cross sections from the measured total cross sections.

The task was done by Institute of Low Energy Nuclear physics, Beijing Normal University, a member of CRAAMD. The details of this work can be seen in the bulletin "CRAAMD-A+M-8".

3. Theoretical calculation

(1) Influences of the Buttle correction on electron collision excitation of CIII was calculated. The R-matrix method is being used to re-calculate the collisional excitation cross sections between the $2s^2\ ^1S$, $2s2p\ ^3P^o$, $^1P^o$ and the $2p^2\ ^3P$, $^1D$, $^1S$ target eigenstates CIII. The wrong CI wavefunctions in earlier work are corrected. The effect of multi-channel coupling has been considered by including the Buttle correction. New results which have complex resonance structures are obtained and the reasons which bring about the result have been discussed.

This work was done by Institute of Atomic and Molecular Physics, Jilin University, Changchun, China. The details of this work can be seen in the bulletin "CRAAMD-A+M-10".

(2) Dielectronic recombination into the lowlying levels of Sodium-like germanium from the Neon-like ground state were calculated by IAPCM, the head institution of CRAAMD. The details of this work can be seen in the bulletin "CRAAMD-A+M-10".

Thank you !

*Appendix 1*

# ELECTRON COLLISION WITH He, Ne, Ar, Xe, AND $H_2$, $N_2$ INTO EXCITED STATES MEASURED BY OMA

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The emission spectra have been measured in collision between electron and He, Ne, Ar, Xe, $H_2$, $N_2$ systems using the Optical Multichannel Analysis System (OMA). The wavelength range is 200 ev-700 ev.

Fig.1 shows the emission spectra of HeI singlet and triplet lines in e + He collision system at 200 ev electron impaact energy.

Fig.2 shows the emission spectra of ArI, ArII lines in e + Ar collision system at 300 ev electron impact energy.

The emission spectra demonstracted one channel of excitation in e + He and e + Ne collision systems.

1. $e + A \rightarrow E + A^{-}(n, l) \rightarrow e + A + h\upsilon(AI)$

where A= He, Ne and two channels of excitation in e + Ar and e + Xe collision systems:

1. $e + B \rightarrow e + B^{-}(n, l) \rightarrow e + B + h\upsilon(BI)$
2. $e + B = 2e + B^{+-}(n, l) \rightarrow 2e + B^{+} + h\upsilon(BII)$

where B = Ar, Xe.

Fig.3 shows the emission spspectra of Balmer lines in e + $H_2$ collision system at 400 ev electron impact energy.

Fig.4 shows the emission spectra of NI lines in e + $N_2$ collision systemat at 200 ev electron impact energy.

The emissiom spectra demonstrated only one channel of excitation in e + $H_2$ and e + $N_2$ collision systems:

1. $e + H_2 \rightarrow e + 2H^{-}(n, l) \rightarrow e + H_2 +$ Balmer $\alpha, \beta, \gamma, \delta$

Balmer $\alpha$ : $\lambda$ = 656.3nm, Balmer $\beta$ : $\lambda$ = 486.1nm

Balmer $\gamma$ : $\lambda$ = 434.0nm, Balmer $\delta$ : $\lambda$ = 410.2nm

2. $e + N_2 \rightarrow e + 2N^{-}(n, l) \rightarrow e + N_2 + h\upsilon(NI)$

Namely, we have only observed the atomic spectra of Balmer lines and NI lines in collision between electron and $H_2$, $N_2$ molecules.

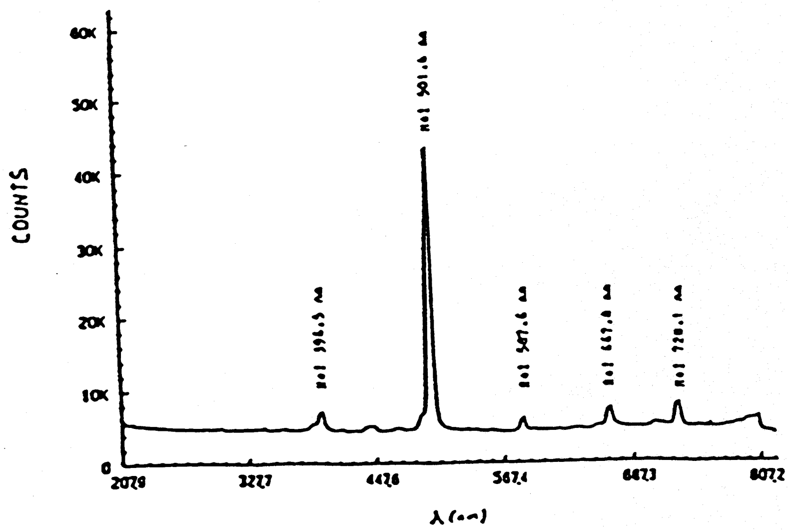


Fig.1 The emission spectra of HeI lines in e + He collision at 200 eV electron impact energy.

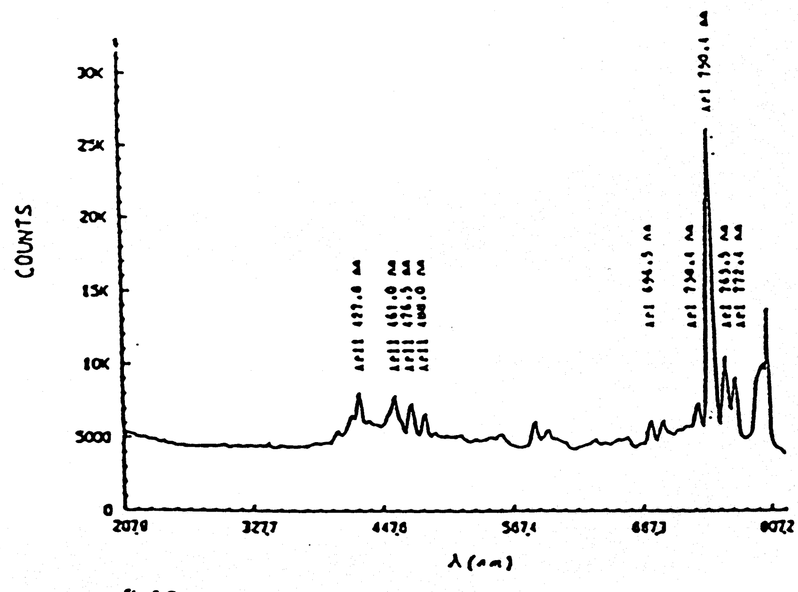


Fig.2 The emission spectra of ArI,ArII lines in e + Ar collision at 200 eV of electron energy.

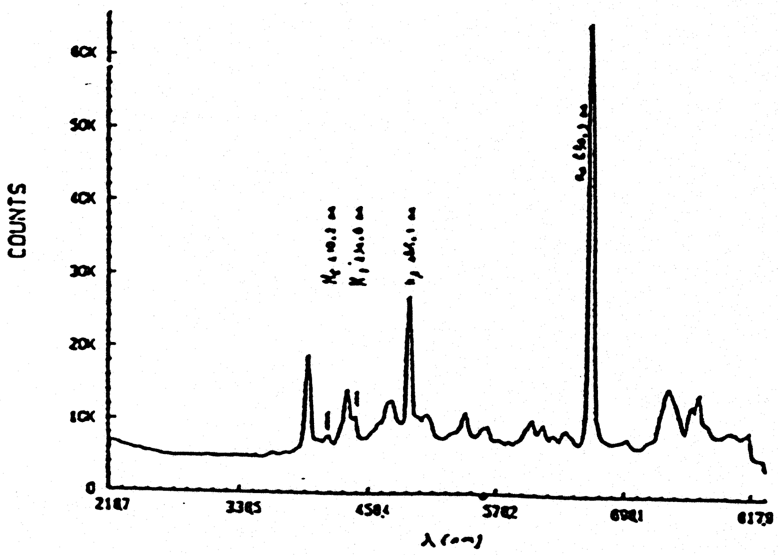


Fig.3 The emission spectra of Balmer lines in e + H$_2$ collision at [illegible] eV of electron energy.

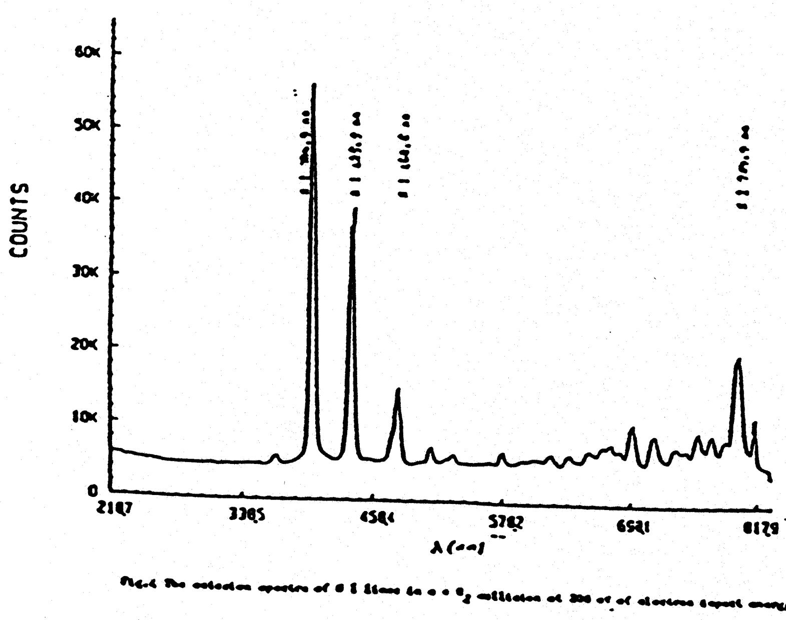


Fig.4 The emission spectra of [illegible] lines in e + [illegible] collision at [illegible] eV of electron impact energy.

## Computational activities on A+M Data at ENEA, Italy

by E.Menapace.

### 1. Electron-ion collision excitation data.

P.L.Ottaviani(1), G.C.Panini(1) and M.Frisoni (3)

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

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

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

### 2. Neutral-ion interaction cross sections and reaction rates.

E.Cupini, A.De Matteis (1)

2.1 Cross sections for plasma-neutral elastic collisions.

Approximate cross sections were computed for proton elastic collisions with atomic hydrogen and helium for energies (see Table 1) of interest in impurity control phisics of advanced fusion devices. For (H, H+) elastic reaction a repulsive potential from the literature (with corrections for misprints in the reference formulas) and, for (He, H+) one, the attractive-repulsive modified Morse potential were adopted. The computed cross sections were fitted with expressions like:

$$\ln \sigma(E_r) = \Sigma\, a_i (\ln E_r)^i$$

i.e. as function of the relative energy $E_r$.

The results were published as ENEA Report and partly on " Il Nuovo Cimento" Vol. 11D, n.10, 1489 (Oct. 1989).

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1. ENEA (INN), Dipartimento Sviluppo Tecnologie di Punta.
2. ENEA (INN), Progetto Materiali Metallici Innovativi.
3. Guest researcher.

Among those :

i) in Table 1 the coefficients "$a_i$" are quoted for (H,H+) and (He, H+) collisions with different values of the cut-off parameter Cmax referred to the approximation limit in the computed integrated cross section;

ii) elastic cross section (approximation Cmax = 0,99) of (H, H+) reaction (full line) and charge-transfer cross section are shown; in fig.3 elastic cross section of (He, H+) for different degrees of approximation were calculated;

iii) energy distributions of atomic H and He after elastic collisions are also presented as typical results from Monte Carlo simulation were estimated.

2.2 Algorithms for stable and fast computation of maxwellian rate coefficients of neutral-ion interactions in a fusion plasma (such as charge exchange, between hydrogen isotopes and between hydrogen and helium isotopes, and ionization by hydrogen isotope ions) developed in the past years and published as ENEA Report, were included in a proper FORTRAN code on ENEA IBM Computing system. Comparison with analytical approximations of the reaction rates by Galbraith et al. (Nucl. Fus. 19, 1047) showed the efficiency of the algorithms.

The referred ENEA Reports are available upon request.

**3. Electron-molecule collision data.**
A.Mengoni(1).

i) In collaboration with T.Shirai (JAERI) the theoretical estimate of electron-polar molecule collision data is in progress. Inclusion of the quadrupole interaction and of the vibrational excitation in the scattering process has been made in the frame of the "Algebraic-Eikonal Approximation".

The computational technique and the corresponding code have been developed for the calculation of differential cross sections within the Glauber diffractive theory, using the algebraic technique (The Vibron Model) for the evaluation of molecular structure quantities.

The calculated data have been extended to the e-HC1 collision process at electron energies of 20 eV. Comparison with the simple FBA (First Born Approximation) has been made.

These and other results are reported in a paper to be published in Phys. Rev. A (1991).

ii) Infrared transition intensities have been estimated in the frame of the Vibron Model for $H^{19}F$, $D^{19}F$, $H^{35}Cl$, $D^{35}Cl$, $H^{79}Br$ and $D^{79}Br$ molecules in collaboration with F. Iachello (Yale and Trento Universities) and A; Leviatan (LANL).

Intensity factors were calculated and compared with experimental data. Different approximations in the dipole operator have been analyzed with the conclusion that a "two-exponential" expansion is sufficient to reproduce the experimental results with satisfactory accuracy.

The paper has been published on Jour. Chem. Phys. 95 (1991), pag. 1449.

iii) The planned activity in the field covers the following arguments:

1) ion- and atom-diatom collision (elastic and inelastic processes). (In the near future).

2) Collision data for electron-polyatomic molecules, possibly releasing the Glauber approximation.

3) Structure of complex (polyatomic) molecules for fusion applications, using algebraic methods.

**4. Light atom interactions on metal surfaces.**

V.Rosato (2), A.Ventura (2) and G.Maino (1)

Microscopic scale simulations via Molecular Dynamics of the behavior of light atoms (H and He) with low incident energies ($E_{in}$<100 eV) interacting on metal surfaces and of the effects induced by the scattering events either on the projectile itself (reflection characteristics, penetration depth, energy losses) and on the target (thermal spikes, creation of surface defects, interaction of absorbed particles with lattice point defects) were estimated, in particular for He atoms impinging on a Ni surface at T=500 K.

In the explored $E_{in}$ range the Binary Collision (BC) approximation does not hold, thus inhibiting the use of codes like MARLOWE, TRIM etc..

The particle and energy reflection coefficients were evaluated, which results to be, particularly in the low energy range, systematically lower than those obtained by extrapolating the BC results. The energy distribution of the reflected particles shows, in the low energy regime, an important contribution at energies higher than the incident ones (gain of energy from the lattice, fig. 1).

It was put in evidence the existence of delayed reflection, i.e. of projectiles whose reflection event takes place well beneath the surface after the creation of lattice defects. Different mechanisms responsible of surface defects creation have been analysed. Thermal spike seems to be the most relevant for $E_{in}$>10 eV.

A strong interaction between He and Ni vacancies (E(He-V) = 2,45 eV) and a weaker one with interstitials in the dumbell configuration (E(He-dumbell) = 0.1 eV) have been estimated. These features can be at the origin of the migration of He atoms toward defective lattice regions, effect which provokes the onset of phenomena like embrittlement and swelling.

Interaction between protons and a Fe surface was estimated too in the same range of energies and at the same temperature of the previous case. An important improvement of this work consists in the introduction of a term in the Hamiltonian which allows to take into account the inelastic energy losses of the charged projectile.

The case of protons is qualitatively different from that of He as proton-metal interaction contains an attractive term which allows the sticking of the projectiles on the metal surface, particularly in the low incident energy regime. In fact it has been observed a sharp decrease of the reflection coefficient $C_R$=0,3 at $E_{in}$=1 eV which, at $E_{in}$=10 eV assumes its maximum value of $C_R$=0,68. For $E_{in}$<1 eV the reflection coefficient drops almost to zero; in these cases, particles remains on the top of the surface placed in the adsorbtion sites.

A FORTRAN code (SCATTER) has been developed and implemented on ENEA IBM computing system. The code has been tested as reliable for light atom interaction data estimate with transition metal surfaces.

TABLE 1

Coefficients in Eq.(7)
(Energies in eV, powers of 10 in parenthesis)

| | $H^+ + H$ | | | $He^+ + H$ | | |
|---|---|---|---|---|---|---|
| $E_r$ | < 60 | < 60 | < 60 | < 8 | < 9 | < 17 |
| $c_{max}$ | 0.95 | 0.97 | 0.99 | 0.95 | 0.97 | 0.99 |
| $a_o$ | -3.319(+1) | -3.306(+1) | -3.283(+1) | -3.391(+1) | -3.386(+1) | -3.371(+1) |
| $a_1$ | -3.428(-1) | -3.250(-1) | -2.937(-1) | -3.723(-1) | -3.612(-1) | -3.429(-1) |
| $a_2$ | -4.132(-2) | -3.713(-2) | -2.997(-2) | -1.022(-1) | -7.097(-2) | -4.477(-2) |
| $a_3$ | -1.032(-2) | -9.023(-3) | -6.621(-3) | -3.315(-2) | -2.014(-2) | -7.551(-3) |

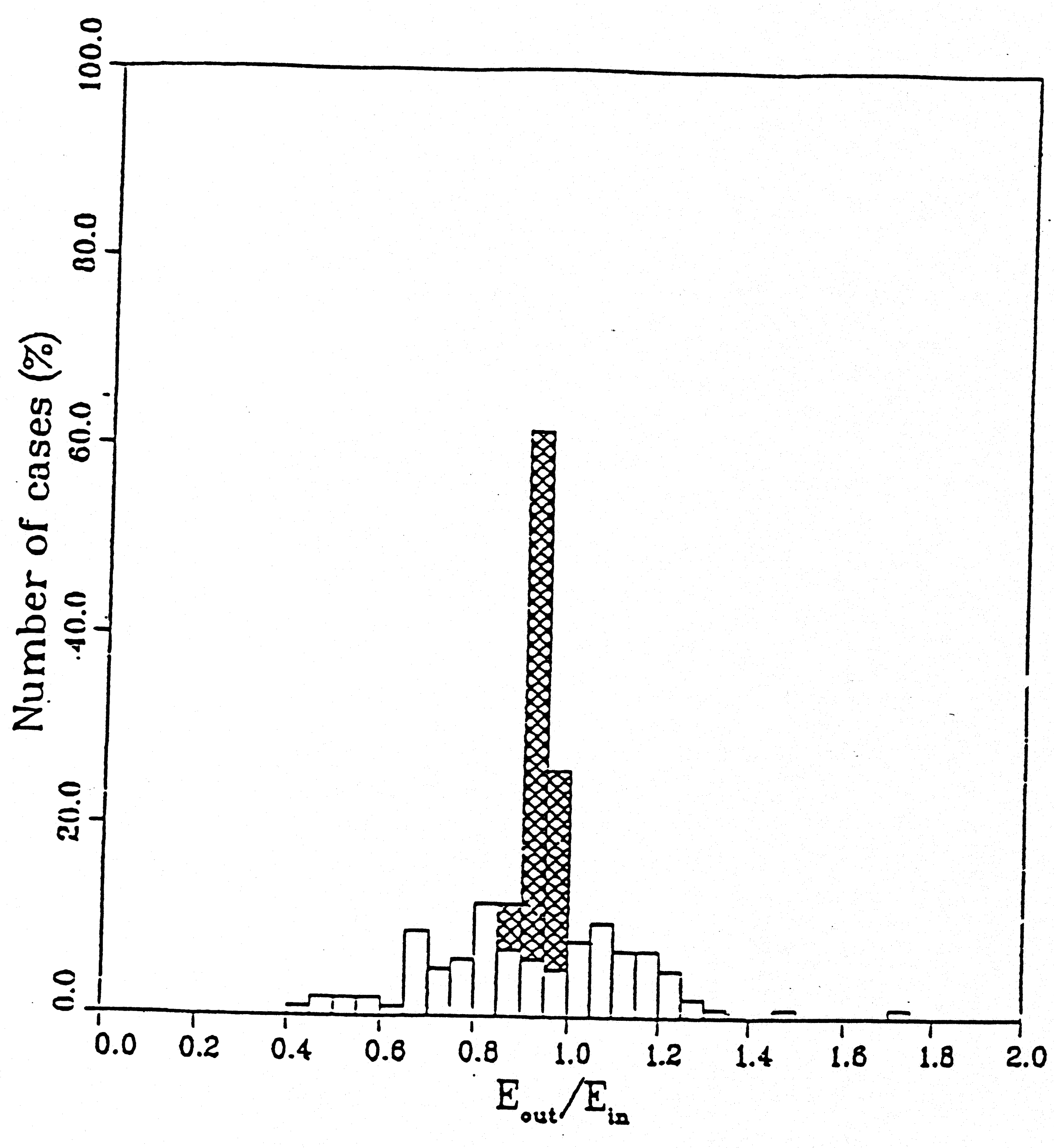


FIG. 1 Energy distribution of reflected He atoms at T=500°K for incident energy E=0,1 eV. Distribution for T=0 is shown for comparison.