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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

IAEA Consultants' Meeting: 8th Atomic and Molecular Data Centre Network Meeting

Vienna, 14, 15 September 1989

SUMMARY REPORT

Prepared by R.K. Janev

November 1989

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Abstract

This Summary Report contains the proceedings and the conclusions of the 8th Atomic and Molecular Dat Centre Network Meeting convened on September 14 and 15, 1989, in Vienna. The Progress Reports of the national atomic and molecular data centres, as well as the presentations on the ALADDIN system developments are also included as Appendices to the present Report.

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1. INTRODUCTION

On September 14 and 15, 1989, the IAEA Atomic and Molecular (A+M) Data Unit convened the regular, 8th Meeting of the Atomic and Molecular Data Centre Network, at the IAEA Headquarters in Vienna. The Meeting was organized to review the ongoing work and the near-future activity programmes of the national centres for atomic data for fusion, to analize the first experiences with the introduction of ALADDIN (the new A+M data exchange and management system) into data centre practices, and to consider some further developments of the system. The Meeting also discussed the next activities of the data centres and the IAEA A+M Data Unit in view of the recent recommendations (October, 1988) given by the Subcommittee on A+M Data for Fusion of the International Fusion Research Council (IFRC) regarding the near- and long-term priorities in the compilation, evaluation and production of A+M data for fusion. The Meeting Agenda is given in Appendix 1.

With two exceptions (Dr. F.J. Smith and Dr. Y. Nakai), all national Data Centres were represented at the Meeting (see Appendix 2: List of Participants). This includes also representatives from the newly established data centres or groups: Dr. Sun Yongsheng, from the Chinese Research Association for Atomic and Molecular Data (CRAAMD), Dr. Yao Jinzhang, from the Atomic Data Group of the Chinese Nuclear Data Centre, Beijing (CNDC), and Dr. V. Piksaikin, from the Atomic Data Group of the Nuclear Data Centre of the Institute for Physics and Energetics in Obninsk (USSR). Appart from the data centre representatives, the Meeting was attended also by Dr. R.E.H. Clark (LANL, USA) who extended ALADDIN to incorporate energy level and transition probability data, and by Dr. R. Hulse (PPPL, USA), the author of ALADDIN.

With respect to the previous Data Centre Network Meeting, held in Oak Ridge National Laboratory two years ago (October, 1987), this meeting was organized under circumstances which have two essential new elements: (1) the conceptual design activities of ITER and the recent developments in fusion research on the existing large tokamaks have introduced new A+M data requirements and certain shifts in A+M data priorities, and (2) adoption of ALADDIN (May, 1988) as a common A+M data exchange and management system. These new circumstances had a strong focussing effect on the recent Data Centre activities and on the programme of the 8th Data Centre Network Meeting. Other new circumstances are the expansion of the Data Centre Network (CRAAMD, CNDC, Obninsk), an overall increase of data evaluation activities, and extension of these activities to particle-surface interaction processes.

2. MEETING PROCEEDINGS

The Meeting Agenda included the following six sections:

Section 1: Ongoing and near-future programmes on A+M data compilation and evaluation in the data centres,

Section 2: IFRC Subcommittee recommendations on near- and long-term priorities in A+M data compilation and evaluation for fusion,

Section 3: The status of ALADDIN system and its introduction in data storage, exchange and management practices,

Section 4: Further developments of ALADDIN system,

Section 5: The ALADDIN System Manual, and

Section 6: Meeting conclusions and adoption of actions.

2.1. Current Data Centre Network Activities

In Section 1 Progress Reports were presented by each of the data centre representatives regarding the activities of the corresponding data centre during the last two years. For completeness, these Progress Reports are reproduced in Appendix 3. Some of the major accomplishments of the data evaluation activities in the A+M data centres include:

A. Spectroscopic data

1) Atomic transition probabilities: Scandium through Manganese (NIST),
2) Atomic transition probabilities: Iron through Nickel (NIST),
3) Spectroscopic data tables for Ti, Cr and Ni (NIST, in ORNL Redbook series, ORNL-6551/VI-3),
4) Spectral tables for the ions Fe VIII through Fe XXVI (NIST - JAERI colaboration),
5) Characteristics of X-ray transitions in multicharged ions of Ar, Cl and K (Kurchatov Institute, Moscow).

B. Collision data

1) Collisions of H, H_2, He and Li atoms and ions with atoms and molecules (prepared by C.F. Barnett, ORNL Redbook vol. 1),
2) Excitation rate coefficients of He and He-like ions (NIFS (ex IPPJ), Nagoya),
3) Electron-impact collision processes of hydrogen molecules (NIFS, Nagoya),
4) Database for H-beam penetration into fusion plasmas (IAEA A+M Data Unit),
5) Evaluated data for electron-impact processes in hydrogen-helium plasmas (Kurchatov Institute, Moscow),
6) Electron excitation collision strengths for Iron ions: FeI through FeXXVI (ENEA, Bologna),
7) Collision strengths for electron excitation of some Ti and V ions (Kurchatov Institute, Moscow).

C) Particle-surface interaction data

1) Sputtering of materials for the first wall and divertor plates of tokamak reactors (Kurchatov Institute, Moscow),
2) Total sputtering yields for monoatomic solids under ion impact (NIFS, Nagoya),
3) Angular distributions of sputtered atoms from monoatomic solids under ion impact (NIFS, Nagoya).

The data and/or bibliographic compilation activities have continued in all data centres. Details on these and other activities in the national data centres and in the IAEA A+M Data Unit are given in Appendix 3.

2.2. Near- and Long-Term Priorities in A+M Data Evaluation

In Section 2 of the Meeting, the participants discussed the Data Centre Network possibilities for implementation of the IFRC Subcommittee recommendations regarding the near- and long-term priorities in the A+M data evaluation for fusion, set at its 5th meeting (October 7-8, 1988) in Vienna. These priorities include:

1. Near-term priorities (1-2 years)

a) Completion of the database for e, H^+-H, H_2, H_2^+ processes (including isotopic variations),
b) Completion of the database for e, H^+, H_2, H-He, He^+, He^{2+} processes,
c) Completion of database for Fe^{q+}-e, H, H_2, He processes,
d) Database for e, H^+, H - C_kH_n, CO_k, $O(O_2)$ and OH processes.

2. Long-term priorities

a) Plasma edge processes (other than those included in 1),
b) Data for e-A^{q+}, A^{q+}-H, H_2, He processes (A=Ti, Cr, Ni) Cu,
c) Data for e-A^{q+}, A^{q+}-H, H_2, He processes (A=Be, B, Si, W),
d) Plasma-wall interaction processes (as specified at the AGM '89).

The Meeting participants accepted the above priorties as an action programme for their future work and deemed necessary to add to the list in 2c) also Mo, V, Al and Ge. They also discussed the question of completion of C^{q+}, O^{q+} and Fe^{q+} databases, and inclusion of data for radiative cooling rates (per atomic species) and data for other processes in these databases. It was concluded that the available evaluated data and the current evaluation (within the data centres) and data production activities (within the ongoing CRP on edge plasma A+M processes) cover most of the requirements mentioned in the above list of priorities.

The basis for accomplishment of the evaluated tasks set by the IFRC Subcommittee list of priorities is as follows:

1) C^{q+}, O^{q+} collisional databases

Data sources: ORNL Redbook vol.5, recent IAEA updates, recent (May, 1988) IAEA Specialists' Meeting (SM) on C^{q+} and O^{q+} (mostly for radiative and dielectronic recombination and state-selective electron capture-SSEC), recent Nagoya compilation on SSEC, recommendations of the recent IAEA SM on atomic database for neutral beam penetrations (April, 1989; for the excitation of H).

New processes to be included in the evaluated database (with respect to ORNL Vol.5):

- radiative and dielectronic recombination (RR + DR),
- state-selective electron capture,
- ion impact excitation of H, (scaling),
- radiative cooling rates (per species).

2) Fe^{q+} collisional database

Data sources: Nucl. Fusion Supplement (1987), Summers' (and others) data on DR, data on excitation of H from the recent IAEA SM on H-beam penetration (April, 1989), ORNL data on charge exchange for $q \leq 5$, new ionization data from Rivarola.

New data to be included (with respect to Nucl. Fus. Supplement):

- DR and RR,
- CX, $q \leq 5$,
- EXC of H by Fe^{q+} (scaling),
- radiative cooling rates.

3) e, H^+ - H, H_2, H_2^+ database

Data sources: ORNL Redbook Vol. 1, Janev et al book (Springer 1987), IAEA H-beam database, results from the ongoing IAEA CRP on plasma edge A+M data.

Particular attention to be paid to: vibrational EXC, particle interchange (PX) reactions, product energy/angular distributions.

4) e, H^+, H, H_2 - He, He^+, He^{2+} database

Data sources: ORNL Redbook Vol. 1, recent Kurchatov Institute e-He data recommendations, Janev et al book (Springer, 1987), results from the ongoing IAEA CRP on edge plasma A+M data.

5) e, H^+, H - C_xH_y (CO, CO_2, O_2, OH) database

Data sources: Nagoya Data Centre Compilations, Langer's PPPL-report, results from the ongoing IAEA CRP on edge plasma A+M data, IAEA evaluations of PX reactions.

6a) A^{q+} - e, H, H_2, He database (A = Ti, Cr, Ni)

6b) B^{q+} - e, H, H_2, He database (B = Be, B, Al, Si, Mo, W, V, Ge)

Collisional data are sparce and not systematically compiled (except for electron-impact ionization). Most of the data have to be yet produced. Actions adopted in producing the required data are given in Section 4 of this Report.

The Meeting participants were of the opinion that in view of the growing interest in Li-beam diagnostics (particularly for the edge plasmas), a database for the neutral Li (including excited states) should be set. Further, in connection with the importance of He-ash transport and exhaust in reactors, setting a separate database for He (He^+, He^{2+}) processes would be useful. The IAEA A+M Data Unit was asked to take appropriate actions along these directions. Establishment of an evaluated spectroscopic database for W was also suggested as a priority. In view of recent fusion research developments, data for Be, B and Ge also aquire certain priority.

2.3. Status and Further Developments of ALADDIN

Discussions in Sections 3-5 were devoted to the status and further developments of ALADDIN and its Manual. The reports from the all Data Centres within Section 3 showed that ALADDIN has been successfully introduced in the data management practices in several of the Data Centres (Oak Ridge, IAEA, Bologna, Los Alamos, GAPHYOR), and that its introduction is underway in the other centres (Nagoya, Kurchatov Institute, Obninsk, CRAAMD, JAERI). No substantial problems with the application of ALADDIN in A+M databases were reported. Data exchange using ALADDIN has so far been accomplished between ORNL and PPPL (Princeton), ORNL and IAEA A+M Data Unit, and IAEA and Bologna (ENEA). All the recommended collisional data sets stored at the IAEA A+M Data Unit (the C^{q+}, O^{q+}, Fe^{q+} - databases, the H-beam penetration database, the Belfast electron-impact ionization database) are now formatted in ALADDIN format. The data in the new ORNL Redbook vol. 1, and the data contained in Janev et al book (Springer, 1989) are also being put in ALADDIN format. The data recently disseminated from the IAEA A+M Data Unit (e.g. to Kurchatov and Obninsk Institutes, ENEA, Cadarache, etc) are all formatted in ALADDIN.

The current status of the ALADDIN system is described in the draft ("zeroth") version of the "ALADDIN Manual", issued by the IAEA A+M Data Unit in June, 1989, and distributed to about 60 institutions and researchers. Discussions in Section 5 revealed that, on general, the draft version of ALADDIN Manual is satisfactory. However, several useful suggestions were made for improvement of the Manual (see Section 3: Meeting Conclusions and Recommendations).

Regarding the future developments of ALADDIN system, all participants provided useful suggestions, which are summarized in Section 3 of this Report. Dr. R. Hulse (PPPL) presented a comprehensive analysis of the possibilities of further enhancement of ALADDIN system, emphasizing the ones which can be implemented by modest efforts. Dr. R.E.H. Clark (LANL) presented extension of ALADDIN to incorporate the atomic structure and transition probability data. The efforts of the IAEA A+M Data Unit to extend ALADDIN system in the field of particle-surface interaction data, actively supported by Dr. E.W. Thomas (Georgia Institute of Technology), were also presented (J.J. Smith, IAEA) at the Meeting. These three presentations are given as Appendix 4 at the end of this Summary Report.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

3.1. Conclusions and Recommendations Regarding Data Evaluation Activities

A. Growth of the A+M evaluated database

1) Despite of manpower and fund problems in most of the national A+M data centres, there is (on average) still a noticeable growth of the A+M data evaluation activities, as evidenced by the number of produced publications during the past two years. This is a result of both enhanced technical possibilities and accummulated experience in the data centres (hence, higher efficiency), but also due to an increased voluntary involvement of experts from atomic physics community in the data evaluation process. (Recent examples are the data evaluation activities undertaken within the IAEA SM on H-beam penetration and the CRP on plasma edge A+M processes).

2) During the past two years, comprehensive evaluated sets of spectroscopic and collisional data have been produced by most of the data centres (ORNL, NIST, Nagoya, Kurchatov Institute, Bologna, Belfast, JAERI, IAEA), and plans for the immediate future indicate that this growth will continue. Contributions to this growth could also be expected from the newly established data centres in China (CRAAMD) and in Obninsk (USSR).

3) The particle-surface interaction data evaluation activities are at present limited to only a few of the data centres (Nagoya, Kurchatov Institute, IAEA and partly ORNL). Enhancement of these activities are expected in the near future through direct involvments of certain fusion laboratories (e.g. IPP Garching) in the evaluation process, and through appropriate co-ordinating actions of the IAEA A+M Data Unit.

4) Experts meetings organized by the IAEA on well defined, purpose oriented databases (e.g. for Li-beam penetration, He-transport and exhaust, Be, etc), and evaluation activities within the IAEA Co-ordinated Research Programmes, may considerably enhance the data evaluation efforts. This method of integration of expertise

potentials outside Data Centre Network has already demonstrated its usefulness and should be further practiced by the IAEA A+M Data Unit.

B. Priorities in the data evaluation work

1) The near- and long-term priorities in the data evaluation work, set up by the IFRC Subcommittee at its last meeting, have been accepted as guidelines in the evaluation activities of the data centres. The data centres will incorporate these priorities in their near- and long-term programmes to the maximum possible extent.

2) The programme of actions oriented towards implementation of IFRC Subcommittee recommendations and adopted by the Data Centre Network (see Section 4 of this Report) is feasible if adequate focussing of data centre efforts is made and provided the IAEA co-ordinated data production and evaluation activities (through CRP's and other forms of action) are successful. Additional priorities (or shifts in priorities), resulting from the very recent fusion research and ITER design work, have been identified (Be-, B-, Li-beams, Ge - data) and included in the future evaluation programme.

3) A degree of flexibility should be retained in the data evaluation programmes in order to respond to urgent A+M data requirements which may come from the ongoing fusion research and, particularly, from the ITER conceptual design activities and R+D plans. In such events, the IAEA A+M Data Unit should take appropriate co-ordinating actions, based on involvment of a broader segment of atomic physics community.

3.2. Conclusions and Recommendations Regarding ALADDIN System

A. ALADDIN Database Development

1) The highest priority should be given to the conversion of the existing A+M data sets which are used in modelling codes into ALADDIN format. All the recommended collision data should be included and consistent sets of data files generated. (A list of plasma modelling codes containing large A+M databases is given in the Attachment to this section).

2) Definition of the labelling schemes required to allow for the inclusion of atomic structure and surface interactions data should be completed.

3) The labelling scheme for particle-surface interaction processes should be completed. The available comprehensive sets of data on physical sputtering and light ion backscattering should be ALADDIN formatted and stored in the IAEA database.

4) Development of a standard set of physics based evaluation functions (fitting forms) is necessary to form the basis of the ALFLIB library.

5) Comprehensive sets of data should be created for use in specific applications (i.e., neutral beam penetration).

B. ALADDIN Software Modifications and Enhancements

1) To allow for the inclusion of numeric data in double precision, the non standard access flag $D must be used. The ALADDIN software must

be modified to read and pass the double precision data in double precision defined fields.

2) The generation of simple linear/log data tables was a feature which was included in the original version of ALADDIN. This should be reintroduced and accessed via the "EV" command. The capability of generating linearly interpolable tables should be refined and accessed via a new "LT" command. The output format of the tables produced from both commands requires modification to include the number of columns and rows which make up the table, stored at the begining of each table. This will allow the tables to be easily read into application codes.

3) The searching algorithms can be improved to allow for searches on numeric values or ranges of values used in labels.

4) When the "SL" command is entered to define new labels for searching the ALADDIN data file using the interactive system, the search labels previously entered can be redisplayed.

5) The possibility of improving the speed of searching of large atomic databases should be investigated.

C. ALADDIN Manual Improvements

In general, the response to the ALADDIN manual was very positive. It was felt that in the following improvements could be made.

1) At the front of the manual a section should be introduced to give a brief overview of ALADDIN which should be followed by the software installation procedures and a tutorial to demonstrate the system.

2) An illustration should be included to demonstrate how the ALPACK routines can be used in a user application code.

3) A change in the labelling conventions for A+M collisional data, which should be reflected in the manual, is that the quantum state descriptions for each heavy particles must be entered. In cases where the state description is irrelevant, a (*) can be introduced.

Attachment

Conversion of Principal Fusion Modelling Codes to ALADDIN Format Data

1) Convert esisting A+M data sets used by plasma codes to ALADDIN format

2) Revise and update ALADDIN data sets with improved data

Neutral Transport	EIRENE - Jülich (Reiter) DEGAS - PPPL (Heifetz)
Convert EIRENE data:	1) Janev book 2) PPPL Methane 3) Jülich H^o multistep 4) Surface data (PPPL fits)
Impurity Transport	MIST - PPPL (Hulse) STRAHL - JET (Behringer)
Tokamak Transport	BALDUR (PPPL)

Convert (generate fits) for MIST ADPAK data, (except substitute better data as already available):

1) TOTAL IONIZATION (Belfast.....)
2) DIELECTRONIC REC & DR (T_e, n_e) (Roszman, Hahn...)
3) RADIATIVE RECOMB.
4) LINE EXCITATION (DIAGNOSTIC) (EMDAT) (He-like, Li-, Be-, Na- ..)
5) RADIATIVE COOLING RATES (LINE+BREM+REC)
6) CHARGE EXCHANGE (σ_{cx}) (TOTAL for RECOMB.)

4. ACTIONS ADOPTED

Processes	Contributors
1) C^{q+} and O^{q+} databases	
a) RR , DR	ORNL (organizer) + ...
b) Cross sections updates	IAEA
c) Rad. Cool. Rates	IAEA (organizer) + ..., (Belfast?)
d) EXC of H(H_2, He) by A^{q+}	IAEA (organizer) + ...
e) SSEC	ORNL, Nagoya, IAEA
2) Fe^{q+} database	
a) RR , DR	Hahn, Summers, Roszman
b) CX (H, H_2, He) , $q \leq 5$	ORNL, IAEA (organizer)
c) ION (H, H_2, He), all q	Rivarola, Lebedev Inst., IAEA
d) EXC (H, H_2, He), all q	IAEA (organizer) + ...
e) Rad. Cool. Rates	IAEA (organizer) + ...
3) e, H^+ - H, H_2, H_2^+ database	
all processes	IAEA, ORNL, Nagoya, edge plasma CRP participants
4) e, H^+, H, H_2 - He, He^+, He^{2+} database	
all processes	IAEA, ORNL, Nagoya, JAERI, Kurchatov, edge plasma CRP participants
5) e, H^+, H - C_xH_y, [CO, CO_2, O_2 ...] database	
a) e - C_xH_y	Nagoya, plasma edge CRP participants
b) H^+, H - C_xH_y	IAEA, CRP participants
6) A^{q+} - e, H, H_2, He (A = Ti, Cr, Ni) database	
a) e - A^{q+} processes	Belfast (ION), Los Alamos (EXC), Kurchatov (EXC), ORNL (organizer) (RR, DR)
b) A^{q+} - H, H_2, He	GAPHYOR + IAEA (CX, ION), IAEA (organizer) (EXC), CNDC (EXC)
c) Rad. Cool. Rates	IAEA (organizer) + ...
7) B^{q+} - e, H, H_2, He (B = V, Mo, W) database	
a) e - B^{q+} processes	Kurchatov (V, EXC), Belfast (ION)
b) B^{q+} - H, H_2, He	GAPHYOR + IAEA (CX, ION), CNDC (EXC)
8) W - spectroscopic data	NIST
9) Li-beam database	
all (high energy) processes	IAEA (organizer)

Appendix 1

Consultants' Meeting: 8th Atomic and Molecular Data Centre Network Meeting

14, 15 September 1989, IAEA Headquarters, Vienna, Austria

Meeting Agenda

Thursday, September 14

9:30 - 9:40 : Opening

Section 1: Ongoing and near-future programmes on A+M data compilation, and evaluation in Data Centres

Chairman: Janev

9:40 - 10:45: Reports from Data Centres:
Wiese (NIST), Phaneuf (ORNL), Tawara (Nagoya)

10:45 - 11:00: Coffee break

11:00 - 12:30: Reports from Data Centres:
Abramov (Moscow), Katsonis (GAPHYOR), Panini (Bologna)

12:30 - 14:00: Lunch

Section 1: (Cont'd)

Chairman: Phaneuf

14:00 - 15:45: Janev (IAEA), Sun Yongsheng (CRAAMD), Yao Jinzhang (CNDC), Piksaikin (Obninsk), Clark (Los Alamos)

15:45 - 16:00: Coffee break

Section 2: IFRC Subcommittee recommendations on near- and long-term priorities in A+M data compilation and evaluation for fusion

Chairman: Tawara

16:00 - 17:30: Discussion of the suggested programmes and task distribution

Friday, September 15

Section 3: The status of the ALADDIN system and its introduction in data storage, exchange and management practices

Chairman: Hulse

9:00 - 10:30: Comments of Hulse and Reports from the IAEA A+M Data Unit and the Data Centres

10:30 - 10:45: Coffee break

Section 4: Further developments of ALADDIN system

10:45 - 12:30: Hulse (PPPL), Clark (LANL), J.J. Smith (IAEA), Data Centre representatives

12:30 - 14:00: Lunch break

Section 5: The ALADDIN System Manual

Chairman: Clark

14:00 - 15:30: Discussion of the content, style, format and preparation of ALADDIN System Manual and adoption of procedures for its future updates and modifications

15:30 - 15:45: Coffee break

Section 6: Meeting Conclusions and Adoption of Actions

Chairman: Janev

15:45 - 17:00: Adoption of actions regarding the A+M data compilation and evaluation activities and the ALADDIN system developments

Consultants' Meeting: 8th Atomic and Molecular Data Centre Network Meeting

14, 15 September 1989, IAEA Headquarters, Vienna

LIST OF PARTICIPANTS

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PROGRESS REPORTS OF THE A+M DATA CENTRES

IAEA A+M DATA UNIT ACTIVITIES: REPORT FOR 1987-89 AND THE CURRENT PROGRAMS

R.K. JANEV

1. Guiding Principles and Main Objectives:

* To establish the IAEA numerical database of recommended A+M data for fusion;
* To establish an A+M data storage and exchange system;
* To conduct activity which reflects both longer- and near-term A+M data needs of fusion research (including ITER);
* To expand the activity to incorporate plasma-material interaction data;
* To strengthen the co-operation between atomic and fusion plasma physics communities;
* To create conditions for stimulation of data generation and evaluation work.

2. Specific Activities in 1988-89

2.1. A+M data exchange system: Establishment and implementation

* Consultants' Meeting (May 1988): Adoption of ALADDIN
* ALADDIN formatting of existing recommended data sets:
  - data for C^{q+}, O^{q+}, Fe^{q+} ions,
  - data for H- beam penetration,
  - some PSI data.
* Draft version of ALADDIN Manual

2.2. Stimulation of data production and evaluation

* CRP on A+M data for edge plasmas
  - 12 participating laboratories
  - Specialists' Meeting on A+M data for edge plasmas (September 11-13, 1989)
* Specialists' Meeting on preparing recommended collision data for H-beam penetration (April, 1989)
* Award of 6 Research Contracts for A+M data generation
* Initiation of an IAEA-ICTP (Trieste) International Workshop on "Computational Methods in Atomic Collision Physics" (First Workshop: 1992).

2.3. Activity extension to PSI processes

* Advisory Group Meeting (April 1989) on plasma-surface interaction (PSI) data for fusion

* Near-term programme in this field established.

* Collection of evaluated data for:

  - Physical sputtering data
  - Light on reflection from surfaces
  - Secondary electron emission

* ALADDIN PSI Dictionary (work in progress)

* Initiation (during 1989/90) of a CRP on erosion rates for fusion materials

2.4. Direct working relations with ITER Team

* Preparation of an Atomic Database for H-beam penetration into ITER plasmas

* Co-operation on the concept of PSI data activities

* Co-operation in the area of A+M data for impurity control and plasma edge studies

2.5. Establishment of a publication medium for A+M and PSI data for fusion

* Establishment of a regular journal-level publication series:

  "Nuclear Fusion" Supplement on A+M and PSI Data for Fusion.

  Vol. 1 on PSI data (in preparation),
  Vol. 2 A+M data for edge plasmas (considered).

3. Current Activities

3.1. Data evaluations

* Database for H-beam penetration into fusion plasmas,

  - based on the recommendations from April' 89 Specialists' Meeting

* Updating of data bases for C^{q+} and O^{q+} ions

* Database for particle interchange reactions in the plasma edge

* Li-beam/plasma interaction database

3.2. Parametrization of evaluated data

* Database for H-beam penetration into fusion plasmas

* C^{q+}, O^{q+} + H, H_2, He CX and ION processes

  - analytic fits with appropriate (physically based) asymptotics at low and high energies

4. Planned Activities (1990-)

4.1. Preparation of Handbooks on recommended data for fusion

* C^{q+}, O^{q+}, Fe^{q+} on H, H_2, He and with e^-

4.2. Work within the joint programme on implementation of IFRC Subcommittee recommendations on priorities in data evaluation (see Attachment 1)

4.3. Preliminary evaluated data bases for:

- Li-beam penetration into plasmas,
- Particle interchange reactions for edge plasmas

4.4. Preparation of regular issues of the Bibliographic Bulletin and other publications (see Attachment 2)

4.5. Meetings preparations (see Attachment 3)

Attachment No. 1

IFRC Subcommittee Recommendations on
Near- and long-term Priorities in A+M Data Evaluation

(from the October 1988 Subcommittee Meeting)

The data evaluation and recommendation work of the A+M Data Unit and Atomic Data Centre Network should be focussed on A+M data most urgently required by the fusion community. In implementing this recommendation, the A+M Data Unit and the A+M DCN should also take into account the actual availability of the A+M data, in order to produce as complete as possible recommended A+M data subsets.

On the basis of these criteria, the following priorities are established:

1. Near-term priorities (1-2 years)

   a) Completion of the database for e, H^+-H, H_2, H_2^+ processes (including isotopic variations)

   b) Completion of the database for e, H^+, H_2, H-He, He^+, He^{2+} processes

   c) Completion of database for Fe^{q+}-e, H, H_2, He processes

   d) Database for e, H^+, H - C_kH_n, CO_k, $O(O_2)$ and OH processes

2. Long-term priorities

   a) Plasma edge processes (other than those included in 1)

   b) Data for e-A^{q+}, A^{q+}-H, H_2, He processes (A=Ti, Cr, Ni) Cu

   c) Data for e-A^{q+}, A^{q+}-H, H_2, He processes (A=Be, B, Si, W)

   d) Plasma-wall interaction processes (as specified at the AGM '89)

Attachment No. 2

IAEA A+M Data Publications in 1990

1.	INDC Report on Atomic Database for Neutral Beam Penetration into Plasmas	January - February
2.	Handbook on Carbon Data	February - March
3.	Handbook on Oxygen Data	February - March
4.	Nuclear Fusion Supplement, Vol. 1: Compendium on Plasma-Surface Interaction Data for Fusion	February - March
5.	INDC Report on Database for Particle Interchange Reactions for Fusion	March - April
6.	INDC Report on Atomic Database for Neutral Lithium Beam Penetration into Plasmas	April - May
7.	Two issues of the A+M Bibliographic Bulletin	May / November
8.	ALADDIN System Manual: Version 0.2	Autumn
9.	Nuclear Fusion Supplement, Vol. 2: Compendium on A+M Data for Fusion Edge Plasmas	October - December
10.	Handbook on Iron Data	November - December

Attachment No. 3

IAEA A+M Data Meetings for 1990

	Title	Tentative Dates and Place
1.	AGM on A+M Data for Metallic Impurities	May 16 - 18, Vienna
2.	CM on Thermal Response of Plasma Facing Materials and Components	June 4 - 6, Vienna or November 26 - 30, Nagoya
3.	CM: 9th A+M Data Centre Network Meeting	September 20 - 21, Vienna
4.	RCM on A+M Data for Fusion Plasma Edge Studies	September 24 - 26, Vienna
5.	TCM: 6th IFRC Subcommittee Meeting	September 27 - 28, Vienna or Satellite to the IAEA plasma conf., Washington

Status Report
Atomic Spectroscopy Data Center at the National Institute of Standards and Technology (NIST)

W.L. Wiese

1. Data Center on Atomic Energy Levels:

   W.C. Martin, Director (30% of his time): critical compilation work
   J. Sugar (30%): critical compilations
   H. Musgrove (100%): literature searches, inquiries, database operation

2. Data Center on Atomic Transition Probabilities

   W.L. Wiese (30% of time): critical compilations
   J.R. Fuhr (100%): literature search, inquiries, critical compilations

Recent events

1) Currently, a database specialist from the NIST Office of Standard Reference Data (OSRD) is assigned to the two data centers to design and test a comprehensive spectroscopic database from the recently produced compilations. Tapes of all these tables are available which are used for computerized type setting but need to be cleared of all editorial marks.

   The first phase of this database work will be to store all atomic energy level data for elements Ca through Ni from the recent "Sugar-Corliss" tables and test various sorting and retrieval precedures.

   Later, spectral transition data, i.e., wavelengths and transition probabilities, will be added.

2) Bibliographical databases, containing annotated literature references, are operational in the Energy level as well as Transition probability data center. At present, the databases are still far from complete, and all older literature references need to be added.

3) Two major compilations of atomic transition probabilities were finally published in late 1988:

   G.A. Martin, J.R. Fuhr, and W.L. Wiese, "Atomic Transition Probabilities: Scandium through Manganese", J. Phys. Chem. Ref. Data 17, Supplement 3, 532 pages (1988).

   J.R. Fuhr, G.A. Martin, and W.L. Wiese, "Atomic Transition Probabilities: Iron through Nickel, "J. Phys. Chem. Ref. Data 17, Supplement 4, 512 pages (1988).

4) "Spectroscopic Data Tables for Ti, Cr and Ni" are scheduled to be published in three separate volumes as an Oak Ridge National Laboratory "Redbook" in October 1989.

5) Joint work with JAERI: Spectral tables for the ions Fe VIII through Fe XXVI have been completed and are in press (J. Phys. Chem. Ref. Data)

Work in progress and near future plans:

a) Energy Level Compilations:

Singly ionized oxygen (OI)
Krypton and Chlorine - all stages of ionization

Plans: Ar and Ge spectra

b) Wavelengths, with energy level classifications:

Mn and Cu, with JAERI

Plans: Na and Mg, with JAERI

c) Transition Probabilities:

Stronger lines of elements with Z > 28, mostly first and sencond spectra

Plans: Update and enlarge data for the elements hydrogen through neon, with all ions.

The recently compiled data for Fe will be put on a diskette and offered for sale by OSRD.

Controlled-Fusion Atomic Data Center

Oak Ridge National Laboratory
U.S.A.

Report on ACTIVITIES 1988 / 1989

R. Phaneuf

1. On-Line Bibliographic Data Base:

   * Up-to-date, with 21,400 entries from 120 journals, covering the period from 1978-present.

   * Input from ORNL atomic physics staff and consultants under contract.

   * Access for on-line searching via local area PC network.

   * Semi-annual updates sent on diskette to IAEA, IPP-Nagoya, JAERI.

   * Trial data base set up on PC at Justus-Liebig University (Giessen).

2. Data Compilation and Evaluation

   * "Redbook" by C. F. Barnett on collisions of H, H_2, He and Li atoms and ions with atoms and molecules (321 reactions) is nearly completed.

   * ALADDIN data base is being assembled for distribution on diskette with "Redbook."

   * "Redbook" by W. Wiese and A. Musgrove (NIST) on spectroscopic data for Ti, Cr, and Ni is being published and will be distributed shortly.

   * Collaboration with R. K. Janev (IAEA) on ALADDIN labelling conventions and dictionary of collision processes.

   * Collaboration with T. Shirai (JAERI) on incorporation of JAERI cross section fits into ALADDIN.

3. Recent Publications

   * "Recommended Cross Sections for Electron Capture and Ionization in Collisions of C^{q+} and O^{q+} with H, He and H_2," R. K. Janev, R. A. Phaneuf, and H. T. Hunter, At. Data Nucl. Data Tables 40, 249-81 (1988).

   * "Atomic and Molecular Data Requirements for Fusion Plasma Edge Studies," H. Tawara and R. A. Phaneuf, Comments At. Mol. Phys. 21, 177-93 (1988).

ATOMIC DATA FOR FUSION

Collisions of H, H_2, He and Li Atoms and Ions with Atoms and Molecules

C. F. Barnett

ORNL-6086 (in preparation)

Contents

Total: 321 reactions

Schedule: completion before the end of 1989

C.1 Excitation Cross Sections for

H + H -> H(2s,2p) + H(Σ)

H(2s)		H(2p)	
Energy (eV/amu)	Cross Section (cm^2)	Energy (eV/amu)	Cross Section (cm^2)
2.0E+03	8.03E-18	4.0E+03	1.62E-17
3.0E+03	9.80E-18	5.0E+03	2.29E-17
4.0E+03	1.15E-17	6.0E+03	2.44E-17
5.0E+03	1.29E-17	7.0E+03	2.47E-17
6.0E+03	1.43E-17	8.0E+03	2.41E-17
7.0E+03	1.51E-17	9.0E+03	2.35E-17
8.0E+03	1.56E-17	1.0E+04	2.28E-17
9.0E+03	1.59E-17	1.5E+04	1.92E-17
1.0E+04	1.60E-17	2.0E+04	1.58E-17
1.5E+04	1.37E-17	3.0E+04	1.17E-17
2.0E+04	1.04E-17		
3.0E+04	6.64E-18		
4.0E+04	4.65E-18		
5.0E+04	3.48E-18		
6.0E+04	2.74E-18		
7.0E+04	2.28E-18		
8.0E+04	2.02E-18		
9.0E+04	1.84E-18		

References: 15, 592, 593, 594, 595, 596, 597, 598

Accuracy: Unknown

Notes: (1) The symbol H(Σ) denotes that the target atom may be left in any [excited] state after the collision. (2) All theoretical treatments of the H + H excitation cross sections are in serious disagreement with experiment and with each other, both in absolute magnitude and energy dependence. For various theoretical treatments see Flannery (Ref. 594 - four state impact parameter method), McLaughlin and Bell (Ref. 595 - close coupling exchange), Shingal, et al. (Ref. 596 - four state semiclassical impact parameter), and Khurana, et al. (Ref. 597 - 2nd Born approximation and also distorted wave Born).

Chebyshev Fitting Parameters for Cross Sections

H(2s) E_{min} = 2.0E+03, E_{max} = 9.0E+04
H(2p) E_{min} = 4.0E+03, E_{max} = 3.0E+04

	A0	A1	A2	A3	A4	A5	A06
H(2s)	-77.1082	-.256046	-.232311	.0701782	-.0315673	.0229762	.00612383
H(2p)	-79.1098	-.784062	-.651723	.0462865	.114234	-.00487654	-.0114391

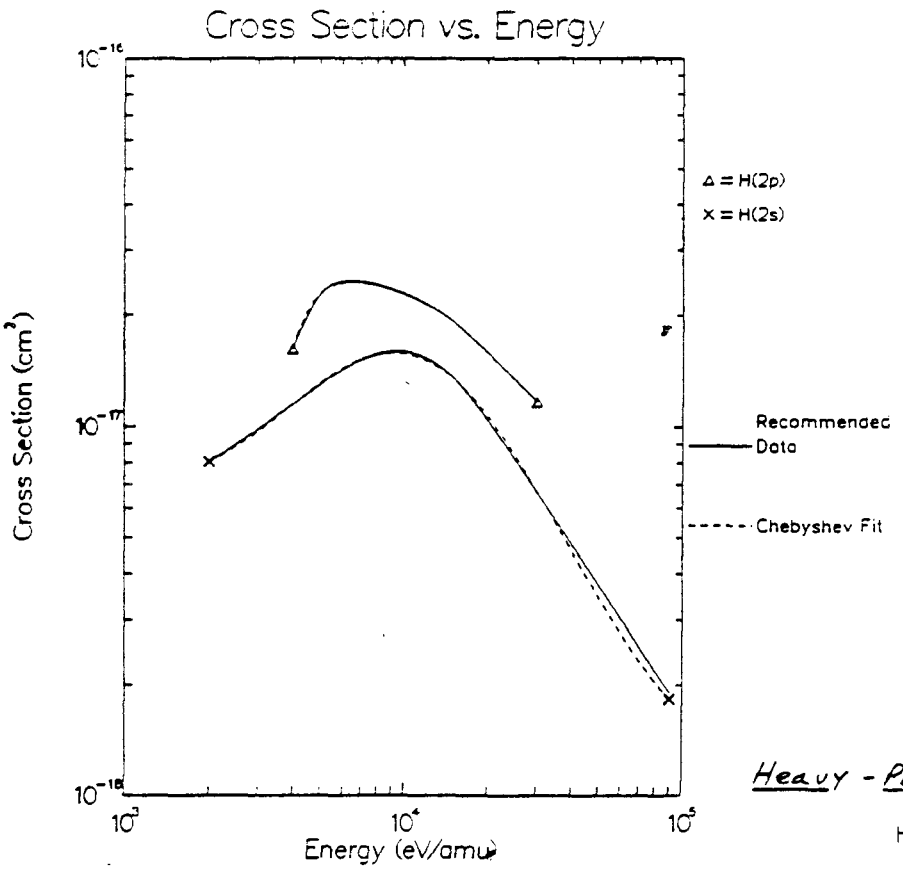
The fit represents the H(2s) cross section with an rms deviation of 1.2%. The maximum deviation is 2.8% at 2.0E+04 eV/amu.

The fit represents the H(2p) cross section with an rms deviation of 0.3%. The maximum deviation is 0.6% at 6.0E+03 eV/amu.

See appendix for Chebyshev fit details.

ALADDIN Categorizations:

EXC H [+0] (G) H [+0] (G) H [+0] (2s) H [+0]
EXC H [+0] (G) H [+0] (G) H [+0] (2p) H [+0]

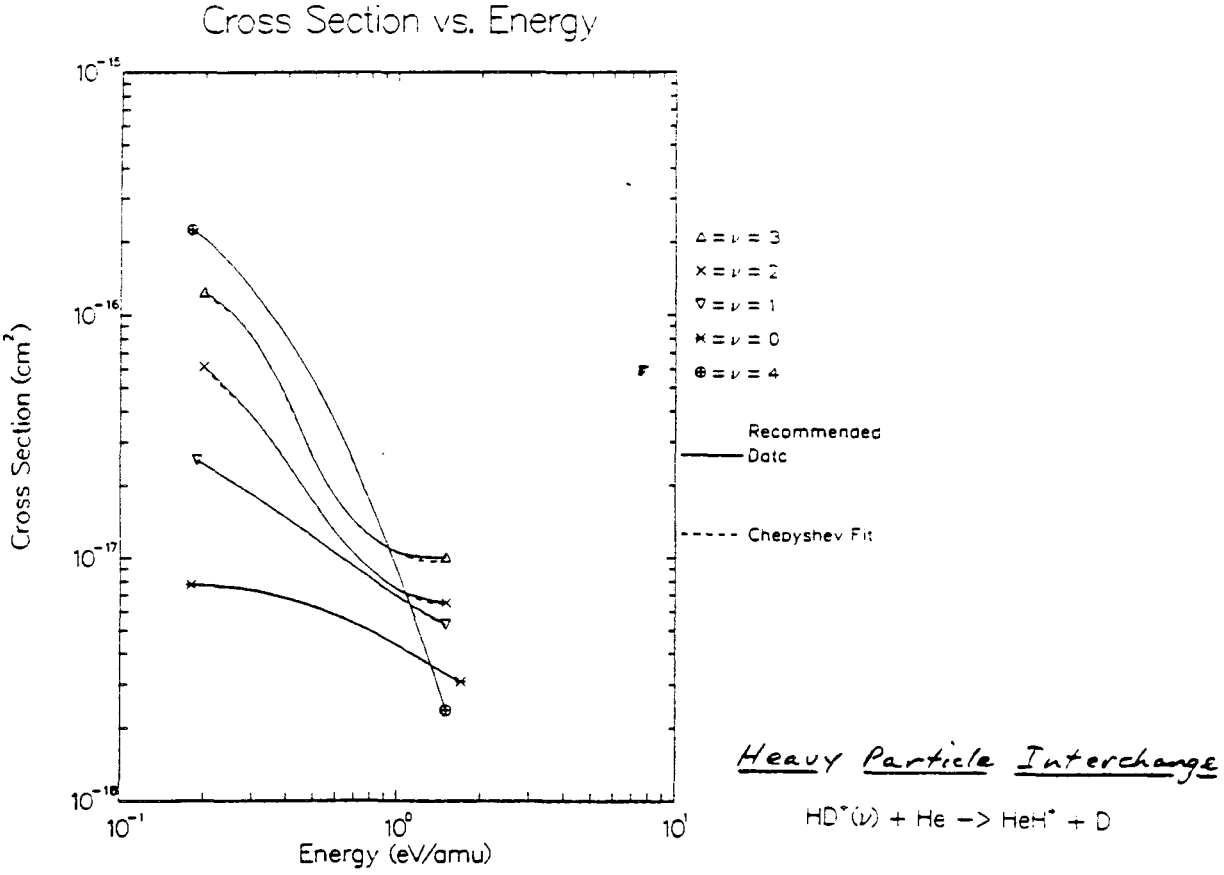


Heavy-Particle Excitation

H + H -> H(2s,2p)

ALADDIN DATA FILE FOR EXCITATION AND LINE EMISSION
ORNL-6086, Chapter C [C.F. Barnett]

```
$ EXC  H [+0] (G)  H [+0] (G)   H [+0] (2s)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.1  #CHEB
-79.1098          -0.784062       -0.651723        0.0462865       0.114234
 -0.00487654      -0.0114391       0.0             0.0  2000.      90000.

$ EXC  H [+0] (G)  H [+0] (G)   H [+0] (2p)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.1  #CHEB
-77.1082          -0.256046       -0.232311        0.0701782      -0.0315673
  0.0229762       -0.00612383      0.0             0.0  4000.      30000.

$ EXC  H [+0] (G)  H [+0] (G)   H [+0] (3s)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.2  #CHEB
-82.579864502     -2.053023577    -0.908966184     0.534100890    -0.2499177
  0.052064214      0.041846298     0.0             0.0    1000.    1000000.

$ EXC  H [+0] (G)  H [+0] (G)   H [+0] (3p)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.2  #CHEB
-81.200477600     -0.954174101    -1.203282118     0.638573289    -0.3283409
  0.026330521      0.071920015     0.0             0.0    1000.    1000000.

$ EXC  H [+0] (G)  H [+0] (G)   H [+0] (3d)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.2  #CHEB
-86.381980896     -0.612847328    -1.478487253     0.754596293    -0.3629288
  0.042892117      0.087654375     0.0             0.0    1000.    1000000.

$ LEM  H [+0]   H [+0]   656.28
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.2  #CHEB
-81.758575439     -1.766494513    -0.933876812     0.519497573    -0.2647967
  0.040677227      0.046427559     0.0             0.0    1000.    1000000.

$ EXC  H [+0] (G)  H(2) [+0]   H [+0] (2s)  H(2) [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.3  #CHEB
! Projectile excitation only
-78.7640          0.402626       -0.287568       -0.08853020       0.009784
-0.0116490        0.0260520       0.0             0.0   2000.      25000.

$ EXC  H [+0] (G)  H(2) [+0]   H [+0] (2p)  H(2) [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.3  #CHEB
! Projectile excitation only
-76.3640 -0.378164  0.0409332 -0.0624297 -0.0180011  0.0197840  0.0125317
 0.0       0.0      5000.      25000.

$ DISEXC  H [+0]  H(2) [+0]   H [+0]   H [+0] (2s)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.3  #CHEB
-80.383300000     0.090421500    -0.109032000     0.028555900    -0.0068929
  0.000520699     0.002897220     0.0             0.0    5000.    25000.

$ DISEXC  H [+0]  H(2) [+0]   H [+0]   H [+0] (2p)  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  C.3  #CHEB
-78.2881  0.202052 -0.276608 -0.0557457  0.03869040 -0.0107516 -0.00871482
 0.0       0.0      5000.      25000.
```



ALADDIN DATA FILE FOR HEAVY-PARTICLE INTERCHANGE REACTIONS
ORNL-6086, Chapter X [C.F. Barnett]

```
$ PX  H [+1]  D(2) [+0]   D [+1]  HD [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.1  #CHEB
-75.6467819214 -3.2291088104  0.4121128917  0.0393397696 -0.2617489398
  0.0012951158  0.1208853275  0.0           0.0      0.45    100.

$ PX  H [+1]  D(2) [+0]   HD [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.1  #CHEB
-82.0488052368 -2.4613640308 -0.2998173237  0.8330806494 -0.3411027491
 -0.0343948416  0.0959802791  0.0           0.0      2.2    100.

$ PX  HD [+1]  D(2) [+0]   HD(2) [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.2  #CHEB
-68.6683044434 -2.9252188206 -1.0689096451 -0.5702099800 -0.1987314671
 -0.0387800001 -0.0184986405  0.0           0.0     0.006    4.3

$ PX  HD [+1]  D(2) [+0]   D(3) [+1]  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.2  #CHEB
-70.3594665527 -3.1182763577 -0.9160673618 -0.4499975443 -0.1941261590
 -0.0628098324 -0.0082232719  0.0           0.0     0.006    4.3

$ PX  HD [+1] (v=0)  He [+0]   HeH [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.3  #CHEB
-79.5223464966 -0.4741957486 -0.1060224026  0.0091071073  0.0041217022
  0.0030853429  0.0034316243  0.0           0.0      0.18    1.7

$ PX  HD [+1] (v=1)  He [+0]   HeH [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.3  #CHEB
-78.0057907104 -0.8027198911  0.0006819559  0.0202372447  0.0018167543
  0.0002085193  0.0019659579  0.0           0.0      0.19   1.5
```

```
$ PX  HD [+1] (v=2)  He [+0]   HeH [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.3  #CHEB
-77.1958007813 -1.2085071802  0.1410915107  0.1016155556 -0.0078602089
 -0.0159890912  0.0143204452  0.0           0.0     0.2   1.5

$ PX  HD [+1] (v=3)  He [+0]   HeH [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.3  #CHEB
-76.1494598389 -1.4227830172  0.2272066027  0.1821492910 -0.0607895106
 -0.0178064369  0.0326453783  0.0           0.0     0.2   1.5

$ PX  HD [+1] (v=4)  He [+0]   HeH [+1]  D [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.3  #CHEB
-75.8801422119 -2.2710402012 -0.3697219193 -0.0086457897  0.0064711664
  0.0010754776 -0.0058953157  0.0           0.0     0.18   1.5

$ PX  H(2) [+1]  He [+0]   HeH [+1]  H [+0]
& CS   EVAL  ACC=?  ORNL-CFADC  DOC=ORNL-6086  H.4  #CHEB
-74.2765960693 -2.0581145287 -0.0177676305  0.1360136420  0.0055540851
 -0.0251696426 -0.0006318173  0.0           0.0     0.56   10.0
```

PROGRESS REPORT 1988/1989 at RIC/IPP-Nagoya and DPC/NIFS

H.Tawara
National Institute for Fusion Science

The Institute of Plasma Physics, Nagoya University, has been reorganized to National Institute for Fusion Science which intends to construct and test a large helical torus system to investigate continuous plasmas. The new Institute, operated by the Ministry of Education, presently occupies the previous location in the campus of Nagoya University and plans to move a new location outside Nagoya city. Thus, atomic and molecular data activities at Research Information Center (RIC) have also been transferred to Data and Planning Center (DPC) of the new Institute.

The followings are our activities pursued in the past years (1988-1989) :

I) AM data activities

1) A recommendation of excitation rate coefficients of helium atoms and He-like ions by electron impact has ben completed.[1]
2) Data are being compiled and evaluated for intensity ratios of various emission lines of O V ions for plasma temperature and density diagnostics.
3) Following our previous comprehensive compilation of data involving hydrogens, an evaluation of hydrogen molecules under electron impact has been completed and a paper describing related data has been submitted to J. Phys. Chem. Ref. Data.[2]
   In order to know the present understanding of plasma processes in torus devices (JT-60 and Heliotron E), a workshop has been organized and a review has been made on AM processes and related AM data in edge plasmas of graphite-covered plasma devices and their carbonization processes.[3]
   Also data are being compiled on hydrocarbon molecules (including CH_4, C_2H_2, etc.,) relevant to edge plasmas in graphite-covered plasma devices.
4) Atomic processes involving low energy, highly charged ions have been reviewed, with the emphasis on ionization/excitation/recombination of ions by electrons, electron capture processes and collisions with solids.[4]
5) Partial electronic stopping cross sections have been calculated for protons in collisions with atoms ranging from He to Xe, shell by shell, based upon wave packet theory.[5] This model can be easily applied to heavy projectiles.

II) Surface data

1) A theory on threshold energy for ion-induced desorption has been developed based upon a few-collision model and an analytical formula for the threshold

energies for any combination of projectile, substrate and adsorbate has been introduced.[6]

2) Topics have been discussed on "near-term" as well as "long term" data activities on plasma-wall interactions in fusion devices.[7] There, it is pointed out that reliable data including synergistic effects, in particular at low energy particle collisions, are urgently necessary under complex conditions as close as possible to those in experimental devices. For doing this, computer simulations should be appropriate.

3) Data for total sputtering yields from monatomic solids under ion impact had previously been published. Data have recently been compiled and reviewed on the angular distributions of sputtered atoms from monatomic solids under ion impact and a convenient empirical formula has been developed.[8]

III) Development of a data base management system

A new data management system incorporating ALADDIN is being developed.

IV) Other activities

1) A comprehensive review has been made on AM physics in fusion research and its relevance in plasma diagnostics and modelling.[9] (Dr. H.W.Drawin stayed with us at Nagoya for Jan. - April, 1988).

References

1. T.Kato and S.Nakazaki, At. Dat & Nucl. Data Tables 42 (1989) 313
2. H.Tawara, Y.Itikawa, H.Nishimura and M.Yoshino, IPPJ-AM-46 (1986) and -55 (1987) ; submitted to J. Phys. Chem. Ref. Data
3. H.Tawara (ed.), IPPJ-AM-59 (1988)
4. H.Tawara, IPPJ-AM-62 (1988) and Conference Proc. No.188, Particles and Fields Series 38 (AIP, ed. by A.Hershcovitch, 1989) p.427
5. T.Kaneko, IPPJ-AM-63 (1989)
6. Y.Yamamura, J.Bohdansky and E.Taglauer, IPPJ-AM-60 (1988)
7. N.Itoh and T.Kawamura (ed.), IPPJ-AM-64 (1989)
8. N.Matsunami et al., At. Data & Nucl. Data Tables 31 (1984) 1 ; Y,Yamamura, T.Takiguchi and H.Tawara, NIFS-AM-1(?) (1989)
9. H.W.Drawin, IPPJ-AM-61 (1988)

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. KURCATOV INSTITUTE OF ATOMIC ENERGY
Moscow, 1989

The more reliable and extensive atomic and molecular data are required to design the reactor-like systems as INTOR and ITER/OTR. The data concerning some elementary processes (for an edge plasmas and for a core plasmas) are reguired. Now the processes in edge plasmas and the processes which affect on the neutral beam penetration (for plasma heating and current drive, E_B>100 keV/amu) are very important. Therefore, the activities in the plasma Physics Department of I.V.Kurchatov Institute of Atomic Energy concerning the (A+M) data problems have been directed, mainly, on these processes.

At present, the activities concerning the collection of bibliographic (A+M) information are in progress. The (A+M) data are being extracted systematically from Soviet publications, including periodicals, monographs, reports and proceedings of All-Union conferences and meetings. These data are transmitted semiannually to the IAEA for the publication in the "International Bulletin on Atomic and Molecular Data for Fusion". Data are collected for the following sections: 1. Energy levels, wavelengths and identification of lines;

2. Transition probabilities;
3. Photon collisions;
4. Electron collisions;
5. Heavy partcile collisions;

6. Surface effects;

7. Plasma impurities;

8. Plasma diagnostics.

The collected data are stored on magnetic tape, and, if necessary, can be printed out and supplied to the scientists of the Kurchatov Institute and other organizations. The activities concerning the file building for the PC IBM-AT are in progress. The copies of the "International Bulletin on Atomic and Molecular Data for Fusion" which we receive from the IAEA, are circulated by us to a number of organizations in the USSR. Now we are also regularly exchanging the (A+M) information with ORNL, Data Information Centre at the Institute of Plasma Physics of Nagoya University, Queen University (Belfast), Culham Laboratory. We hope this exchange will continue and further develop.

We are currently engaged in the compilation of numerical (A+M) data for fusion. The data for the cross-section of large number transitions in helium atom due to electron collisions are compiled and analyzed in the Reference book by V.A.Abramov, L.A.Vainstein, G.I.Krotova and A.Yu.Pigarov "The Recommended Atomic Data for Hydrogen and Helium Plasmas" [1]. The data which have been published in the period 1978-1987 are compiled in this edition. This reference book contains also the results of calculations for cross-sections and rates for 155 transitions with n=1-5 which have been performed using the numerical code "ATOM". The data concerning the electron collisions strengths for some transitions in Ti^{+q} and V^{+q} are collected in [2]. The results of the calculations of characteristics of X-ray lines in Argon ions, chlorine ions and potassium ions are presented in [3]. These data are required for experimental data interpretation which have been obtained on modern tokamaks due to X-ray diagnostics. The results of extensive calculations of the sputtering yield for different

combinations target+projectile are collected in [4].It should be noted that these results are twice averaged: over incidence angle and over energy distribution (the distortion of the distribution function is taken into account).

Apart from the collection and the dissemination of the available bibliographic and numerical data, in the Kurchatov Institute the experimental activity concerning the reactor-relevant processes are being carried out. Dr M.I.Guseva and her collaborators have measured the sputtering yields (including composite materials) taking into account some new interesting effects (especially, synergetic effect). The modernization of the "ATOS" device has been performed by V.A.Belyaev and his group. The total electron capture cross-sections for C^{+q}+H reactions at electron-volts (up to 1 keV) energies will be measured at this device.

The impact of different data bases for elementary processes which affect the neutral beam penetration on ITER/OTR design have been considered by V.A.Abramov and A.Yu.Pigarov.

At present the most important problem is the exchange of data between national centres due to tremendous required data files. The exchange problem leads to the problem of unique exchange format. The estimation of possibilities of a new format "ALLADIN" which has been developed in PPPL is being carried out now. The discussion concerning the "ALLADIN" will give a possibility to estimate of potential possibilities and, may be, the "ALLADIN" format will be recommended for different centres and laboratories. All the aspects of (A+M) data problem require the consolidation of international cooperation between the national centres and IAEA and also require to find the new forms of cooperation (especially, for such an important problem as the problem of the evaluation of existing data).

REFERENCES

1. V.A.Abramov et al. "The Recommended Data for Hydrogen and Helium Plasmas", Central Institute for Information in Atomic Sciences, 1987.

2. V.A.Abramov, T.I.Zhukova "The Collision Strengths for Electron Excitation of Different Transitions in Some Titanium and Vanadium Ions", Central Institute for Information in Atomic Sciences, 1986.

3. P.S.Kiselyus, A.V.Kuplyauskene, Z.B.Rudzikas, V.A.Abramov, V.S.Lisitsa, "The Characteristics of X-Ray Transitions in Multi-Charged Ions of Ar, Cl, K", Central Institute for Information in Atomic Sciences, 1985.

4. V.A.Abramov et al. "The sputtering of Materials for First Wall and Divertor Plates in Tokamak Reactor", Preprint IAE-4463/8, 1987.

THE USSR ACTIVITIES IN THE FIELD OF THE ITER/OTR-RELEVANT ELEMENTARY PROCESSES

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I.V. KURCHATOV INSTITUTE OF ATOMIC ENERGY

Moscow, 1989

The investigations of fusion-relevant atomic and molecular interactions are carried out by specialists of the USSR Academy of Sciences, the Ministry for Higher Education and also by specilaists of some institutes of State Committee for Utilization of Atomic Energy and some Ministries.

The studies are coordinated by the Scientific Council of the USSR Academy of Sciences "Physics of electronic and atomic collisions" (Chairman is corresponding of member V.V.Afrosimiv). Council of the USSR Academy of Sciences "Plasma Physics". The total amount of the institutions involved in the cooperation is 35 (the institutions of the USSR Academy of Sciences and the Ministry of Higher Education are 29). The list of the institutions is given below.

THE INSTITUTIONS OF THE USSR ACADEMY OF SCIENCES AND THE ACADEMIES OF SCIENCES OF THE SOVIET REPUBLICS

1. A.F.Ioffe Institute	Leningrad
2. P.N.Lebedev Institute	Moscow
3. Institute of General Physics	Moscow
4. Institute of Chemical Physics	Moscow
5. Institute of Physical Chemistry	Moscow
6. Solid State Physics Institute	Chernogolovka, Moscow region
7. Institute of Mechanical Problems	Moscow
8. Space Studies Institute	Moscow
9. Nuclear Physics Institute	Gatchina, Leningrad region

10. IZMIRAN (Institute of Terrestrial Magnetics and radio-waves propagation)	Troitsk, Moscow region
11. Centre of Surface and Vacuum Studies	Moscow
12. Institute of Spectroscopy	Troitsk, Moscow region
13. Institute of Oil-Chemical Synthesis	Moscow
14. Physical Studies Institute	Erevan
15. Institute of Physics	Riga
16. Institute of Physics	Vilnuis
17. Electronics Institute	Tashkent
18. The Uzhgorod Department of the Institute for Nuclear Studies	Uzhgorod

THE INSTITUTIONS OF THE MINISTRY FOR HIGHER EDUCATION

19. Voronezh State University	Voronezh
20. Latvian State University	Riga
21. Leningrad State University	Leningrad
22. Moscow State University	Moscow
23. Petrozavodsk State University	Petrozavodsk
24. Tbilisi State University	Tbilisi
25. Uzhgorod State University	Uzhgorod
26. Chuvashian State University	Cheboksary
27. Moscow Aviation Institute	Moscow
28. Moscow Engineering Physics Institute	Moscow
29. Moscow Energetic Institute	Moscow
30. Institute of Nuclear Physics of the Moscow State University	Moscow

INSTITUTES OF THE STATE COMMITTEE FOR UTILIZATION OF ATOMIC ENERGY AND SOME MINISTRIES

31. I.V. Kurchatov Institute of Atomic Energy	Moscow
32. Theoretical and Experimental Physics Inst.	Moscow
33. Dubna Institute for Nuclear Studies	Dubna Moscow region

34.Institute of Graphite Materials	Moscow region Moscow
35.Institute of Structural Materials	Leningrad

TABLES I-Y show the main scientific interests of the institutions.

Topic: Electron-Hydrogen and Electron-Carbon-Hydrogen Interactions

Solid State Physics Institute	Loss and capture of electron by hydrogen atom
A.F.Ioffe Institute	Hydrogen excitation (theory)
Institute of Physics (Riga)	Hydrogen excitation (theory)
Institute of Oil Chemical Synthesis	Carbon-Hydrogen Ionization
Physical Studies Institute	Autoionization States

Topic: Electron-impurities interactions TABLE II

Institute of Nuclear Physics of Moscow State University	Helium ionization
P.N.Lebedev Institute	Ionization and excitation (theory)
Institute of Physics (Riga)	H-like ions excitations (Riga)
General Physics Institute	Be-like and more complex ions ionization and excitation (theory)
Institute of Physics (Vilnuis)	Iron group ions ionization and excitation (theory)
Moscow Energetic Institute	Metal atoms ionization and excitation (Mo,Cu,Ni)
Uzhgorod Department of the Institute for Nuclear Studies	Impurity ions excitation
Uzhgorod State University	Multi-charged ions (Ti^{+3}) ionization
Electronics Institute	Ionization during the electron capture by multi-charged ions
Chuvashian State University	Electron scattering on metastable atoms
Petrozavodsk State University	Helium metastable states

TABLE III

Heavy Particle interactions

A.F.Ioffe Institute Institute for Nuclear Studies	Charge-exchange
Kurchatov Institute	Charge-exchange. Sputtering. Multicharged ions.
Spase Studies Institute	Ionization and charge-exchange
Tbilisi State University	Ionization and charge- exchange at V= $(2 \cdot 4)\,10^7$ cm s^{-1}
Institute of Nuclear Physics of the Moscow State University	Ionization nad charge exchange at V= $(6 \cdot 8) \cdot 10^8$ cm s^{-1} Multiple ionization at fast collisions Loss and capture of electron by proton.
P.N.Lebedev Institute	Charge-exchange (theory)
Leningrad State University	Charge-exchange (theory)
Voronezh State University	Charge-exchange (theory)
Petrozavodsk State University	Helium metastable states
Institute of Physics (Riga)	Multicharged ions
Latvian State University	Multicharged ions
Institute of Mechanics Problems	Ion-atom collisions
Institute of Chemical Physics	Ion-molecule collisions
Centre of Surface and Vacuum Studies	Ionization of metallic atoms
A.F.Ioffe Institute Institute of Nuclear Physics (Gatchina)	Isotopic exchange in hydrogen isotopes mixtures

TABLE IY

Plasma-surface interactions

Institute of Physics (Riga)	Binary collisions with atoms of first wall
Institute of Nuclear Physics of the Moscow State University	Sputtering energy range is (0, 1-1) keV

Kurchatov Institute	Sputtering (theory) Sputtering (experiment) Blistering Composite materials sputtering (experiment) Sputtering with fission fragments (theory)
Electronics Institute	Ion bombardment
Moscow Aviation Institute	Sputtering (experiment)
Institute of Chemical Physics	Ion bombardment
Institute of Graphite Materials	Composite materials sputtering
Institute of Structural Materials	Structural Materials sputtering
Uzhgorod Department of the Institute of Nuclear Studies	Ion bombardment
Moscow Engineering-Physics Institute	Ion bombardment Particle reflection Ion implantation

TABLE Y

Topic: Energy levels and transition probabilities

Institute of Spectroscopy	**Energy levels, wavelengths, transition probabilities (theory and experiment)**
Institute of Spectroscopy	Energy levels, wavelengths, transition probabilities (theory and experiment)
Leningrad State University	Transition Probabilities
Institute of Nuclear Physics of the Moscow State University	Energy levels, wavelengths, transition probabilities (theory)
Institute of Physics (Vilnuis)	Energy levels, wavelengths, transition probabilities (theory)
Kurchatov Institute	Energy levels (theory)
A.F.Ioffe Institute	Energy levels (theory)

Finally, we wuld like to note some recent results of the (A+M) investigations which may be interesting for the ITER/OTR design.

A.F.Ioffe Institute:

The device for the study of an interaction of He and He^{+} with atoms and molecules (~ 1 MeV/amu)is constructed. This device may be used to study the α-particle thermalization process.

The particle- spectroscopic diagnostic method is developed. The base for this diagnostic method of impurity ions in fusion plasmas is the record of intensity of spectral lines excited due to impurity bare ions charge-exchange on the atoms of doping beam. It is shown that the plasma collisions lead to the equipartitation of levels of H-like impurities ions. The effective rates of spectral lines change (up to 5 times).

The code for the collisional re-population of levels is developed. This method have been tested on ASDEX and JET.

Institute of Nuclear Physics of the Moscow State University:

The cross-sections of electron capture by proton and the cross-sections of electron loss by atoms and negative hydrogen ions during the transportation through different gases at $U = 8\ 10^{8} cm\ s^{-1}$ are measured. It is shown that the relations between the electron capture cross-sections in different gases are quantitatively reproduced by the Oppengeimer-Brinkman-Kramers calculations. The model for the calculation of the charge composition of molecular hydrogen beam after the passage of a film at E 100 keV/amu.

P.N.Lebedev Institute:

The code "ATOM" is developed; it gives the possibilities to calculate the radiative transition probabilitie, the cross-sections (rates) of excitation, ionization and recombination (direct radiative and dielecronic) processes by electron impact. This code is valid for the atoms and ions.

I.V.Kurchatov Institute:

The interactions of multicharged ions with surface are investigated. It is shown that the sputtering yields of metals by single-charged ions and multicharged ions are about equal, whereas the sputtering yields of dielectric by multicharged ions are greater (up to 3 magnitude of order).

Centre of surface and vacuum studies:

The method of absolute measurements of metallic atoms ionization cross-sections is developed (the method accuracy is 5%).

GAPHYOR DATA CENTRE

Progress Report 1988 - 1989

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1. FACTUAL DATA BASE

1.1. Some statistics

As of the 1st September 1989, the number of entries in the files were distributed as follows:

a) The entries for one, two, three and four elements files for each section is given in the table 1.

Table 1. Number of entries

Section . 1 . 2 . 3 . 4 . 5 . .						
File	structure	phot.coll.	e coll.	heavy part.	macrosc.	Totals
1 element	34420	6240	11392	6651	4291	62994
2 elements	44202	5028	4232	32819	7039	93320
3 elements	20033	2192	725	17835	2485	43270
4 elements	4153	439	82	5004	774	10452
Totals	102808	13899	16431	62309	14589	210036

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

Table 2. Entries per Process for each section

(for process code see Appendix 1)

. structure		. phot. coll.		. e coll.		. heavy part. coll.		. macroscopic. propert.	
EN	57773	AN	1647	SN	1023	SN	997	PV	1023
CP	258	SN	491	SC	401	SC	500	FT	1530
DP	2714	SC	270	EL	1545	EL	758	VR	158
NP	737	EL	170	EX	4101	EN	1626	ZT	120
PE	2238	FF	79	ER	439	EX	2366	CO	123
VR	26007	EX	1533	DX	179	ER	1047	DN	591
TR	10147	ER	397	XX	354	DX	7155	VI	681
IN	706	DX	95	DO	39	XX	2074	CT	781
DT	191	XX	64	IN	4310	DO	271	TD	265
DS	1278	DO	77	RC	187	TE	1970	PE	269
XX	27	IN	5355	RR	141	IN	6338	EN	2406
EA	732	DT	427	RE	88	DT	871	DM	56
		DS	2871	RO	63	RI	443	RN	935
Tot.	102808	NL	134	RD	385	10	4830	FE	336
		PR	289	RS	536	20	198	CE	156
				AT	1441	LN	3056	ME	610
		Tot.	13899	DT	53	MP	146	DE	173
				DS	813	LP	3590	PI	483
				BS	197	IR	12819	AT	448
				PR	136	AS	3737	DT	67
						DS	2404	PC	66
				Tot.	16431	IH	835	FI	29
						AH	174	MI	858
						DH	89	DI	182
						KE	602	DA	40
						PR	2800	RC	100
						IA	77	RR	84
						ID	536	RE	21
								RO	7
						Tot.	62309	RD	3
								RS	0
								RI	4
								LA	908
								MD	92
								ST	984
								Tot.	14589

1.2. Gas-phase Chemical Physics Data Base

The GAPHYOR data base has been published by Elsevier North Holland in its entirety in three separate volumes. The table of contents of these books are given in Appendix 1. The introduction provides a detailed description of the present state of GAPHYOR.

1.3. Recent Technical Developments

The description of a number of reactants was improved and new processes were introduced. Samples of the corresponding hard copy output are provided:

Shell structure description

ELEMENTS AA	S E	INITIAL STATE MOL 1	MOL 2	MOL 3	PR	FINAL STATE MOL 4	MOL 5	MOL 6	INFO	AN	JO	VO	PAGE	AU	GEOG
* 8A = Fe Co Ni *															
Fe	1	Fe 22+*	1,3		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA
Fe	1	Fe 23+*	1,2		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA
Fe	1	Fe 23+*	1,1,1		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA
Fe	1	Fe 24+*	0,2		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA
Fe	1	Fe 24+*	0,1,1		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA
Fe	1	Fe 24+*	0,1,0,1		IN	e			P :R	87	IPPJ	REPT	AM49	KATO T	JAAINA

(total number of records: 292)

Neutral or ionized clusters

ELEMENTS AA	BB	CC	DD	S E	INITIAL STATE MOL 1	MOL 2	MOL 3	PR	FINAL STATE MOL 4	MOL 5	MOL 6	INFO	AN	JO	VO	PAGE	AU	GEOG
* H = H D T p- * 4A = C Si Ge Sn Pb * 5A = N P As Sb Bi * 6A = O S Se Te Po *																		
H	C	N	O	1	/HCO2-/HCN/n	n=01-09		EN	HCN	/HCN/n/HCO2-		B E	BB	JPC	92	2738	MEOT-NER M	USMDGA
H	C	N	O	1	/H3C2O2-/HCN/n	n=01-09		EN	/H3C2O2-/HCN/n	HCN		B E	BB	JPC	92	2738	MEOT-NER M	USMDGA
* H = H D T p- * 4A = C Si Ge Sn Pb * 5A = N P As Sb Bi * 7A = F Cl Br I At *																		
H	C	N	F	1	/H3CF/N2/n/v	n=01-02		EN				B E	BB	ZP/D	10	347	CELII F G	USCAPA
H	C	N	F	1	/F-/H3C2N/n	n=01-07		EN	H3C2N	/H3C2N/n/F-		B E	BB	JPC	92	3943	HIRAOKA K	JAYNKO
H	C	N	C1Br	1	/DD-/H3C2N/n	n=01-08		EN	H3C2N	/H3C2N/n/DD-		B E	BB	JPC	92	3943	HIRAOKA K	JAYNKO
H	C	N	I	1	/I-/H3C2N/n	n=01-05		EN	H3C2N	/H3C2N/n/I-		B E	BB	JPC	92	3943	HIRAOKA K	JAYNKO
* H = H D T p- * 4A = C Si Ge Sn Pb * 6A = O S Se Te Po * 7A = F Cl Br I At *																		
H	C	O	234	1	/DD-/HCO/n	n=01-09		EN	HCO	/HCO/n/DD-		B E	BB	JPC	92	2738	MEOT-NER M	USMDGA

(total number of records: 461)

Molecules absorbed on a surface

ELEMENTS AA	BB	CC	DD	S E	INITIAL STATE MOL1	MOL2	MOL3	PR	FINAL STATE MOL4	MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* H = H D T p- * 4A = C Si Ge Sn Pb * 6A = O S Se Te Po * 8A = Fe Co Ni *																		
H	C		S	FeNi 4	H4CS	(DD)		IR	(DD)H4CS	(DD)H3C	(DD)HS	K2-L/E	BB	JFI	84	3027	ALHAIDARY	IQBAJA
H	C		S	FeNi 4	H4CS	(DD)		IR	(DD)H4CS	(DD)H3CS	(DD)H	K2-L/E	BB	JFI	84	3027	ALHAIDARY	IQBAJA
* H = H D T p- * 4A = C Si Ge Sn Pb * 6A = O S Se Te Po * 8B = Ru Rh Pd *																		
H	C		S	Pd 4	H4CS	(Pd)		IR	(Pd)H4CS	(Pd)H3C	(Pd)HS	K2-L/E	BB	JFI	84	3027	ALHAIDARY	IQBAJA
H	C		S	Pd 4	H4CS	(Pd)		IR	(Pd)H4CS	(Pd)H3CS	(Pd)H	K2-L/E	BB	JFI	84	3027	ALHAIDARY	IQBAJA

(total number of records: 3193)

Isoelectronic series

ELEMENTS AA	S E	MOL1	INITIAL STATE MOL2	MOL3	PR	MOL4	FINAL STATE MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* 10 *															
	1	AA(N=29)*	Z=38-60		TR	AA(N=29)	Z=38-60		UI T	BB	ADND	39	157	BIEMONT E	BELICC
	1	AA(N=04)*	Z=04-26		TR	AA(N=04)	Z=04-26		UI R	BB	ZP/D	9	143	TRABERT E	DBNWBC
	1	AA(N=29)*	Z=38-60		TR	AA(N=29)*	Z=38-60		UI T	BB	ADND	39	157	BIEMONT E	BELICC

(total number of records: 1603)

Homonuclear sequences

ELEMENTS AA	S E	MOL1	INITIAL STATE MOL2	MOL3	PR	MOL4	FINAL STATE MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* R = He Ne Ar Kr Xe Rn *															
Xe	3	e	Xe n+	n=02-06	IN	2e	Xe n+	n=03-07	SO J R	BB	IPPJ	REPT	AMB2	TAWARA H	JAAICH
Ne	3	e	Ne n+	n=05-09	IN	2e	Ne n+	n=06-10	CO J R	BB	JRD	17	1285	LENNON M A	UKIRBE
Ar	3	e	Ar n+	n=05-06	IN	2e	Ar n+	n=06-07	CO L R	BB	JRD	17	1285	LENNON M A	UKIRBE
Ar	3	e	Ar n+	n=09-13	IN	2e	Ar n+	n=10-14	KO J R	BB	JRD	17	1285	LENNON M A	UKIRBE
Ar	3	e	Ar n+	n=15-17	IN	2e	Ar n+	n=16-18	KO J R	BB	JRD	17	1285	LENNON M A	UKIRBE

(total number of records: 1462)

1.4. 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 our 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.

2. NUMERICAL DATA ACTIVITIES

2.1. Numerical data files

A system for storage and retrieval of numerical data has been implemented for use with IBM compatible microcomputers. It includes only processes involving one or two atoms and possibly photons and electrons, i.e. records of GAPHYOR 1 and 2 files. The bibliographic part of the system is contained in three tables following the mainframe implementation of GAPHYOR. These tables are using all the GAPHYOR system conventions as implemented in its edition by Elsevier. This part of the system is regularly used in the Astrophysical Laboratory at Meudon for keeping a bibliographic file for photoionization used for the needs of the international astrophysical project Opacity. The numerical data file of the system comprise evaluated charge transfer and ionization cross sections of ions colliding with H° and He°. The standard commercial data base system Rbase for DOS has been used as a basis for this implementation. Consequently, data handling and transfer under standard ASCII format files or other common commercial form files (e.g. .DB) is straightforward. It is to be noted that this system is giving full satisfaction, being fully relational and retrieving with remarkable speed in INTEL 80386 based microcomputers. Another commercial support is now used for building an atomic data base at Livermore Laboratory. In order to be able to implement our data base also in mainframe computers we are considering to further use as support Oracle, successfully used by NIST for a number of data bases.

Numerical data included in the Belfast-Daresbury data bank are also implanted at one of the major computing facilities of the Paris region (CIRCE). In collaboration with the Astrophysical Laboratory at Meudon the procedural part of this data bank has been installed at CIRCE; part of the numerical values contained will be stored in microcomputer and will eventually be merged with the numerical GAPHYOR file.

2.2. Meudon meeting

The GAPHYOR data centre collaborated with the Meudon Astrophysical Laboratory in preparing an international meeting held at Meudon (4 to 6 September 1989), supported by the French National Research Centre (CNRS). The programme comprise review and assessment of atomic data for fusion and astrophysics (mainly cross sections for electron and photon collisions) and data bank management items.

2.3. Theoretical data production

Our project of calculation and evaluation of atomic data is going on. This project was initiated as a collaborative programme with

the Royal Holloway College, University of London and the Institute of Physics, University of Belgrade.

Initially, a review report has been prepared to assess the recent achievements in atomic data measurement, calculation and evaluation. This report was published in a special issue of Nuclear Fusion. It mainly reviews the work produced under the Coordinated Research Programme (CRP) on 'Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas' conducted by the Atomic Data Unit of the IAEA under Dr. Katsonis responsibility; it also includes all the conclusions and recommendations of the CRP, as was suggested by the IFRC A+M data subcommittee. In order to keep pace with the fast developments in this field, subsequent work has also been included in the report.

Numerical calculations of charge transfer and ionization cross sections are under way. After a long stage of checking, the CTMC code for Monte Carlo type calculations developed by M. R. C. McDowell and his collaborators and subsequently modified at Orsay is now finalized. Charge transfer and ionization cross sections for collisions of neon ions with hydrogen have been calculated.

These calculations were realized in a CDC computer in Grenoble and in a PC hosting a Definicon accelerator board based on a 68020 CPU and a 68882 FPU running SVS Fortran under DOS compatible kernel and represent the equivalent of several hundreds of CRAY computing hours.

We are now calculating the same cross sections for metallic ions (Ti, V, Kr, Mn, Fe, Co, Ni). This will complete our commitment with the CEA of Cadarache to produce urgently needed data for fusion. We are also considering to produce data needed for plasma diagnostics in the JET tokamak at Culham (see meetings discussions).

2.4. Data storage and exchange

The system Aladdin provided by the IAEA (version 1.0) was implanted and tried in microcomputers under various 32 bits compilers. The system was compiled and linked without problem with the NDP Fortran working under Phar Lap DOS Extender (see Appendix 2) after adding the necessary END statements in the source files ALCOM and ALPCOM. On the contrary it needs major modifications in order to be compiled with the SVS Fortran, although it is a standard Fortran 77 compiler. Further tests on Aladdin are under way.

CONTENTS OF OTHER VOLUMES

Part A: Systems with one element

Part B: Systems with two elements

Part C: Systems with three or four elements

CONTENTS

ACTIVITIES IN THE A+M DATA AT ENEA-BOLOGNA

M.Frisoni[1] P.L.Ottaviani-ENEA Bologna, Italy

The work about a systematic collection of experimental and theoretical data for electron-ion ionization, excitation and recombination processes is going on.

The elements considered are typically those present in the plasma as impurities coming from structural materials which are recognized to play an important role on both radiative power losses and plasma energy confinement.

For the present time carbon, oxygen, iron and nickel are considered.

The aim of this work is to provide a comprehensive and continuously updated collection of the existing data in literature on the most relevant electron-ion collisional processes in plasmas, as a necessary step in order to obtain "recommended" data.

For any electron-ion process and for each element characterized by its Z-value, all the ions are considered and the data are accordingly selected. Such data have been organized in files which are read by a computer code in order to obtain cross sections and rate coefficients, both in tabular and graphical form suitable for easy comparison.

A sequence of values of the independent variable (temperature, incident electron energy etc.) is chosen in order to make easy the interpolation.

For each ion a bibliography is also supplied specifying in addition, for theoretical data, the approximation used; see figure 1.

As an example of the organization of the entire data base, we present here the relevant steps that have been adopted for the collection of data on electron impact excitation collision strengths of iron ions from Fe XXVI to Fe I (ENEA reports RT/TIB/89/3, RT/TIB/89/12):

1. For each ion the compilation is 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. Since resonance cross sections are not easy to handle for tabulating, plotting and comparing, non resonant collision strengths only are considered, whereas resonance effects are included in excitation rate coefficients.

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 are 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 are minimized.

Figure caption.: In figure 2 at the top of each table the charge state, the type of transition and the threshold energy (ΔE_{ij} = DE) are shown. The LS coupling notation is used. The threshold energy of the transition is derived from the critical compilations of spectroscopic data and from recent references found in literature. However, the values of threshold reported must not be considered as the recommended ones.

The incident electron energy values in threshold unit (E/DE = x) are listed in the first column. These values are equally spaced in logarithmic x-scale. The resulting collision strengths are listed in the subsequent columns which show at their top the reference label and the threshold energy used by the authors. Generally, each table is followed by the corresponding plot where the same notation and units are used.

Plots are obtained by means of the PLOTTAB code.

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[1] Guest researcher

REFERENCES

1) M.Jones, Mon.Not.R.Astr.Soc. 169,211 (1974). (DWX)

2) M.S.Pindzola,S.L.Carter, Phys.Rev A22,898 (1980). (RDWX)

3) R.Mewe,J.Schrijver,J.Sylvester, Astron.Astrophys. 87,55 (1980); R.Mewe, Astron.Astrophys. 20,215 (1972). (FIT)

4) R.E.H.Clark,N.H.Magee Jr.,J.B.Mann,A.L.Merts, Astrophys.J. 254,412 (1982). (FIT-DWX)

5) S.Nakazaki,T.Hashino, J.Phys. B15,2295 (1982). (CBX)

6) F.Bely-Dubau,J.Dubau,P.Faucher,A.H.Gabriel, Mon.Not.R.Astr. Soc. 198,239 (1982). (DWX)

7) J.B.Mann, Atom.Data Nucl.Data Tables 29,407 (1983). (DWX)

8) D.H.Sampson,S.J.Goett,R.E.H.Clark, Atom.Data Nucl.Data Tables 29,467 (1983). (CBX)

9) A.K.Pradhan, Phys.Rev. A28,2113 (1983). (RDWX,CC)

10) A.K.Pradhan, Phys.Rev. A28,2128 (1983). (RDWX,CC)

11) L.Steenman-Clark,P.Faucher, J.Phys. B17,73 (1984). (DWX)

12) R.Mewe,E.H.B.M.Gronenschild,G.H.J.van der Oord, Astron. Astrophys.Suppl.Ser. 62,197 (1985). (FIT)

13) A.K.Pradhan, Astrophys.J.Suppl.Ser. 59,183 (1985). (RDWX,CC)

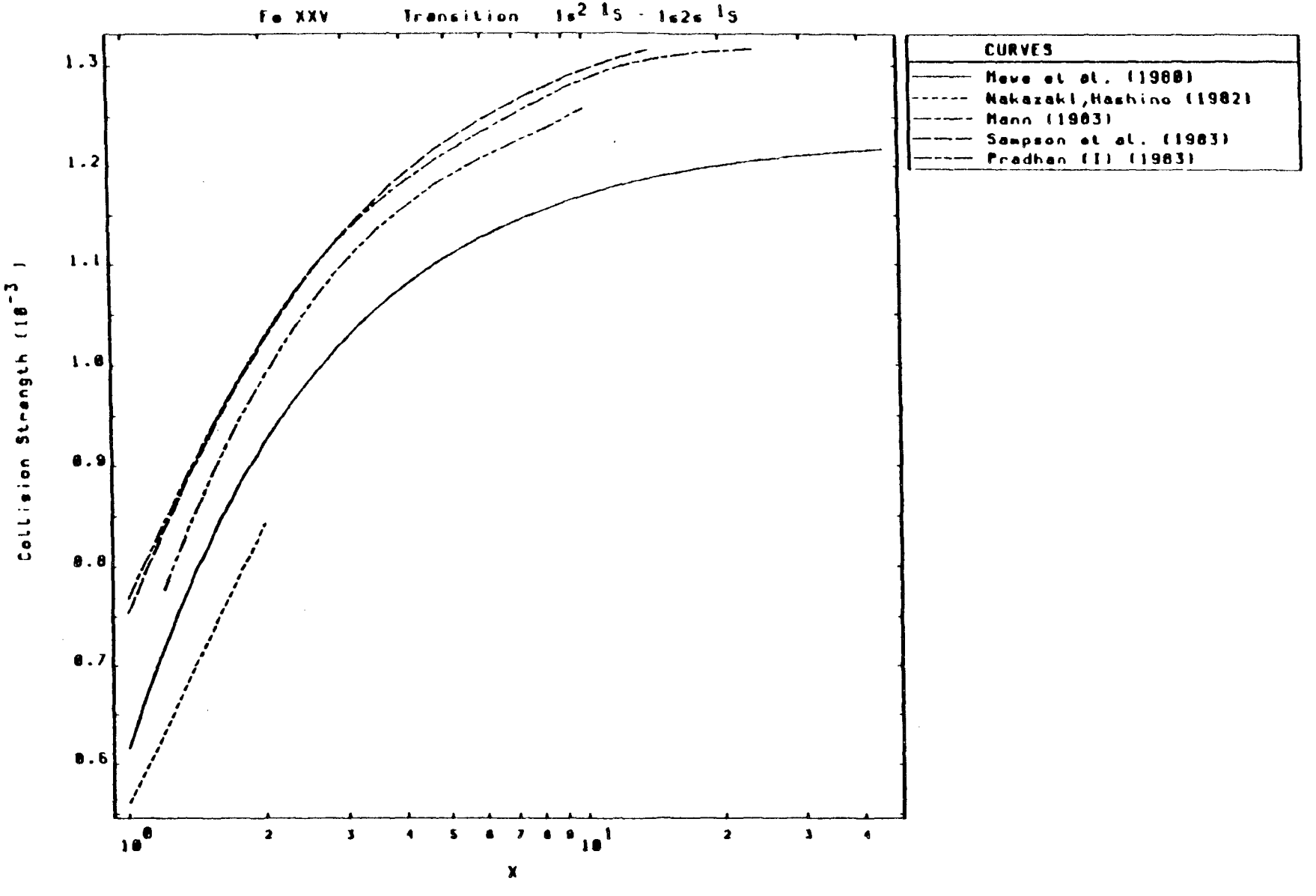
14) N.R.Badnell, J.Phys. B18,955 (1985). (DWX)

15) P.Faucher,J.Dubau, Phys.Rev. A31,3672 (1985). (DWX)

16) H.Zhang,D.H.Sampson, Astrophys.J.Suppl.Ser. 63,487 (1987). (CBX)

COLLISION STRENGTHS FE XXV $1s^2\ ^1S$ - $1s2s\ ^1S$ DE=6670(eV)

E/DE	1) DE=6677.4	3) DE=6670.0	4) DE=6668.0	5) DE=6620.7	6) DE=6670.0	7) DE=6697.9	8) DE=6676.5	9) DE=6674.7	14) DE=6675.0
1.000		6.157E-04	5.521E-04	5.606E-04		7.683E-04	7.531E-04		
1.100	6.166E-04	6.716E-04	6.108E-04	5.971E-04	6.914E-04	8.073E-04	7.968E-04		7.711E-04
1.200	6.596E-04	7.183E-04	6.617E-04	6.324E-04	7.196E-04	8.425E-04	8.351E-04	7.768E-04	8.086E-04
1.300	7.018E-04	7.577E-04	7.062E-04	6.661E-04	7.515E-04	8.743E-04	8.689E-04	8.162E-04	8.416E-04
1.400		7.916E-04	7.455E-04	6.975E-04	7.900E-04	9.032E-04	8.988E-04	8.508E-04	8.709E-04
1.600		8.465E-04	8.114E-04	7.532E-04	8.386E-04	9.529E-04	9.496E-04	9.082E-04	9.200E-04
1.800		8.893E-04	8.645E-04	8.014E-04	8.826E-04	9.939E-04	9.908E-04	9.534E-04	9.604E-04
2.000		9.235E-04	9.080E-04	8.426E-04	9.187E-04	1.028E-03	1.025E-03	9.895E-04	9.925E-04
2.200		9.515E-04	9.444E-04		9.486E-04	1.056E-03	1.054E-03	1.020E-03	1.020E-03
2.400		9.748E-04	9.753E-04		9.744E-04	1.080E-03	1.078E-03	1.046E-03	1.043E-03
2.600		9.945E-04	1.002E-03		9.972E-04	1.100E-03	1.099E-03	1.067E-03	1.063E-03
2.900		1.019E-03	1.035E-03		1.027E-03	1.124E-03	1.125E-03	1.094E-03	1.089E-03
3.200		1.039E-03	1.063E-03		1.050E-03	1.144E-03	1.147E-03	1.116E-03	1.110E-03
3.500		1.055E-03	1.086E-03		1.069E-03	1.160E-03	1.165E-03	1.134E-03	1.127E-03
3.800		1.069E-03	1.105E-03		1.085E-03	1.174E-03	1.181E-03	1.148E-03	1.142E-03
4.100		1.081E-03	1.122E-03		1.098E-03	1.186E-03	1.194E-03	1.161E-03	1.154E-03
4.500		1.094E-03	1.141E-03		1.113E-03	1.199E-03	1.209E-03	1.174E-03	1.168E-03
4.900		1.106E-03	1.157E-03		1.127E-03	1.210E-03	1.222E-03	1.185E-03	1.180E-03
5.400		1.117E-03	1.174E-03		1.140E-03	1.223E-03	1.235E-03	1.197E-03	1.193E-03
5.900		1.127E-03	1.188E-03		1.152E-03	1.233E-03	1.246E-03	1.206E-03	
6.400		1.135E-03	1.200E-03		1.161E-03	1.243E-03	1.255E-03	1.215E-03	
7.000		1.143E-03	1.212E-03		1.171E-03	1.252E-03	1.265E-03	1.223E-03	
7.700		1.151E-03	1.224E-03		1.180E-03	1.262E-03	1.274E-03	1.232E-03	
8.400		1.158E-03	1.234E-03		1.187E-03	1.271E-03	1.282E-03	1.241E-03	
9.200		1.164E-03	1.244E-03		1.194E-03	1.279E-03	1.289E-03	1.250E-03	
10.000		1.170E-03	1.252E-03		1.199E-03	1.286E-03	1.295E-03	1.258E-03	
11.000		1.175E-03	1.260E-03			1.293E-03	1.301E-03		
12.000		1.180E-03	1.267E-03			1.298E-03	1.307E-03		
13.000		1.184E-03	1.273E-03			1.302E-03	1.311E-03		
14.000		1.187E-03	1.278E-03			1.305E-03	1.315E-03		
16.000		1.193E-03	1.286E-03			1.310E-03			
18.000		1.197E-03	1.293E-03			1.313E-03			
20.000		1.201E-03	1.298E-03			1.314E-03			
22.000		1.203E-03	1.303E-03			1.315E-03			
24.000		1.206E-03	1.306E-03			1.316E-03			
26.000		1.208E-03	1.309E-03						
29.000		1.210E-03	1.313E-03						
32.000		1.212E-03	1.316E-03						
35.000		1.214E-03	1.318E-03						
38.000		1.215E-03	1.321E-03						
41.000		1.216E-03	1.322E-03						
45.000		1.218E-03	1.324E-03						


Fe XXV Transition $1s^2\ ^1S - 1s2s\ ^1S$
Collision Strength (10^{-3})
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
10^0
2
3
4
5
6
7
8
9
10^1
2
3
4
X
CURVES
Neve et al. (1980)
Nakazaki,Hashino (1982)
Mann (1983)
Sampson et al. (1983)
Pradhan (I) (1983)

The Status of A+M Data Research for Fusion in CRAAMD

Sun Yongsheng

(IAPCM, Beijing)

OUTLINE

- The brief situation on CRAAMD;
- The several tasks being already in progress in CRAAMD:
  1. Experiments;
  2. Theoretical calculations;
  3. A+M database;
- Funds;
- Hope!

I. The brief situation on Chinese Research Association for A+M Data.

In order to fit the needs of certain new technology fields, especially for magnetic and inertial confinement fusion, Laser fusion and so on, "Chinese Research Association for A+M Data" (CRAAMD) was established in Beijing in 1987.

Up to now, ten institutions of the whole country have joined CRAAMD, they are:

(1) Institute of Applied Physics and Computational Mathematics (IAPCM, Beijing)
(2) The Department of Modern Physics Fudan University (Shanghai)
(3) Institute of Low Energy Physics and Department of Physics, Beijing Normal University (Beijing)
(4) Nuclear Physics Division of Institute of Atomic Energy (Beijing)
(5) Institute of High Temperature and High Pressure Physics, Chengdu University of Science and Technology (Chengdu City, Sichuan Province
(6) Institute of Physics, Academia Sinica (Beijing)
(7) Institute of Atomic and Molecular Physics, Jilin University (Changchun City, Jilin Province)
(8) Center of Basic Physics, University of Science and Technology of China (Hefei City, Anhui Province)
(9) Institute 207, The Second Academy, Ministry of Aerospace (Beijing)
(10) Department of Applied Physics, National University of Defence Technology (Changsha City, Hunan Province).

IAPCM is the leading instituation of CRAAMD.

Although the Ten joining CRAAMD are not all institutions of researching A+M physics, they are really the principal ones in China. There are about 200 people making research on A+M data in CRAAMD. Many chinese well-known

atomists have joined CRAAMD, such as, theoretical atomists Profs. Gou Qingquan, Li Jiaming and experimental atomists Yang Fujia, Wang Renguang etc.

II. The several tasks being already in progress.

1. Experiment:

(1) Electron Impact Ionization of Atomic Ions.

This task is undertaken by Department of Modern Physics, Fudan University. The persons in charge: Prof. Yang Fujii and Tang Jiayong. Their experimental facilities have been already fixed. They are debugging them now. By the end of this year or the beginning of next year, they will get the first set of the measured cross-section for the reaction

$$He^{+} + e \rightarrow He^{++} + 2e \quad .$$

After 1990, they will measure the electron impact ionization cross-sections of H-like (C^{+5}), He-like (C^{+4}) and those of Ge^{+}, Kr^{+} etc.

(2) Electron- and ion-impact excitation of atoms

This task is undertaken by the Institute of Physics (Beijing), Academia Sinica. The persons in charge: Prof. Liu Jiarui and Pan Guangyan.

Up to now, they have done many experiments on collisions between atoms and ions, such as:

$$He^{+} + Ne \rightarrow He^{*} + Ne^{+*}$$

$$He^{+} + Ar \rightarrow \quad ; \quad Ne^{+} + He \rightarrow \quad ;$$

$$Ar^{+} + T \rightarrow \quad ; \quad \ldots\ldots\ldots \quad .$$

and collisions of double charged ions: He^{2+} + Ne (or Ar) → ... etc. They have investigated many processes in these collisions. Their task ahead is to measure electron impact excitation.

(3) Ionic spectroscopy.

This task is undertaken by the Institute of Atomic Energy. Dr. Yao will talk about it in detail.

2. Theoretical Calculations.

The tasks of theoretical calculations are undertaken by IAPCM and Jilin University.

(1) Jilin University works on electron impact ionization and ionic spectroscopy. Relativistic effects are rigorously considered in their work. In ionic spectroscopy calculations, they used the MCDF (Multiple Configuration Dirac-Fock) code given by Grant. In the research of electron impact ionization, they used the approach of Prof. Sampson and Dr. Zhang (Hueng Lin) and the MCDF code. They have already calculated the rate coefficients of Na-like ions and Ne-like ions of several elements (such as: iron, selenium, molybedenum, cobalt etc).

(2) IAPCM

IAPCM is a comprehensive institute. There are 4 groups (25 people) engaged in research on A+M physics in IAPCM. One of them works on ionic spectroscopy; another works on electron impact; the third group studies the basic theory of A+M physics; the fourth one compiles A+M data and put them into the database. Our calculations rest on the series of R.D. Cowan's code. In the calculations of ionic spectroscopy, we used Cowan's code directly. In electron impact problems, we are building up our own codes, using Cowan's wave functions and energy levels. We have already calculated a number of electron impact and ionic spectroscopy data for several elements (such as Ge, Se, Fe, Al, etc).

(3) A+M database:

Our compilation group has compiled lots of electron impact data in the last two years. We are studying the ALADDIN system now. All the A+M data will be put into the computer. There is a SUN (computer) working station in our Institute. It has 3 Mini-computers, the computers are:

i) Sun-4-280, memory 32 MB, hardware 892 MB
ii) Sun-4-110, memory 8 MB, hardware 892 MB
iii) Sun-386i, memory 4 MB, hardware 327 MB

The Sun-386i is the special computer for A+M database. The 3 computers are being netted. Our database just starts on a step.

Our compilation also just starts on a step. I have brought the first issue of our reports (CRAAMD). It's a paper on compilation of electron impact data. Be kind enough to give us your opinions.

III. Funds

In order to support the research of A+M data for fusion, National Foundation Committee of Natural Science and Chinese General Company of Atomic Energy have supplied quite a lot of funds for CRAAMD, since it was established (1987).

IV. Our Hope.

We hope to make our contributions to the development of the International Atomic Data Centre Network. We would like to establish professional relations with all A+M data centres in the world and to learn their advanced experiences from them. We hope to get help and advice from A+M Data Unit of IAEA.

Finally I would say that you all are welcome to China, welcome to our Institute. Thank you!

Activities of the Belfast Data Centre (The Queen's University of Belfast) for Atomic and Molecular Physics Processes Relevant to Fusion

Michael J. Higgins, and Prof. F.J. Smith

1. Introduction

This report contains a brief account of the work carried out by the Belfast Data Centre in the two year period ranging from November 1987 to November 1989. A short description of each one of the projects undertaken by the data centre during this period is presented under the appropriate heading. The report concludes by outlining the planned direction of the centre's efforts in the year ahead.

2. Electron Impact Ionization of Atoms

The collection, storage and fitting of data and the production of recommended cross section and rate coefficient data on the electron impact single ionization of atoms and ions, of the high-Z elements from copper to uranium (inclusive), was completed. A report on the compiled data was forwarded to the Culham laboratory (UKAEA) and is now in the process of being published as Culham Report CLM-R294. The report is titled 'Atomic and Molecular Data for Fusion, Part 3. Recommended Cross Sections and Rates for Electron Impact Ionization of Atoms and Ions: Copper to Uranium'.

3. Scaled Electron Impact Ionization Cross Section Data for Molybdenum and its Ions

At the request of Mr. Harrison, then at Culham, we carried out an investigation into the possibility of producing scaled cross section data for all of the ionization stages of molybdenum. The preliminary results of this investigation were forwarded to Mr. Harrison at Garching.

4. Electron Impact Excitation Rates for Iron and its Ions

An in-depth look was taken at the possibilities of producing a more 'physically realistic' analytic form for fitting the available data on the excitation rates of iron and its ions (as opposed to the simple polynomial fitting procedure employed by some authors). Consultation with experts in this field has been sought, as to possible solutions to this problem.

5. ALADDIN Atomic Data Interface Software

The Mk 1.0 version of the ALADDIN data interface code (received in August of this year) is now operational on the data centre's local mainframe computer.

6. Electron Impact Ionization/Dissociation of Selected Molecules

The Culham laboratory has recently requested that our efforts be directed towards the task of producing a current data compilation on the ionization/dissociation processes resulting from electron collisions with 21 preselected diatomic and polyatomic molecules (considered to be of importance in the plasma/containment vessel boundary region of fusion plasmas). The processes to be covered include total ionization, single ionization, double ionization and dissociative ionization and the energy of interest is that between threshold and 500eV.

A comprehensive literature search, spanning the period April 1987 (i.e. from the time when the original critical survey of this topic was completed by this laboratory) to the present, has just been completed. The accumulation of new data is now well under way.

7. Future Plans

The main effort of the Belfast Data Centre in the forthcoming months will be directed towards completion of the molecular ionization project. This will include the collection and storage of all relevant data, followed by a critical appraisal of the collated data by experts in this field of study. Upon consultation with these experts, the data sets, chosen by them, will be fitted using an appropriate analytic form and recommended cross section data produced. The conclusion of this project will take the form of a report to be produced at some stage in the forthcoming year.

REPORTS ON ALADDIN DEVELOPMENTS

Future Development of the ALADDIN System

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Three areas of ALADDIN development can be identified

1. Entry of comprehensive data into ALADDIN format and further practical adoption of ALADDIN by a wide range of users

2. Refinement and enhancement of ALADDIN labeling schemes

3. Modifications and enhancements to the basic ALADDIN data format and/or code structure

These three areas of activity are listed in a logical sequence, with highest priority given to continued data entry (item 1). Expanded data sets will help encourage wider application of ALADDIN, and taken together, expanded data sets and applications will provide the most reliable guidance as to development required in the other two areas.

1. Entry of comprehensive data into ALADDIN format and widespread practical adoption of ALADDIN

- First priority is broadened base of ALADDIN data and widespread adoption
  - larger database will itself encourage applications and help establish ALADDIN as a standard format
  - develop expanded applications to atomic structure data, surface data, etc.
  - develop a standard set of physics-based, fast to evaluate fitting forms (also affects labeling and ALFLIB software)
  - provide comprehensive sets of data for specific applications, rather than organizing data by source or atomic physics
- ALADDIN v1.0 manual an important milestone
  - keep documentation as computer files for simultaneous distribution with ALADDIN ?

- add sample code ALP_EX.FOR (Hulse) which shows complete working example of ALPACK interface in a user's code

- Enhanced "secondary" distribution of ALADDIN data and software
  - handle via atomic data centers, others from ALADDIN user's group
  - establish ALADDIN data and software access via MFENET and other computer networks
  - provide debugged software and media translation for other major computers beyond IBM PC

    VAX, Cray, Macintosh, Sun, etc. FORTRAN compatibility

    media compatibility (5 1/4" floppies, 3 1/2" floppies, 9 track tape, etc. as most appropriate for each target machine)

- Continued development of ALADDIN connections to existing fusion and non-fusion atomic physics data resources is important
  - LANL atomic physics database system(s) (Clark)
  - LLNL atomic physics database system(s) (Cauble, Walling)
  - Skip Morgan / NIST grant to organize plasma processing data
  - fit current PPPL impurity rate subroutine (ADPAK) output
  - setup facility for automated generation of extensive ALADDIN data sets from atomic physics codes ?
  - astrophysics ?

- Magnetic fusion impurity transport codes
  - PPPL impurity transport code (Hulse)
  - need complete set of rates for impurity modeling !
  - data buffering system needs to be developed and explored

- Develop other user applications
  - surface data an important area for new ALADDIN applications

2. Refinement and enhancement of ALADDIN labeling schemes

- Require no modification of basic ALADDIN format or software

- Refinements to existing labeling scheme based on discussion of experience using ALADDIN at atomic data centers and elsewhere

- Templates to simplify understanding hierarchical labeling schemes
  - this is an important labeling feature we should agree on at this meeting
- Support broadened ALADDIN applications by developing labeling schemes for important data types not emphasized in original ALADDIN scope
  - new indexing label scheme to support atomic structure data (R.E.H. Clark)
  - surface data

3. Modifications and enhancements to the basic ALADDIN data format and/or code structure

- Fundamental changes unnecessary
  - original ALADDIN format and software well accepted
  - continued attention to goals of simple and straightforward code
  - avoid changes ("creeping featurism") unless warranted by serious difficulties
- I will focus on ALADDIN data format/software functionality issues in three areas
  - searching
  - handling double precision fitting coefficients
  - output of tabular data
- "Double precision" and "tabular data" issues are addressed by different solutions than those incorporated in IAEA v1.0 as changes from the original ALADDIN software

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)

Double precision fitting coefficients

- IAEA v1.0 addressed the issue of double precision coefficients by converting all ALFLIB function variables to double precision (along with other changes)
  - usually single precision = (REAL*4) = 32 bits (~ 7 decimal places), double precision = REAL*8 = 64 bits (~ 16 decimal places)
  - but note that on Cray, single precision = 64 bits !

- Use of double precision should be strongly discouraged
  - double precision is unnecessary; a different fit type and single precision coefficients can always be used
  - double precision leads to fits which are overly sensitive to evaluation errors
  - double precision complicates data types in ALADDIN and codes
  - double precision very slow
  - only need is to accomodate existing data sets which use double precision coefficients and which cannot be immediately converted to single precision fitted forms

- Standardize ALADDIN coefficients as single precision real numbers as in original version

- Treatment of double precision coefficients as a special data type in the coefficient field falls within the intended use of the ALADDIN $ access label

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

Output of data in tabular form

- Main issue is adding the ability to generate tabular data with intervals automatically selected so as to guarantee linear interpolation to a specified accuracy ("LINTAB" procedure)
- LINTAB feature was substituted for original "EV" command function in IAEA v1.0 to provide this capability
- Simple linear / log data point generation as per original "EV" command should be still supported
- Restore TAB1D as important basic data type
- LINTAB output can best be generated using a new "LT" command
  - write LINTAB output as ALADDIN data entry
  - optionally, write LINTAB output as "EV" command style columnar output to terminal or a file

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
```

New "LT" command to provide additional tabular data output with formally specified interpolation accuracy

- "LT" command functionality should be available in parallel with, rather than in place of, original "EV" command

- Can be added in modular fashion via new subroutine ALLT to process "LT" command

- Primary output as ALADDIN entries
  - duplicate ALADDIN header from input entry
  - change data type to #TAB1D
  - add Boolean label "LINTAB" to identify as LINTAB data
  - add Boolean label "LTACC=xx" to carry accuracy of interpolation (not necessarily that of original data !)

- write new entry to usual ALADDIN data output file (requires no new file open/close code)

- Also options for columnar output to terminal or data file
  - follow new format of EV command output for consistency
  - write columnar data to usual "EV" data output file (requires no new file open/close code)

An additional option (?): Output of automatically-generated subroutine with embedded tabular data

- Variation on LINTAB generation of ALADDIN output file, subroutine would be created which calls TAB1D with embedded data

- Would provide "stand-alone" subroutines which could return atomic data with no need to call ALADDIN system at all after initial generation of subroutine using ALADDIN interactive code

- Result would be 3 parallel paths to get ALADDIN data into codes
  - use ALPACK and ALFLIB subroutine package to access standard ALADDIN data files
  - use ALADDIN "LT" command to convert data of various types to linearly interpolatable data values in #TAB1D format, then read data files using ALPACK and just TAB1D routine for simple & fast linear interpolation to access data originally in many fitted forms
  - ALADDIN-generated subroutines with embedded LINTAB data & documentation compiled into codes

Code fragment for stand-alone subroutine with embedded data

```
SUBROUTINE XYZFCN (PX, PY, ERRMSG, DOC)
COMMON /XYZCF/ CF, NCF
COMMON /XYZDOC/ DOC
.....
CALL ALTAB1(PX, CF, NCF, PY, ERRMSG)
.....
END
- - - - -
BLOCK DATA XYZDAT
COMMON /XYZCF/ CF(###), NCF
COMMON /XYZDOC/ DOC
CHARACTER*80 DOC
```

DATA CF / ... {DATA VALUES} ... /
DATA NCF / {NUMBER OF CF'S} /
DATA DOC /"BRIEF INTERNAL DOCUMENTATION OF DATA"/
END

(THE ABOVE IS MEANT TO BE ONLY A SUGGESTIVE OUTLINE)

Organizational approach to implementation of proposed ALADDIN data format / software changes

- R. Hulse to (finally) write CPC paper, including new ALADDIN v1.1
  - description of design philosophy behind ALADDIN and resulting ALADDIN structure
  - description of fundamental ALADDIN data format, interactive code functionality, and use of ALPACK
  - reference IAEA for details of current IAEA labeling scheme, available data with supporting fit subroutines, and future development (including incorporation of ALLT command)
- ALADDIN v1.1 attributes:
  - based on original (Hulse v1.0) ALADDIN software
  - original EV command included, slightly enhanced output file format
  - new searching (added numeric search and substring wild card features)
  - double precision via $D
  - dummy "LT" command subroutine ALLT, establishing framework for "LINTAB" implementation
- J. Smith to add "LINTAB" capability via self-contained "LT" command subroutine ALLT
  - generate LINTAB output to ALADDIN format, terminal or data file
  - possibly also develop embedded-data subroutine output feature
- IAEA developed subroutines (ALLT & added ALFLIB fitting routines) combined with Hulse v1.1, released and documented with labeling updates as IAEA v1.1L

v1.1 = "CORE" ALADDIN software.

v1.1L "optional packages"
↑ LINTAB

Summary of General Points for Discussion

- Data entry and ALADDIN applications
  - types of data currently entered
  - interfaces with other atomic database systems
  - expansion to include new types of data, such as atomic structure data, surface data, etc.
  - standard set of fitting forms (also affects labeling and ALFLIB software)
  - data needed to make up comprehensive "application-oriented" data sets
  - incorporation into modeling codes and other user's application codes
- Labeling Scheme
  - refinement of existing labeling scheme
  - templates
  - support of important new data types
- ALADDIN data format / software
  - new search capability on labels as real numbers, substring wild cards
  - double precision coefficients supported as special coefficient field via new access label $D
  - tabular data output

    "EV" command file format

    "LT" command, including ALADDIN format output, possible embedded data subroutines

Postscript: Other Ideas

- "Update" code
  - automatically revise a user's mixed IAEA & private data type files to update w/ new IAEA standard data
  - nice idea, but not immediately important and implementation unclear

- Graphical output
  - probably prohibitively complex for IAEA support, due to lack of graphics standards
  - users will typically have their own graphics options to apply to ALADDIN output anyway
- Faster searching for larger atomic physics databases
  - ALADDIN labeling approach does not lend itself to typical commercially available RDBM software
  - object-oriented databases are under development, may prove useful in the future as they mature
  - search kernel (ALPACK) might be customized for different computer systems for increased speed

ATOMIC STRUCTURE AND RADIATIVE PROCESSES IN ALADDIN FORMAT

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LOS ALAMOS NATIONAL LABORATORY

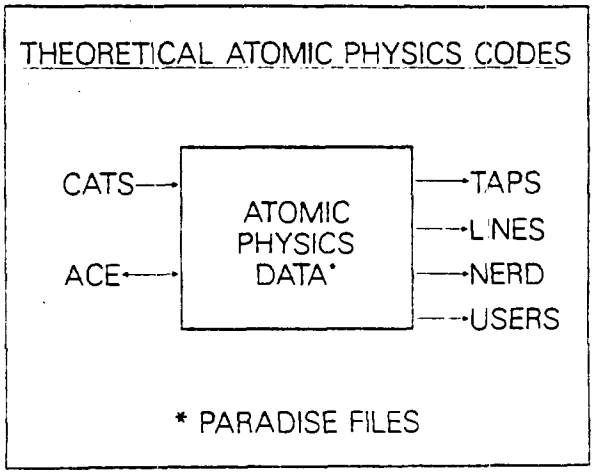
OVERVIEW

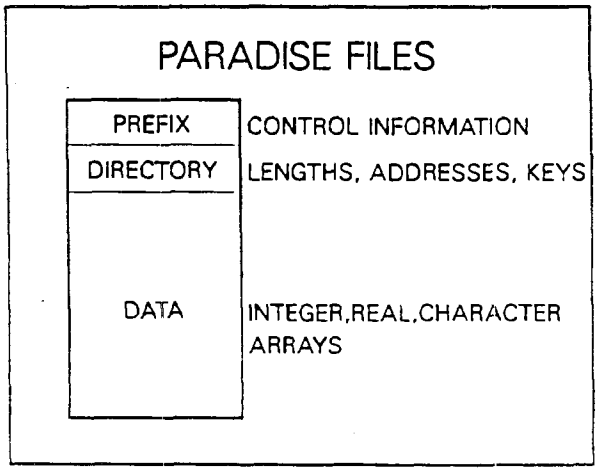
I. LOS ALAMOS SYSTEM OF CODES

II. ATOMIC STRUCTURE DATA

III. COLLISION PROCESSES

IV. RADIATIVE PROCESSES





```
command
? levels
levels
```

index	config #	mult, l Cowan	TAPS	j	energy	configuration				
1	1	4p	4p	0.5	0.0000000e+00	1s 2	2s 2	2p 5	3s 1	3c
2	1	4p	4p	1.5	9.1150591e-01	1s 2	2s 2	2p 5	3s 1	3c
3	1	4f	4f	4.5	2.1416869e+00	1s 2	2s 2	2p 5	3s 1	3c
4	1	4p	4p	2.5	2.4625876e+00	1s 2	2s 2	2p 5	3s 1	3c
5	1	4f	4f	3.5	2.8959361e+00	1s 2	2s 2	2p 5	3s 1	3c
6	1	4f	4f	2.5	3.8914948e+00	1s 2	2s 2	2p 5	3s 1	3c
7	1	4f	4f	1.5	5.2265226e+00	1s 2	2s 2	2p 5	3s 1	3c
8	1	4d	4d	3.5	5.8302288e+00	1s 2	2s 2	2p 5	3s 1	3c
9	1	2p	2p	0.5	5.8547868e+00	1s 2	2s 2	2p 5	3s 1	3c
10	1	2f	2f	2.5	6.1037504e+00	1s 2	2s 2	2p 5	3s 1	3c
11	1	2p	2p	1.5	7.4091451e+00	1s 2	2s 2	2p 5	3s 1	3c
12	1	2f	2f	3.5	9.1859249e+00	1s 2	2s 2	2p 5	3s 1	3c
13	1	2d	2d	2.5	1.1279426e+01	1s 2	2s 2	2p 5	3s 1	3c
14	1	4d	4d	0.5	1.1453687e+01	1s 2	2s 2	2p 5	3s 1	3c
15	1	4d	4d	1.5	1.2656579e+01	1s 2	2s 2	2p 5	3s 1	3c
16	1	4f	2d	1.5	1.6040943e+01	1s 2	2s 2	2p 5	3s 1	3c
17	1	4d	4d	2.5	1.6321547e+01	1s 2	2s 2	2p 5	3s 1	3c
18	1	2d	2d	2.5	1.7296977e+01	1s 2	2s 2	2p 5	3s 1	3c
19	1	2f	2f	3.5	1.7599001e+01	1s 2	2s 2	2p 5	3s 1	3c
20	1	2d	2d	1.5	2.0286537e+01	1s 2	2s 2	2p 5	3s 1	3c
21	1	2f	2f	2.5	2.2683116e+01	1s 2	2s 2	2p 5	3s 1	3c
22	1	2p	2p	0.5	2.5016638e+01	1s 2	2s 2	2p 5	3s 1	3c
23	1	2p	2p	1.5	2.6753170e+01	1s 2	2s 2	2p 5	3s 1	3c

```
command
? mixl 7
mixl 7

index    j        component    configuration

   7     1.5    6.3153e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4F
               -4.2193e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4D
               -9.1447e-02  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4P
               -5.3165e-01  ( 2p5   2P)  2P  ( 3s1   2S)  1P  ( 3d1   2D)  2D
               -3.5669e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  2D
                6.7732e-02  ( 2p5   2P)  2P  ( 3s1   2S)  1P  ( 3d1   2D)  2P
                1.7642e-02  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  2P

command
? mixl 16
mixl 16

index    j        component    configuration

  16     1.5    7.3853e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4F
                1.4476e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4D
               -4.4527e-02  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  4P
                5.7133e-01  ( 2p5   2P)  2P  ( 3s1   2S)  1P  ( 3d1   2D)  2D
                2.9348e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  2D
               -4.8034e-02  ( 2p5   2P)  2P  ( 3s1   2S)  1P  ( 3d1   2D)  2P
                1.2954e-01  ( 2p5   2P)  2P  ( 3s1   2S)  3P  ( 3d1   2D)  2P
```

command
? levels 1 to 20
levels 1 to 20

index	config #	mult, l Cowan	mult, l TAPS	j	energy	configuration
1	1	6d	6d	0.5	0.0000000e+00	1s 2 2s 1 2p 3 3d 1
2	1	6d	6d	1.5	8.9082165e-02	1s 2 2s 1 2p 3 3d 1
3	1	6d	6d	2.5	2.2143454e-01	1s 2 2s 1 2p 3 3d 1
4	1	6d	6d	3.5	4.1495395e-01	1s 2 2s 1 2p 3 3d 1
5	1	6d	6d	4.5	7.5952445e-01	1s 2 2s 1 2p 3 3d 1
6	1	4d	4d	2.5	1.3190053e+01	1s 2 2s 1 2p 3 3d 1
7	1	4d	4d	1.5	1.3469957e+01	1s 2 2s 1 2p 3 3d 1
8	1	4d	4d	0.5	1.4020622e+01	1s 2 2s 1 2p 3 3d 1
9	1	4d	4d	3.5	1.4097141e+01	1s 2 2s 1 2p 3 3d 1
10	1	4f	4f	1.5	3.3741378e+01	1s 2 2s 1 2p 3 3d 1
11	1	4f	4f	2.5	3.4804874e+01	1s 2 2s 1 2p 3 3d 1
12	1	4f	4f	3.5	3.6187305e+01	1s 2 2s 1 2p 3 3d 1
13	1	4g	4g	2.5	3.7303500e+01	1s 2 2s 1 2p 3 3d 1
14	1	4f	4g	3.5	3.7833103e+01	1s 2 2s 1 2p 3 3d 1
15	1	4g	4g	4.5	3.7944301e+01	1s 2 2s 1 2p 3 3d 1
16	1	4d	4d	0.5	3.9058058e+01	1s 2 2s 1 2p 3 3d 1
17	1	4d	4d	1.5	3.9755600e+01	1s 2 2s 1 2p 3 3d 1
18	1	4f	4f	4.5	3.9799151e+01	1s 2 2s 1 2p 3 3d 1
19	1	4g	4g	5.5	4.1069699e+01	1s 2 2s 1 2p 3 3d 1
20	1	4d	4d	2.5	4.1257273e+01	1s 2 2s 1 2p 3 3d 1

command
? mixl 12
mixl 12

index j

12 3.5

component	configuration									
-9.9085e-02	(2s1	2S)	2S	(2p3	4S)	5S	(3d1	2D)	6D
-6.1958e-01	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4G
6.4230e-01	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4F
3.8004e-01	(2s1	2S)	2S	(2p3	2P)	3P	(3d1	2D)	4F
-3.5378e-02	(2s1	2S)	2S	(2p3	4S)	3S	(3d1	2D)	4D
-9.5234e-02	(2s1	2S)	2S	(2p3	4S)	5S	(3d1	2D)	4D
6.8080e-02	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4D
-1.5139e-01	(2s1	2S)	2S	(2p3	2P)	3P	(3d1	2D)	4D
-3.2118e-02	(2s1	2S)	2S	(2p3	2D)	1D	(3d1	2D)	2G
7.5715e-02	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	2G
4.0477e-02	(2s1	2S)	2S	(2p3	2D)	1D	(3d1	2D)	2F
-4.6409e-02	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	2F
-2.6384e-02	(2s1	2S)	2S	(2p3	2P)	1P	(3d1	2D)	2F
-1.4149e-02	(2s1	2S)	2S	(2p3	2P)	3P	(3d1	2D)	2F

command
? mixl 14
mixl 14

index j

14 3.5

component	configuration									
-1.9042e-02	(2s1	2S)	2S	(2p3	4S)	5S	(3d1	2D)	6D
6.6222e-01	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4G
6.6378e-01	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4F
-1.4784e-01	(2s1	2S)	2S	(2p3	2P)	3P	(3d1	2D)	4F
3.0248e-02	(2s1	2S)	2S	(2p3	4S)	3S	(3d1	2D)	4D
9.1602e-03	(2s1	2S)	2S	(2p3	4S)	5S	(3d1	2D)	4D
1.4513e-01	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	4D
-2.1216e-01	(2s1	2S)	2S	(2p3	2P)	3P	(3d1	2D)	4D
3.0356e-02	(2s1	2S)	2S	(2p3	2D)	1D	(3d1	2D)	2G
1.1299e-02	(2s1	2S)	2S	(2p3	2D)	3D	(3d1	2D)	2G

```
$aladdin>>
? de

 entry sequence number =        1

   1[$ CONFIGS Fe [+22]                                                                    ]
   2[& EN ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ=1          #CFGTAB                           ]
   3[!1.   CONFIGURATION INDEX, NSHELL, TOTAL ENERGY(eV)                                   ]
   4[!2.   n, l, w, SHELL ENERGY(eV) FOR EACH SHELL                                        ]
   5[!     REPEAT 1 AND 2 FOR ALL CONFIGURATIONS                                           ]
   6[       1       2 -2.2109530409e+04                                                    ]
   7[  1  0  2  8.5690e+03  2  0  2  1.9459e+03                                           ]
   8[       2       2 -2.1977050573e+04                                                    ]
   9[  1  0  2  8.5283e+03  2  1  2  1.8733e+03                                           ]
  10[       3       3 -2.2053139743e+04                                                    ]
  11[  1  0  2  8.5483e+03  2  0  1  1.9491e+03  2  1  1  1.8897e+03                     ]

$aladdin>>
? ev

     configuration #   1
   shell       energy
   1s2         8.5690000e+03
   2s2         1.9459000e+03
   total configuration energy =  -2.2109530e+04

     configuration #   2
   shell       energy
   1s2         8.5283000e+03
   2p2         1.8733000e+03
   total configuration energy =  -2.1977051e+04

     configuration #   3
   shell       energy
   1s2         8.5483000e+03
   2s1         1.9491000e+03
   2p1         1.8897000e+03
   total configuration energy =  -2.2053140e+04
```

```
$aladdin>>
? de

 entry sequence number =        2

   1[$ TERMS Fe [+22]                                                    ]
   2[& EN ORIG TAPS-36  DOC-TAPS 09/11/89 SEQ-1          #TERMTAB        ]
   3[!1.    TERM INDEX, NSHELL, E(eV)                                    ]
   4[!2.    n, l, w, BLS, BLL, SCRS, SCRL FOR EACH SHELL                 ]
   5[!      REPEAT 1 AND 2 FOR EACH TERM                                 ]
   6[        1        1 -6.5956507e+00                                  ]
   7[  2  0  2  0.0  0  0.0  0                                           ]
   8[        2        2  4.6537573e+01                                  ]
   9[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  1.0  1               ]
  10[        3        2  8.5949982e+01                                  ]
  11[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  0.0  1               ]
  12[        4        1  1.2322586e+02                                  ]
  13[  2  1  2  1.0  1  1.0  1                                          ]
  14[        5        1  1.4326416e+02                                  ]
  15[  2  1  2  0.0  2  0.0  2                                          ]
  16[        6        1  1.6843997e+02                                  ]
  17[  2  1  2  0.0  0  0.0  0                                          ]

$aladdin>>
? ev

listing of ls-terms
 index    energy      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
```

```
 1[$ LEVELS Fe [+22]                                                          ]
 2[& EN ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ=1          #LEVTAB                ]
 3[!1.   LEVEL INDEX, J, NSHELL, E(eV)                                        ]
 4[!2.   n, l, w, BLS, BLL, SCRS, SCRL FOR EACH SHELL                         ]
 5[!     REPEAT 1 AND 2 FOR ALL LEVELS                                        ]
 6[       1  0.0     1 -6.5956507e+00                                        ]
 7[  2  0  2  0.0  0  0.0  0                                                  ]
 8[       2  0.0     2  3.6571950e+01                                        ]
 9[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  1.0  1                      ]
10[       3  1.0     2  4.0540601e+01                                        ]
11[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  1.0  1                      ]
12[       4  2.0     2  5.2128881e+01                                        ]
13[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  1.0  1                      ]
14[       5  1.0     2  8.5949982e+01                                        ]
15[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  0.0  1                      ]
16[       6  0.0     1  1.1200468e+02                                        ]
17[  2  1  2  1.0  1  1.0  1                                                 ]
18[       7  1.0     1  1.2094761e+02                                        ]
19[  2  1  2  1.0  1  1.0  1                                                 ]
20[       8  2.0     1  1.2683706e+02                                        ]
21[  2  1  2  1.0  1  1.0  1                                                 ]
22[       9  2.0     1  1.4326416e+02                                        ]
23[  2  1  2  0.0  2  0.0  2                                                 ]
24[      10  0.0     1  1.6843997e+02                                        ]
25[  2  1  2  0.0  0  0.0  0                                                 ]
```

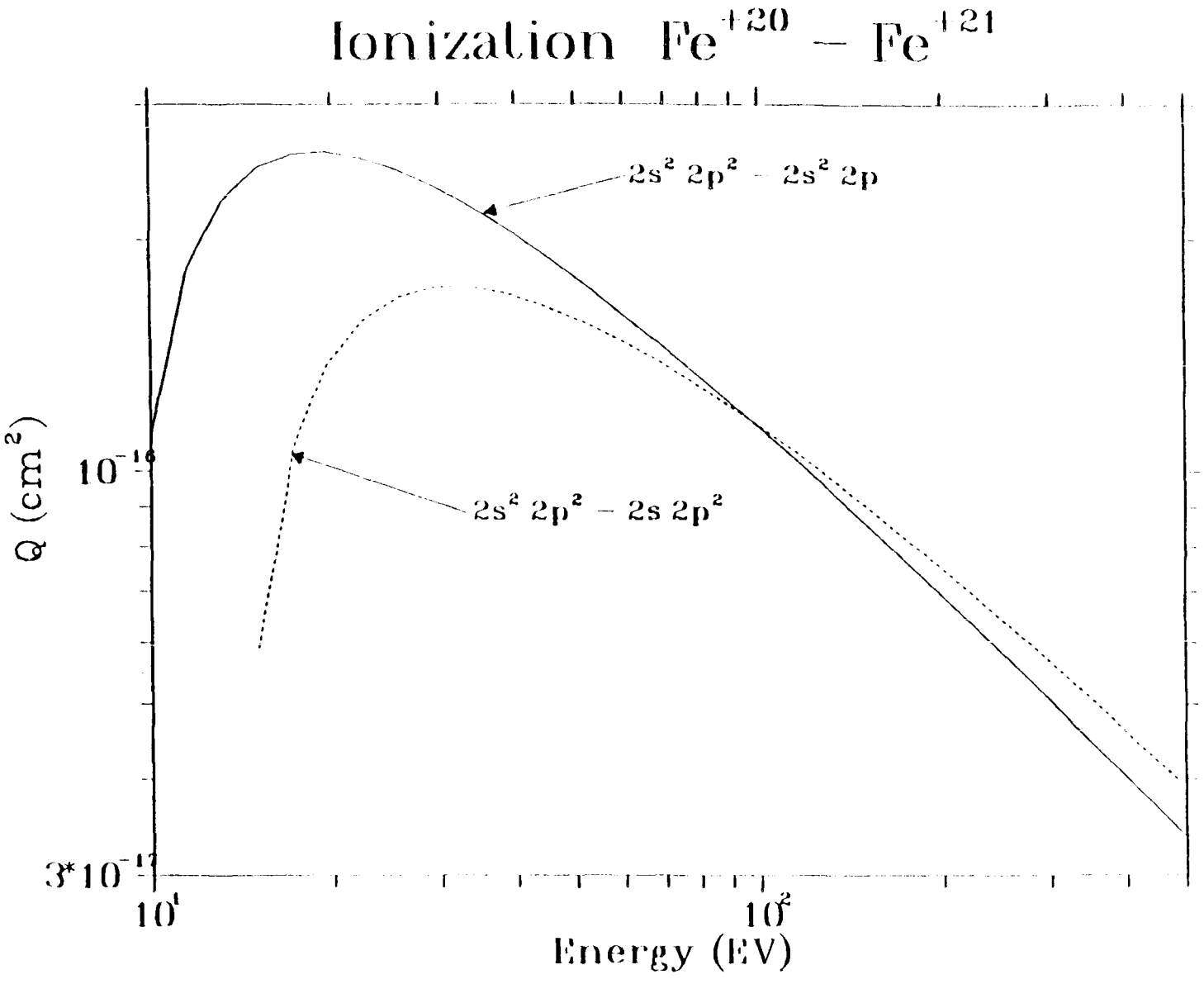
```
$aladdin>>
? ev

listing of fine structure energy levels
 index   j      energy      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
```

```
$aladdin>>
? de

 entry sequence number =        4

   1[$ MIXLEV Fe [+22]  (1)                                                    ]
   2[& MIX ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ=1          #MIXTAB             ]
   3[!1.    J, NMIX, ENERGY                                                   ]
   4[!2.    NSHELL, COEFFICIENT                                               ]
   5[!3.    n, l, w, BLS, BLL, SCRS, SCRL FOR ALL SHELLS                      ]
   6[!      REPEAT 2 AND 3 FOR ALL COMPONENTS (NMIX IN NUMBER)                ]
   7[  0.0      3 -6.5957e+00                                                 ]
   8[      1  9.8008e-01                                                     ]
   9[  2  0  2  0.0  0  0.0  0                                                ]
  10[      1  2.3430e-02                                                     ]
  11[  2  1  2  1.0  1  1.0  1                                               ]
  12[      1  1.9720e-01                                                     ]
  13[  2  1  2  0.0  0  0.0  0                                               ]

$aladdin>>
? ev

 mixing for level with j, energy =  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
```

```
$aladdin>>
? de

 entry sequence number =        6

   1[$ MIXLEV Fe [+22]  (3)                                                    ]
   2[& MIX ORIG TAPS-36  DOC-TAPS 09/11/89 SEQ-1          #MIXTAB             ]
   3[!1.    J, NMIX, ENERGY                                                   ]
   4[!2.    NSHELL, COEFFICIENT                                               ]
   5[!3.    n, l, w, BLS, BLL, SCRS, SCRL FOR ALL SHELLS                      ]
   6[!      REPEAT 2 AND 3 FOR ALL COMPONENTS (NMIX IN NUMBER)                ]
   7[  1.0      2  4.0541e+01                                                 ]
   8[      2  9.8651e-01                                                     ]
   9[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  1.0  1                    ]
  10[      2  1.6371e-01                                                     ]
  11[  2  0  1  0.5  0  0.5  0    2  1  1  0.5  1  0.0  1                    ]

$aladdin>>
? ev

 mixing for level with j, energy =  1.0  4.0541e+01

 coefficient   basis state
  9.8651e-01  ( 2s1   2S)  2S  ( 2p1   2P)  3P
  1.6371e-01  ( 2s1   2S)  2S  ( 2p1   2P)  1P
```

```
$ EXC e Fe [+24]  (1)       e Fe [+24]  (2)
& XCS ORIG TAPS-35  DOC=TAPS 08/22/89 SEQ=1          dw        LEVELS #TAB1D
!  E (eV),  Q (cm**2)
  7.0000e+03  3.6423e-23  7.8661e+03  2.7072e-23  8.8393e+03  1.9980e-23
  9.9329e+03  1.4646e-23  1.1162e+04  1.0667e-23  1.2543e+04  7.7220e-24
  1.4095e+04  5.5591e-24  1.5838e+04  3.9813e-24  1.7798e+04  2.8383e-24
  2.0000e+04  2.0152e-24
$ EXC e Fe [+24]  (1)       e Fe [+24]  (3)
& XCS ORIG TAPS-35  DOC=TAPS 08/22/89 SEQ=1          dw        LEVELS #TAB1D
!  E (eV),  Q (cm**2)
  7.0000e+03  1.3443e-22  7.8661e+03  1.1129e-22  8.8393e+03  9.3820e-23
  9.9329e+03  8.0584e-23  1.1162e+04  7.0517e-23  1.2543e+04  6.2800e-23
  1.4095e+04  5.6778e-23  1.5838e+04  5.1969e-23  1.7798e+04  4.8037e-23
  2.0000e+04  4.4722e-23
$ EXC e Fe [+24]  (1)       e Fe [+24]  (5)
& XCS ORIG TAPS-35  DOC=TAPS 08/22/89 SEQ=1          dw        LEVELS #TAB1D
!  E (eV),  Q (cm**2)
  7.0000e+03  3.9902e-22  7.8661e+03  4.2754e-22  8.8393e+03  4.5011e-22
  9.9329e+03  4.6596e-22  1.1162e+04  4.7555e-22  1.2543e+04  4.7959e-22
  1.4095e+04  4.7847e-22  1.5838e+04  4.7286e-22  1.7798e+04  4.6365e-22
  2.0000e+04  4.5144e-22
$ EXC e Fe [+24]  (1)       e Fe [+24]  (4)
& XCS ORIG TAPS-35  DOC=TAPS 08/22/89 SEQ=1          dw        LEVELS #TAB1D
!  E (eV),  Q (cm**2)
  7.0000e+03  1.8212e-22  7.8661e+03  1.3536e-22  8.8393e+03  9.9898e-23
  9.9329e+03  7.3228e-23  1.1162e+04  5.3334e-23  1.2543e+04  3.8610e-23
  1.4095e+04  2.7795e-23  1.5838e+04  1.9907e-23  1.7798e+04  1.4192e-23
  2.0000e+04  1.0076e-23
$ EXC e Fe [+24]  (1)       e Fe [+24]  (5)
& DXS1 ORIG TAPS-35  DOC=TAPS 08/22/89 SEQ=1         dw        LEVELS #TAB1D
!      IMPACT ELECTRON ENERGY (eV)
!  ANGLE(degrees),  Q (cm**2/sr)
  2.0000e+04
  0.0000e+00  1.0932e-21  1.0000e+01  8.6965e-22  2.0000e+01  3.6216e-22
  3.0000e+01  1.1945e-22  4.0000e+01  4.1577e-23  5.0000e+01  1.6940e-23
  6.0000e+01  8.0691e-24  7.0000e+01  4.3460e-24  8.0000e+01  2.5933e-24
  9.0000e+01  1.7013e-24  1.0000e+02  1.2189e-24  1.1000e+02  9.4338e-25
  1.2000e+02  7.7788e-25  1.3000e+02  6.7433e-25  1.4000e+02  6.0780e-25
  1.5000e+02  5.6487e-25  1.6000e+02  5.3891e-25  1.7000e+02  5.3041e-25
  1.8000e+02  5.4176e-25
```

```
 1[$ GF Fe [+22]                                                              ]
 2[& GF ORIG TAPS-36  DOC-TAPS 09/11/89 SEQ-1          LEVELS #GFTAB          ]
 3[!     WAVELENGTH(nm), DELTAE(eV), gf, LEVEL1, LEVEL2                       ]
 4[  2.6304e+01  4.7136e+01  1.7674e-03       1       3                       ]
 5[  1.3397e+01  9.2546e+01  1.5445e-01       1       5                       ]
 6[  1.7349e+01  7.1464e+01  5.6051e-02       3       6                       ]
 7[  4.7587e+01  2.6055e+01  9.3264e-04       5       6                       ]
 8[  9.6940e+00  1.2790e+02  2.5377e-04       3      10                       ]
 9[  1.5030e+01  8.2490e+01  1.0497e-01       5      10                       ]
10[  1.4694e+01  8.4376e+01  6.4364e-02       2       7                       ]
11[  1.5420e+01  8.0407e+01  4.4769e-02       3       7                       ]
12[  3.5427e+01  3.4998e+01  5.3662e-04       5       7                       ]
13[  1.8016e+01  6.8819e+01  6.5621e-02       4       7                       ]
14[  1.4367e+01  8.6296e+01  8.4551e-02       3       8                       ]
15[  3.0324e+01  4.0887e+01  3.0209e-02       5       8                       ]
16[  1.2070e+01  1.0272e+02  5.1795e-03       3       9                       ]
17[  2.1633e+01  5.7314e+01  1.7186e-01       5       9                       ]
18[  1.6596e+01  7.4708e+01  1.5655e-01       4       8                       ]
19[  1.3605e+01  9.1135e+01  6.9726e-02       4       9                       ]

$aladdin>>
? ev

   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
```


Ionization $Fe^{+20} - Fe^{+21}$
$2s^2\ 2p^2 - 2s^2\ 2p$
$2s^2\ 2p^2 - 2s\ 2p^2$
Q (cm^2)
10^{-16}
$3*10^{-17}$
10^1
10^2
Energy (EV)

```
$aladdin>>
? de

 entry sequence number =        1

   1[$ CONFIGS Ar [+0]                                                          ]
   2[& EN ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ=1          #CFGTAB                ]
   3[!1.   CONFIGURATION INDEX, NSHELL, TOTAL ENERGY(eV)                        ]
   4[!2.   n, l, w, SHELL ENERGY(eV) FOR EACH SHELL                             ]
   5[!     REPEAT 1 AND 2 FOR ALL CONFIGURATIONS                                ]
   6[       1        6 -1.4391078598e+04                                        ]
   7[  1  0  2  3.2517e+03  2  0  2  3.4718e+02  2  1  6  2.6993e+02           ]
   8[  3  0  2  4.2242e+01  3  1  5  2.3785e+01  4  0  1  4.1744e+00           ]

$aladdin>>
? ev

     configuration #   1
   shell       energy
   1s2         3.2517000e+03
   2s2         3.4718000e+02
   2p6         2.6993000e+02
   3s2         4.2242000e+01
   3p5         2.3785000e+01
   4s1         4.1744000e+00
   total configuration energy =  -1.4391079e+04
```

```
$aladdin>>
? de

 entry sequence number =        2

   1[$ CONFIGS Ar [+1]                                                          ]
   2[& EN ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ=1          #CFGTAB               ]
   3[!1.    CONFIGURATION INDEX, NSHELL, TOTAL ENERGY(eV)                       ]
   4[!2.    n, l, w, SHELL ENERGY(eV) FOR EACH SHELL                            ]
   5[!      REPEAT 1 AND 2 FOR ALL CONFIGURATIONS                               ]
   6[        1        5 -1.4386917316e+04                                       ]
   7[  1  0  2  3.2574e+03  2  0  2  3.5286e+02  2  1  6  2.7563e+02           ]
   8[  3  0  2  4.7822e+01  3  1  5  2.9395e+01                                 ]
   9[        2        6 -1.4369399705e+04                                       ]
  10[  1  0  2  3.2663e+03  2  0  2  3.6143e+02  2  1  6  2.8411e+02           ]
  11[  3  0  2  5.3658e+01  3  1  4  3.5825e+01  4  0  1  1.0801e+01           ]

$aladdin>>
? ev

     configuration #   1
   shell       energy
   1s2         3.2574000e+03
   2s2         3.5286000e+02
   2p6         2.7563000e+02
   3s2         4.7822000e+01
   3p5         2.9395000e+01
   total configuration energy =  -1.4386917e+04

     configuration #   2
   shell       energy
   1s2         3.2663000e+03
   2s2         3.6143000e+02
   2p6         2.8411000e+02
   3s2         5.3658000e+01
   3p4         3.5825000e+01
   4s1         1.0801000e+01
   total configuration energy =  -1.4369400e+04
```

```
$aladdin>>
? de

 entry sequence number =        5

   1[$ ION e Ar [+0]    (1)       2e Ar [+1]    (1)                              ]
   2[& XCS ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ1=1         SEQ2=1                 ]
   3|CONFIGS BIEN #ION1D                                                        ]
   4[!      TRANSITION ENERGY (eV)                                              ]
   5[!      IMPACT ELECTRON ENERGY (eV), Q (cm**2)                              ]
   6[  4.1613e+00                                                               ]
   7[  5.0000e+00  3.4948e-16  1.0000e+01  7.8463e-16  1.5000e+01  7.2702e-16
   8[  2.0000e+01  6.3994e-16  3.0000e+01  5.0220e-16  4.0000e+01  4.1002e-16
   9[  5.0000e+01  3.4584e-16  6.0000e+01  2.9889e-16  8.0000e+01  2.3504e-16
  10[  1.0000e+02  1.9370e-16  2.0000e+02  1.0324e-16  5.0000e+02  4.3117e-17
  11[  1.0000e+03  2.1902e-17                                                   ]

$aladdin>>
? ev

ionization cross sections - transition energy =   4.1613e+00

     x           y
 5.00000e+00 3.49480e-16
 1.00000e+01 7.84630e-16
 1.50000e+01 7.27020e-16
 2.00000e+01 6.39940e-16
 3.00000e+01 5.02200e-16
 4.00000e+01 4.10020e-16
 5.00000e+01 3.45840e-16
 6.00000e+01 2.98890e-16
 8.00000e+01 2.35040e-16
 1.00000e+02 1.93700e-16
 2.00000e+02 1.03240e-16
 5.00000e+02 4.31170e-17
 1.00000e+03 2.19020e-17
```

```
$aladdin>>
? de

 entry sequence number =        6

   1[$ ION e Ar [+0]   (1)      2e Ar [+1]   (2)                          ]
   2[& XCS ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ1=1        SEQ2=1           ]
   3[CONFIGS BIEN #ION1D                                                 ]
   4[!     TRANSITION ENERGY (eV)                                        ]
   5[!     IMPACT ELECTRON ENERGY (eV), Q (cm**2)                        ]
   6[  2.1679e+01                                                        ]
   7[  5.0000e+00  0.0000e+00  1.0000e+01  0.0000e+00  1.5000e+01  0.0000e+00
   8[  2.0000e+01  0.0000e+00  3.0000e+01  1.3062e-16  4.0000e+01  1.8128e-16
   9[  5.0000e+01  1.9533e-16  6.0000e+01  1.9629e-16  8.0000e+01  1.8580e-16
  10[  1.0000e+02  1.7178e-16  2.0000e+02  1.1940e-16  5.0000e+02  6.3490e-17
  11[  1.0000e+03  3.7043e-17                                            ]

$aladdin>>
? ev

ionization cross sections - transition energy =   2.1679e+01

     x           y
 5.00000e+00 0.00000e+00
 1.00000e+01 0.00000e+00
 1.50000e+01 0.00000e+00
 2.00000e+01 0.00000e+00
 3.00000e+01 1.30620e-16
 4.00000e+01 1.81280e-16
 5.00000e+01 1.95330e-16
 6.00000e+01 1.96290e-16
 8.00000e+01 1.85800e-16
 1.00000e+02 1.71780e-16
 2.00000e+02 1.19400e-16
 5.00000e+02 6.34900e-17
 1.00000e+03 3.70430e-17
```

```
$aladdin>>
? de

 entry sequence number =        3

   1[$ PHOTION Ar [+0]    (1)       e Ar [+1]    (1)                              ]
   2[& XCS ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ1=1          SEQ2=1                 ]
   3[CONFIGS PIG #ION1D                                                          ]
   4[!      TRANSITION ENERGY (eV)                                               ]
   5[!      PHOTON ENERGY (eV), Q (cm**2)                                        ]
   6[  4.1613e+00                                                                ]
   7[  5.0000e+00  1.0766e-19  1.0000e+01  7.4686e-21  1.5000e+01  1.4070e-20
   8[  2.0000e+01  1.4252e-20  3.0000e+01  1.2534e-20  4.0000e+01  1.1052e-20
   9[  5.0000e+01  9.8818e-21  6.0000e+01  8.9056e-21  8.0000e+01  7.3152e-21
  10[  1.0000e+02  6.0649e-21  2.0000e+02  2.6938e-21  5.0000e+02  5.6891e-22
  11[  1.0000e+03  1.4835e-22                                                   ]

$aladdin>>
? ev

ionization cross sections - transition energy =   4.1613e+00

     x            y
 5.00000e+00 1.07660e-19
 1.00000e+01 7.46860e-21
 1.50000e+01 1.40700e-20
 2.00000e+01 1.42520e-20
 3.00000e+01 1.25340e-20
 4.00000e+01 1.10520e-20
 5.00000e+01 9.88180e-21
 6.00000e+01 8.90560e-21
 8.00000e+01 7.31520e-21
 1.00000e+02 6.06490e-21
 2.00000e+02 2.69380e-21
 5.00000e+02 5.68910e-22
 1.00000e+03 1.48350e-22
```

```
$aladdin>>
? de

 entry sequence number =        4

   1[$ PHOTION Ar [+0]    (1)       e Ar [+1]    (2)                          ]
   2[& XCS ORIG TAPS-36  DOC=TAPS 09/11/89 SEQ1=1         SEQ2=1              ]
   3[CONFIGS PIG #ION1D                                                       ]
   4[!     TRANSITION ENERGY (eV)                                             ]
   5[!     PHOTON ENERGY (eV), Q (cm**2)                                      ]
   6[  2.1679e+01                                                             ]
   7[  5.0000e+00  0.0000e+00  1.0000e+01  0.0000e+00  1.5000e+01  0.0000e+00
   8[  2.0000e+01  0.0000e+00  3.0000e+01  7.7916e-18  4.0000e+01  1.2508e-18
   9[  5.0000e+01  6.0172e-19  6.0000e+01  7.1217e-19  8.0000e+01  9.1382e-19
  10[  1.0000e+02  8.9814e-19  2.0000e+02  4.0223e-19  5.0000e+02  5.5117e-20
  11[  1.0000e+03  8.9401e-21                                                 ]

$aladdin>>
? ev

ionization cross sections - transition energy =   2.1679e+01

     x           y
 5.00000e+00 0.00000e+00
 1.00000e+01 0.00000e+00
 1.50000e+01 0.00000e+00
 2.00000e+01 0.00000e+00
 3.00000e+01 7.79160e-18
 4.00000e+01 1.25080e-18
 5.00000e+01 6.01720e-19
 6.00000e+01 7.12170e-19
 8.00000e+01 9.13820e-19
 1.00000e+02 8.98140e-19
 2.00000e+02 4.02230e-19
 5.00000e+02 5.51170e-20
 1.00000e+03 8.94010e-21
```

RUNNING ALADDIN AT ENEA-BOLOGNA

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Abstract

Operating experience in running ALADDIN did not give raise to particular problems. The code has been compiled with three FORTRAN compilers both on Personal Computer and on IBM mainframe. The errors flagged out in the compilation are listed.

Using ALADDIN on Personal Computer

Compiling

As test computer an IBM PS 2 70 386 has been used. The code has been submitted to two compilers, whose diagnostics follow.

Ryan - McFarland Professional FORTRAN Compiler (Vers. 1.0): The only error flagged out by this compiler (and by all compilers) is a wrong statement at line 753 (a line composed by all =). With a C in column 1 the problem disappeared.

Microsoft FORTRAN 4.1 Compiler An extra comma inserted in a implicit Fortran statement has been flagged out in subroutine ALTB1D between statement labels 350 and 360.

Running

The version produced by Ryan-McFarland compiler did not run: the generated diagnostic is here reproduced.

```
C:\ALADDIN>aladdin

INPUT FILE NAME ? examples.dat

QUERY DICTIONARY FILE NAME (C/R FOR NONE)? amco1.dic

ALADDIN>> ?

ERROR:  INVALID ACCESS LABEL LINE

ALADDIN>> s

STARTING SEARCH AT ENTRY SEQUENCE NUMBER       2
ERROR:  INVALID ACCESS LABEL LINE

ALADDIN>>
```

The Microsoft version of ALADDIN reproduced the sample problem (EXAMPLES.DAT entry no.7) with all significant figures.

Using ALADDIN on mainframe

Compiling

ALADDIN were compiled with IBM VS FORTRAN Version 3.0 on an IBM 3090.30E and three errors were revealed:

- line 753 of illegal (#) characters - the same error revealed on PC
- an illegal format statement between statements numbers 350 and 360 in subroutine ALT1BD - the sequence 2,(is illegal, comma must be omitted - as detected by Microsoft compiler
- a blank record exists after the END card of ALADDIN main programme.

Running

The version on mainframe generated the correct output with all significant figures too.

A PROPOSAL FOR THE ALADDIN DICTIONARY AND CONVENTIONS FOR PARTICLE-SURFACE INTERACTION PROCESSES

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A. Discussion of Particle-Surface Interactions

Process Specification

Particle surface collisions do not necessarily fit the simple $A+B \rightarrow A^*+B^*$ format of a binary atomic collision. Consider some of the processes which can occur when H^+ is incident on a copper surface. In each of the following processes are listed the observed product as the first entry on the post collision side.

i. Reflection of the projectile:

$$H^+ + Cu\ (surf) \rightarrow H^+ + Cu\ (surf)$$

ii. Sputtering of the target:

$$H^+ + Cu\ (surf) \rightarrow Cu + Cu\ (surf)$$

One has no knowledge of the fate of the H^+.

iii. Implantation (retention, trapping) of the projectile:

$$H^+ + Cu\ (surf) \rightarrow H\ (trapped) + Cu\ (surf)$$

iv. Desorption of an adsorbed surface species could be described as:

$$H^+ + O\ (adsorbed) + Cu\ (surf) \rightarrow O + Cu\ (surf)$$

We have here four separate processes involving H^+ on Cu where the observed species is different in each case and where the post-collision condition of the target is unknown and largely irrelevant.

Two modifications to the indexing scheme that might be helpful in particle surface interactions.

Firstly, one should write as the first reaction product the species that is observed. The second reaction product should be listed the same as the original target. In most processes the post collision behavior is governed by the interaction of an escaping isolated species (the first reaction product) with the original surface (the second reaction product); thus the ordering makes sense. As in atomic data the specification of post collision products may be omitted if the reaction is unambiguously specified by the process name and reactants.

Secondly it may be of value to follow the species chemical symbol by an indication of its state of aggregation written in parenthese. Typically the state would be:

surface	(surf)
adsorbed	(ads)
trapped	(trap).

In this manner one follows the convention of listing charge, excited and molecular state for atoms. A chemical symbol without a state of aggregation represents a free species (which is the way they are currently listed in atomic data). Specification of aggregation state would eliminate ambiguities in searches by reactant species.

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)
B.9.	Secondary electron ejection by electrons	SEE	e+B(surf)→e+B(surf)
B.10.	Secondary electron ejection by electrons energy distribution	SEEENER	e+B(surf)→e+B(surf)
B.11.	Sputtering by atoms leading to molecule emission (total) (chemical sputtering)	SATM	A+B(surf)→M+B(surf)
B.12.	Sputtering by molecules leading to atom emission (total)	SMTA	M+B(surf)→A+B(surf)

B.13.	Sputtering by molecules leading to molecule emission (total)	SMTM	M_1+B(surf)→M_2+B(surf)
B.14.	Synergistic sputtering (total)	SST	

Group C. Projectile Penetration and Retention

C.1.	Stopping power for atoms	STA	A+B(surf)→A+B(surf)
C.2.	Range of atoms	RA	A+B(surf)→A+B(surf)
C.3.	Stopping power for electrons	STE	e+B(surf)→e+B(surf)
C.4.	Trapping of atoms	TA	A+B(surf)→A(trap)+B(surf)
C.5.	Re-emission of atoms/molecules	REMA	A+B(surf)→A+B(surf)
C.6.	Adsorption (sticking) of atoms/ molecules	ADSA/M	A/M+B(surf)→A/M(ads)+B(surf)

Group D. Other Processes of Interest

D.1.	Desorption by atoms	DESA	A+B(ads)+C(surf)→B+C(surf)
D.2.	Desorption by electrons	DESE	e+B(ads)+C(surf)→B+C(surf)
D.3.	Desorption by photons	DESP	hν+B(ads)+C(surf)→B+C(surf)
D.4.	Thermal desorption	DEST	Temp+B(ads)+C(surf)→B+C(surf)

Notes: One might consider whether A.4., A.5. and B.4. should be subdivided into 3 groups each covering total, processes leading to a specific excited state and processes leading to a specific charge state.

E. Conventions about Order of Reactants and Products

(a) Initial reaction channel: reactants

1. The projectile always appears first.
2. The target should be followed by its state of aggregation. Generally this is surf for a solid. Rarely will this be ads for adsorbate.
3. In cases where the target is a adsorbate one treats the notation in the order projectile, adsorbate, substrate.
4. In general there is no need to specify the quantum or charge state of the target.

(b) Final reaction channel: product

1. The product observed (whether projectile or target) is always shown first.
2. The second product is the target (or substrate) with the designation surf.
3. If the reaction is uniquely specified by the process label and reactants the indication of reaction products is not necessary and may be omitted.

F. Quantities of Data

The most relevant quantity is a coefficient (# of events per incident particle). Sometimes this may be averaged over a particle energy distribution. Frequently the coefficient is differentiated in angle or in free particle energy distribution. On rare ocassions a cross section is used. Range and stopping power have special types of quantity. (See Table 6).

Table 6. Quantities of Data

No.	Resolved Process	Comment	Abbreviation
1.	Coefficient	Integrated over all exit angles and energies	C(Y?)C_R,C_N
2.	Coefficient differential in angle	Integrated over all exit energies	CXA
3.	Coefficient differential in energy	Integrated over all exit angles	CXE
4.	Rate cofficient for Maxwellian distribution		CMAX
5.	Cross section		XS
6.	Stopping power		DE/DX
7.	Range		R

C. Additional Labels

For collisions on solids there are certain additional parameters that are essential for specification of the process. These generally need not be searchable but listing on the label or as a second label should be mandatory. These would include:

1. Angle of incidence on target (measured from normal). Possible label ANGLE IN =

2. Angle of exit from target (measured from normal). Possible label ANGLE OUT =

3. Energy of projectile impact. E IN =

4. Energy of particle exit. E OUT =

5. Crystalline nature of target. CRYSTAL = . A response would be SINGLE (singel crystal) or POLY (polycrystalline).

6. Target temperature. TEMP =

For some situations the responses would be:

ALL Integrated over all angles (or energies). - as in 2 and 4.

VAR. Indicating that this item is a variable and that the data table is a function of that variable.

H. Other Labels

The other reference labels listed on page 8 of INDC(NDS)-211/GA, and their order, can remain the same for surface data.