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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Second Meeting of the Atomic and Molecular Data Centre Network

Fontenay aux Roses, 23-24 May 1980

SUMMARY REPORT

Edited by
K. Katsonis
Atomic and Molecular Data Unit
Nuclear Data Section
International Atomic Energy Agency

November 1980

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

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Abstract

Summary report of the Second A+M Data Centre Network (DCN) meeting convened by the IAEA Nuclear Data Section at the CEA Laboratory at Fontenay-aux-Roses, France, 23–24 May 1980. The meeting was attended by 20 representatives from centres and groups from six Member States concerned with the coordinated international management of atomic and molecular data pertinent to controlled fusion research and technology.

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List of Abbreviations

A+M	Atomic and Molecular.
DCN meeting	Data Centre Network meeting.
FRG/IPP	Max-Planck-Institut für Plasmaphysik, Garching bei München, FRG.
FRG/FIZ	Fachinformationszentrum, Eggenstein-Leopoldshafen, FRG.
FR/Orsay	Laboratoire Physique des Plasmas of the University of Paris, Orsay, France.
GAPHYOR	GAz-PHYsique-ORsay, a computerized retrieval system on properties of atoms, molecules and gases.
IAEA	International Atomic Energy Agency.
IFRC	International Fusion Research Council.
JPN/JAERI	Japan Atomic Energy Research Institute, Tokai mura, Japan.
JPN/Nagoya	Institute of Plasma Physics, Nagoya University, Nagoya, Japan.
NDS	Nuclear Data Section.
TC meeting	Technical Committee meeting.
UK/QUB	Queen's University, Belfast, Northern Ireland, United Kingdom.
US/JILA	Joint Institute for Laboratory Astrophysics, Boulder, Colorado, United States.
US/NBS	National Bureau of Standards, Washington D.C., USA.
US/ORNL	Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
US/PPP	Plasma Physics Laboratory, Princeton University, Princeton, N.J., USA.
USSR/IAE	Institut Atomnoi Energii I.V. Kurchatova, Moscow, USSR

SUMMARY OF THE MEETING

1. Introduction

The Second A+M Data Centre Network (DCN) meeting was convened by the IAEA Nuclear Data Section at the CEA laboratory at Fontenay-aux-Roses, France, on 23 and 24 May 1980. The meeting was attended by 20 representatives from centres and groups from six Member States concerned with the coordinated international management of atomic and molecular data pertinent to controlled fusion research and technology. The list of participants is given in Appendix I.

After the selection of Prof. F.J. Smith from the Queen's University of Belfast (UK/QUB) to chair the meeting, the proposed Agenda, given in Appendix II was adopted without modification.

Discussions during the meeting concerned the technical aspects of the cooperation between the members of the data centre network established in the first A+M data centre meeting held in Vienna in May 1977 (see Report INDC(NDS)-88). Data centres participating in the network and their responsibles are listed in Appendix III.

The meeting came to a number of conclusions on the development of the international effort in numerical A+M data for fusion and assigned a number of specific actions (see Appendix IV). Specifically, the meeting established agreements for the cooperation between existing A+M centres and groups and the IAEA NDS-A+M Data Unit with regard to the International Bulletin, the bibliographic data indexes and the assessment and exchange of evaluated A+M data.

2. Actions arising from the First Data Centre Network meeting

It was agreed that the actions listed in Appendix 4 of the minutes of the First Data Centre Network (DCN) meeting held in Vienna from 9 to 13 May 1977 (see Report INDC(NDS)-88/GB) were nearly all implemented by the persons concerned, with the exception of one or two that turned out to be impossible to fulfil.

3. Reports of the A+M Data Centres and Groups

Information about the work performed at the A+M data centres and groups was already given in the first DCN meeting. J.J. Schmidt, head of the Nuclear Data Section (NDS), summarized the work in progress in the Agency's A+M Data Unit. Detailed information on it is given in Appendix V. Brief presentations given by the centre representatives are presented in Appendix VI.

4. Future Role and Programme of the IAEA A+M Data Unit

The meeting supported the recommendations from the Working Group for International Cooperation of the preceding Second Technical Committee (TC) meeting on A+M Data for Fusion. In view of these recommendations it was decided that the working document V.2 (see Appendix V), constituting a proposal for the future role and programme of the IAEA A+M Data Unit, has to be revised with the understanding that the Unit will not collect non-evaluated data. The final version of this document will be distributed to all participants of the meeting as soon as prepared.

5. International Bulletin on A+M Data for Fusion

The meeting participants agreed that the IAEA A+M Bulletin is used extensively, considered it to be a useful bibliographic source for A+M data for fusion, and complimented the Agency. The Agency was asked to take into account the recommendations of the preceding Technical Committee meeting and incorporate them into the future issues of the Bulletin. It was left to the expertise of the A+M Data Unit to decide on further improvements of the Bulletin.

As key issue discussed was the scope of the atomic collision section of the Bulletin. At issue was whether or not the criteria used for CIAMDA and for the Bulletin should be identical. The present criteria were developed by the A+M Data Unit taking into account the recommendations of the Joint IFRC/INDC Subcommittee on A+M Data for Fusion. A description of the criteria was presented by K. Katsonis and F.M. Smith at the Nagoya Seminar on Atomic Processes in Fusion Plasmas (1979) and in Bulletin No. 10, Appendix I (1979). Primarily, the criteria provide restrictions for collisions data as to reactant species (Bulletin No. 5, p. 48) and energy range of interest to fusion. Some of the participants expressed a desire to significantly restrict the number of collisions papers cited in the Bulletin through stringent use of an additional criterion - that the papers should contain actual data of direct and immediate use to fusion. Application of this criterion was recognized as problematic to the IAEA A+M Data Unit in two regards: (1) requiring a somewhat subjective judgement by some reviewers, and (2) prohibiting the Bulletin from serving directly as an update to CIAMDA which would then be of broader scope. In addition, other participants felt that such reduction of citations would compromise the Bulletin and preferred the present broader scope. This issue was not completely resolved so that implementation of the suggestions was left to the discretion of the IAEA A+M Data Unit.

Additional specific suggestions for the improvement of the A+M Data Bulletin were made,

- Cover more journals.
- Restrict or reduce the reactants list.
- Consider to expand the scope of the Bulletin to include all data related to surface effects and diagnostics.

- Include reviews and other A+M information pertinent to fusion research, as well as analytical formulas derived for the calculation of certain data.

- Include an author list of the references appearing in the part "Other Literature" (IV.).

In answer to comments related to the scope of data in the Bulletin, it was pointed out that the data considered for input to the Bulletin were restricted to a specific set of reactions involving a limited set of atoms and molecules in a defined energy range which conformed to the needs of fusion research. The criteria for fusion relevance used in determining this set, were developed by the A+M Data Unit taking into account the recommendations of the Joint IFRC/INDC Subcommittee on A+M Data for Fusion, and in Consultation with representatives of the fusion research community. A complete description of the criteria used was described in a paper by K. Katsonis and F.J. Smith presented at the Nagoya Seminar on Atomic Processes in Fusion Plasmas (see also Bulletin No. 10, Appendix I).

The Unit was instructed by the meeting participants to examine carefully the information included in the Bulletin, and to revise periodically the criteria used to determine fusion relevance, taking fusion research developments into account.

A preliminary report of a completeness comparison of the IAEA Bulletin with the US-produced Bulletin on Atomic Data for Fusion was presented by the A+M Data Unit. A final report of this comparison is expected to be issued by the IAEA in the near future.

The meeting recommended to the Agency to produce periodically compendia of previous issues of the Bulletin. These compendia should include the bibliographic information on structure, collision, and plasma-surface interactions and should be distributed mainly to the data centres.

With regard to surface effects it was decided to expand the corresponding part of the Bulletin by extending the list of periodicals scanned for that purpose, and by revising the indexing used for the Bulletin input on the basis of the Recommendations of the Working Group on Surface Effects of the Technical Committee meeting. In addition, it was deemed desirable to obtain the collaboration of data centres already involved in the collection of plasma-surface effects data; as a result the Garching laboratory (FRG/IPP) offered to communicate monthly to the Agency the bibliographic information collected for the preparation of the "Surface and Vacuum Physics Index" in collaboration with the Fachinformationszentrum in Karlsruhe (FRG/FIZ). The Karlsruhe data centre agreed in principle to cooperate in the retrieval of the fusion-oriented information from the corresponding computer file. The Oak Ridge and Nagoya data centres agreed to help in establishing criteria for the selection of data considered to be of interest to fusion.

It was suggested that all data centres involved in plasma-surface interaction data collection should send to the Agency their views on the fusion pertinence criterion as soon as possible. The Agency agreed to distribute these suggestions among the data centres. Prof. Abramov from the Kurchatov Institute in Moscow (USSR/IAE) presented a classification scheme for plasma-surface interaction data (see Appendix V.3.)

Drs. Kato and Itikawa presented in a working paper the database and retrieval display system of A+M data for fusion of IPP/Nagoya (Appendix V.4.).

Finally, it was recognized that inclusion of macroscopic plasma properties references in the Bulletin was not warranted at this time.

6. Data Indexes

6.1. CIAMDA

The contributions of numerous data centres to the production of CIAMDA was acknowledged. The main external sources for its production were the tapes provided by the JILA Atomic Collision Information Centre, the Oak Ridge National Laboratory and the Orsay Plasma Physics Laboratory (GAPHYOR system). Bibliographic data collected by the IAEA for the preparation of the first ten issues of the Bulletin as well as contributions from Japan, UK, and the USSR were also included.

It was decided that the master file used for the production of CIAMDA could become available to the other data centres of the network. It was however stipulated that whenever one of the centres used the CIAMDA master file, it would have to include in any produced listing an acknowledgement of its IAEA origin and a mention of the names of the organizations that participated in its production.

6.2. Structure data index

W. Wiese (US/NBS) pointed out that a number of comprehensive structure data indexes are available from US/NBS and it was agreed that there was no need for an additional structure data index. It was suggested that a compendium of structure data references retrieved from the Bulletin file could be useful. This compendium could be distributed to the network.

6.3. Surface data index

The Garching group agreed that IAEA could have its surface index file (on tape). It would then be up to IAEA to apply a selection criterion to this file in order to create an index. G. Ebel (FRG/FIZ) offered to search the surface index for fusion-relevant references. This effort would be related with the preparation of the plasma-surface interaction part of the A+M Bulletin.

7. International Effort in Numerical A+M Data for Fusion

The primary reason given by the IFRC for the creation of an international atomic and molecular data programme was the need of the fusion community for critically reviewed data on atomic and ionic collision processes of importance to nuclear fusion research, which could be used as a common data base by all fusion laboratories. To substantiate these needs, the IAEA convened two international meetings (Culham in 1976 and Fontenay-aux-Roses in 1980) which had as its main objectives the identification of the data needed by the fusion community and the assessment of the status of existing data. As a result of these studies, it became evident that emphasis was required in the compilation and evaluation of atomic collision data as well as plasma-surface interaction data.

At this meeting, the prepresentatives of the data centres agreed, that initially (at least until the next Data Centre Network meeting) the IAEA effort should give priority to the compilation of evaluated atomic collision data. Furthermore, the A+M Data Centre Network recommended that numerical data which would eventually form the body of an "evaluated A+M collision data file", be reviewed by a selected group of scientists, and that no unevaluated numerical A+M collision data be distributed by the IAEA.

7.1. Functions and services of the IAEA A+M Data Unit

The following summarizes the meeting discussions on the A+M Data Unit activities concerning primarily the numerical A+M collision data, their evaluation, compilation, exchange and dissemination.

a) Promotion of A+M collision data evaluation

- The meeting recommended that IAEA promote the evaluation of A+M collision data by means of IAEA Research Contracts and Agreements in context of coordinated research programmes. It was considered preferable to have the evaluation performed by atomic physics specialists in residence at fusion research laboratories or relevant data centres.

- Progress of IAEA sponsored, as well as other reviews and evaluations should be communicated directly to all members of the A+M Data Centre Network, and to the atomic physics and fusion communities through notices in the A+M Data Bulletin.

b) Collection of numerical A+M data by the IAEA

- The IAEA A+M Data Unit should collect all existing A+M collision data, initially whatever is available at other centres, and gradually building up a body of evaluated collision data.

- In order to assist the A+M Data Unit in this effort, the data centres represented at this meeting agreed to send to the Agency a list of evaluations of data pertinent to fusion that they are aware of. It was also agreed that when the data centres have evaluated data to make them available to the Agency as soon as possible.

- The A+M Data Centre Network agreed to a free exchange of all (experimental and evaluated) A+M data between all members of the network.

- Preliminary results of a data base survey, identifying the type of numerical data compiled by all members of the A+M Data Centre Network, which had been initiated by J. Rumble (IAEA/NDS), are shown in Appendix VII.

- In addition, the A+M Data Unit was also encouraged to make a compilation of reports and review papers which include empirical formulas for the calculation of important A+M data. The data centre network agreed to send any related information to the IAEA. It was recommended that such reports and review papers be indexed and included in the A+M Data Bulletin for Fusion.

c) Compilation of evaluated numerical A+M data by the IAEA

- The IAEA should initiate the compilation of evaluated A+M collision data which have been reviewed and approved by experts who are to be appointed by the A+M Data Subcommittee of the IFRC.

- The evaluated A+M collision data are to be compiled into a well defined and documented computer file (or library) in an internationally agreed upon exchange format. The A+M Data Unit should maintain the library up-to-date and as comprehensive as possible.

- A committee, consisting of E.C. Beaty (US/JILA), F.J. Smith (UK/QUB) and K. Katsonis (IAEA/NDS) was formed to devise an exchange format for the storage of evaluated A+M collision data, which would also be used for the exchange of these data between centres. A preliminary proposal of such a format is to be circulated among the members of the A+M Data Centre Network before the next DCN meeting.

- It was also mentioned that the evaluated A+M collision data stored in the evaluated data library will be indexed in the CIAMDA A+M collision data index.

- Although rate coefficients are directly applicable to fusion needs, it was agreed that reaction data was more usefully stored as cross-sections. Conversion of the data to rate coefficients for specific applications can easily be performed by the user. A number of such programmes are currently in use (e.g. at Princeton and Oak Ridge).

- It was also recommended that the evaluated reaction data be fully documented as regards its origin and evaluation history, and that the data themselves have uncertainties assigned whenever possible. Proposed units for the cross sections and the corresponding energy were cm^2 and eV.

d) Dissemination of the evaluated data

- The evaluated data will be available from the IAEA free of charge in a suitable user format upon request.

APPENDIX I

Second Atomic and Molecular Data Centre Network Consultants' Meeting

Paris, France, 23-24 May 1980

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APPENDIX II

International Atomic Energy Agency

Second Atomic and Molecular Data Centre Network Consultants' Meeting

Paris, France, 23-24 May 1980

PROPOSED AGENDA

1. Introductory items: Selection of chairman, approval of the agenda.

2. Actions from the first Data Centre Network Meeting, Vienna, 9 - 13 May 1977.

3. Reports from existing A+M data centres and groups.

4. Future role and programme of the IAEA A+M Data Unit.

5. A review of the scope and classification scheme of the International Bulletin on Atomic and Molecular Data for Fusion, especially for * plasma-surface interaction data and macroscopic plasma properties*.

6. Discussion of Indexes to Atomic and Molecular Data for Fusion.

   a) Collision data (CIAMDA)
   b) Structure data
   c) Plasma-surface interaction data

7. International effort in numerical A+M data for fusion: generation, compilation, evaluation, exchange and dissemination.

   a) Proposed role of IAEA A+M Data Unit
   b) Role of the other A+M data centres
   c) Role of atomic physics research groups
   d) Exchange format for numerical data.

8. Summary of actions, conclusions and recommendations of the meeting.

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* These items have also been discussed by separate working groups of the preceding Second Technical Committee Meeting on Atomic and Molecular (A+M) Data for Fusion.

APPENDIX III

DATA CENTRES AND RESPONSIBLES

Centre Code	Address	Head of Project or Centre
FR/Orsay	Université Paris Sud Laboratoire de Physique des Gaz et des Plasmas F-91405 Orsay, Cedex	Prof. J.L. Delcroix
FRG/FIZ	Fachinformationszentrum Energie,Physik,Mathematik GmbH D-7514 Eggenstein-Leopoldshafen 2	Dr. G. Ebel
FRG/IPP	Max-Planck-Institut für Plasma Physik D-8046 Garching bei München	Dr. H. Verbeek
IAEA/NDS	Nuclear Data Section International Atomic Energy Agency P.O.B. 590 A-1011 Vienna	Dr. J.J. Schmidt
JPN/Nagoya	Research Information Center Institute of Plasma Physics Nagoya University Nagoya 464, Japan	Dr. Y. Itikawa
JPN/JAERI	JAERI Nuclear Data Center Tokai-Mura, Naka-gun Ibaraki-ken, 319-11 Japan	Dr. Yohta Nakai
UK/QUB	Department of Computer Science The Queen's University Belfast, BT7 1NN Northern Ireland, UK	Prof. F.J. Smith
UK/Culham	Culham Laboratory U.K. A.E.A. Abingdon, Oxon OX14 3DB U.K.	Dr. N. Peacock

Centre Code	Address	Head of Project or Centre
US/NBS-AT	Data Centers on Atomic Transition Probabilities and Atomic Line Shapes and Shifts Optical Physics Division National Bureau of Standards Washington, D.C. 20234, USA	Dr. W.L. Wiese, Dr. G.A. Martin
US/NBS-EL	Atomic Energy Levels Data Center Optical Physics Division National Bureau of Standards Washington, D.C. 20234,USA	Dr. W.C. Martin Dr. W.L. Wiese
US/JILA	Atomic Collision Cross Section Information Center Joint Institute for Laboratory Astrophysics University of Colorado Boulder, Col. 80302, USA	Dr. E.C. Beaty
US/ORNL	Physics Division Oak Ridge National Laboratory P.O.B. X Oak Ridge, Tenn. 37830, USA	Dr. D.H. Crandall
USSR/IAE	Institut Atomnoi Energii I.V. Kurchatova 46 Ulitsa Kurchatova Moscow, D-182, USSR	Dr. Yu.V. Martynenko

APPENDIX IV

ACTIONS RESULTING FROM THE SECOND A+M DATA CENTRE NETWORK MEETING

1.	NDS/A+M Data Unit	Revise the working document VI.2 "Future IAEA programme on A+M data for fusion" in view of the recommendations of the preceding second TC meeting, with the understanding that the Unit will not collect non-evaluated data. Distribute the final version to all participants of the DCN meeting.
2.	"	Expand the list of scientific journals scanned for the preparation of the IAEA International Bulletin on A+M Data for Fusion, especially for the plasma-surface interaction.
3.	"	Revise periodically the fusion relevance criterion used in the preparation of the IAEA Bulletin.
4.	"	Prepare a report on the comparison of the IAEA Bulletin with the Bulletin produced jointly by US/ORNL and US/NBS.
5.	"	Produce periodically compendiums of the previous issues of the Bulletin and distribute them to the data centres.
6.	FRG/IPP, FRG/FIZ	Cooperate with NDS/A+M Data Unit to establish a retrieval system from the plasma-surface interaction file they are producing, to be used in the preparation of the corresponding part of the IAEA Bulletin and/or the preparation of bibliographic indexes.
7.	All data centres	Send to the Agency their views on plasma-surface interaction data considered of fusion interest.
8.	NDS/A+M Data Unit	Create a comprehensive file of available <u>evaluated</u> data of relevance to fusion and make it available to users and data centers.
9.	"	Ask IFRC to suggest or appoint experts to judge on 1. the quality of the data coming out after an evaluation work in a special topic and 2. whether the work is sufficient for the data needs.

10.	NDS/A+M Data Unit	Use the IAEA contracting facilities to have atomic physics specialists spend time in fusion laboratories to perform prioritary data evaluation.
11.	"	Promote review reports (starting with collision processes) to be used as a basis for evaluations of data.
12.	"	Prepare a comprehensive IAEA report, describing the status of evaluated data that could be useful to fusion on the basis of the information that will be gathered in Vienna.
13.	"	Prepare a compilation of review papers including empirical formulas, reports, etc., non-indexed in the International Bulletin on A+M Data for Fusion because of the broad information they contain.
14.	All data centres	Send to the Agency a list of evaluations of data pertinent to fusion that they are aware of. Make available to the Agency the result of any work on data evaluation once the work is finished.
15.	US/ORNL, JPN/Nagoya UK/QUB	Send to IAEA their file of evaluated data whenever available.
16.	All data centres	Send to IAEA all available documents related with the data activities.
17.	"	Contribute to the preparation of a Data Base Survey by informing NDS/A+M Data Unit of all known data centres or working groups that are collecting A+M data for fusion and specify the data that are collected.
18.	Beaty, Smith, Katsonis	Elaborate an A+M data exchanging format to be used among A+M data centres. Prepare a report on the result of this work and submit it to the next DCN meeting.

APPENDIX V

WORKING DOCUMENTS

APPENDIX V

V.1. THE HISTORICAL DEVELOPMENT OF THE ATOMIC AND MOLECULAR DATA UNIT OF THE IAEA NUCLEAR DATA SECTION

A. Lorenz, K. Katsonis, J. Rumble, J.J. Schmidt
IAEA, Nuclear Data Section

The International Fusion Research Council (IFRC) at its fifth meeting, held on 16 November 1974 in Tokyo, recognized the vital importance and need for a coordinated world-wide atomic and molecular (A+M) data service to ensure the successful development of fusion technology. On this premise, it recommended that the International Atomic Energy Agency (IAEA) perform a survey of existing data banks, and consider adding atomic and molecular data for fusion to the scope of its existing nuclear data programme.

In response to this IFRC recommendation, the Director General of the IAEA asked the Nuclear Data Section (NDS) to review the needs and to perform a world-wide survey of existing compilation activities concerned with atomic and molecular data for fusion. To assist in this task, members of the International Nuclear Data Committee (INDC) and of the IFRC were invited to convey to NDS any information on existing and planned compilations, evaluations and publications of A+M data in their own country. A report was written by NDS in cooperation with the IAEA Physics Section and published as INDC(NDS)-67/NF. At the same time the Director General instructed NDS to convene a small consultants' meeting to assess the needs and availability of A+M data for plasma research and fusion technology, and to advise him on the size and scope of an IAEA programme in this field. This meeting took place on 21 - 22 July 1975 in Vienna.

At that meeting, after a detailed review of the NDS report, the consultants unanimously stressed the immediate and expanding needs for A+M data for fusion and concurred that the present national activities do not adequately meet the demand.

The consultants concluded that the IAEA was a particularly suitable organization to provide a central and international service for the co-ordination, compilation and evaluation of A+M data for fusion. As the IAEA already provided an international service in the nuclear data field, it was outstandingly well equipped to extend its activities to include A+M data for fusion. In their conclusions, the consultants recommended that the IAEA immediately establish an international programme for A+M data for fusion.

As a consequence of this consultants' meeting, the Director General of the IAEA indicated that, conditional upon positive recommendations of the IFRC and the INDC, he would be prepared to support an extension of the Agency's nuclear data programme to include the compilation, analysis and dissemination of A+M data for fusion.

In due course, following the recommendations of both IFRC and INDC in 1976, an Atomic and Molecular Data Unit was established within the IAEA Nuclear Data Section for a trial period of two years (1977-1978) beginning January 1977. At the same time, to help him evaluate this programme and review its progress and achievements, the Director General appointed a Joint IFRC/INDC Subcommittee on A+M Data for Fusion for the two-year trial period of the programme.

In November 1976, upon the recommendation of the IFRC, the IAEA convened the first international meeting on Atomic and Molecular Data for Fusion at the Culham Laboratory in the UK. The goals of this meeting were to identify specific data requirements for A+M data in fusion technology and to initiate an international cooperative effort on the systematic compilation and dissemination of A+M data relevant to fusion research and technology. The proceedings of this meeting were published in Physics Letters (Section C) Vol. 37C in February 1978, and were also released as an IAEA Technical Report IAEA-199 in 1977.

The participants of the Culham meeting confirmed the needs for A+M data, and recognized that the scope of this work is so large that no single Member State could adequately do it alone. It was therefore agreed to create a network of data centres which would cooperate in the collection, evaluation, and dissemination of A+M data required by the fusion community, and be coordinated by the IAEA Nuclear Data Section.

At the first meeting of the Joint IFRC/INDC Subcommittee, which met immediately after the Advisory Group Meeting at the Culham Laboratory, the initial tasks of the A+M Data Unit were specified as follows:

- compilation, publication and distribution of a quarterly bulletin on newly measured or calculated fusion-related A+M data and associated information;

- creation and publication of an international index of references to atomic collision data; and

- formulation of a common system for the exchange of bibliographic and numerical A+M data between existing or planned atomic and molecular data centres.

The first two points of this recommended programme were implemented by the A+M Data Unit and formed the basis for its activities in the first three years of its operation (1977-79). To assist the A+M Data Unit in accomplishing these tasks, a first meeting of the A+M Data Centre Network was held in Vienna in May 1977 (see IAEA report INDC(NDS)-88/GB). The results of this meeting consisted primarily in initial agreements between members of the A+M Data Network and the IAEA A+M Data Unit regarding (a) the content and publication schedule of the "International Bulletin on Atomic and Molecular Data for Fusion", (b) the format, information content and physics scope of the "Bibliographic A+M Collision Data Index", (c) the extent and timing of the contributions of participating data centres' bibliographic data files to the Agency's Index, and (d) an exchange of views regarding a potential format for the exchange of evaluated A+M collision data.

The Joint IFRC/INDC Subcommittee met four times during the trial period of the IAEA A+M programme. The programme was judged by the Subcommittee to be proceeding according to the recommendations except for a delay in the completion of the Index to Atomic Collision Data. The proposed future programme of the Unit, namely the continuation of the publication of the International Bulletin on Atomic and Molecular Data for Fusion, the completion of the Computer Index of Atomic and Molecular Data, the creation of an evaluated A+M data file for fusion and the coordination of the network of data centres was supported. The Subcommittee felt that the response from the scientific fusion community had been very positive, that the programme was needed, and that the IAEA was uniquely qualified to implement this programme; it recommended that the programme be made a regular IAEA programme from 1 January 1980 onwards. These conclusions and recommendations of the Subcommittee were endorsed by IFRC and INDC and submitted to the IAEA.

During 1979, the A+M data programme was evaluated by the IAEA, and following its official approval by the policy organs of the Agency, the programme was regularized as of January 1980.

Until the end of these initial years, the A+M Data Unit, with a staff complement of three professionals and two clerical staff, has published 12 issues of the quarterly International Bulletin on A+M Data for Fusion distributed free of charge to approximately 750 recipients world-wide, and has produced the first publication of the comprehensive computerized bibliographic index to A+M collision data relevant to fusion acronymed "CIAMDA", covering the years 1950 - 1979.

Apart from continuing the International Bulletin and keeping the CIAMDA file up-to-date the major area of future work planned by the A+M Data Unit is the coordination of the collection, evaluation, and dissemination of evaluated numerical A+M collision data and reaction rates for their use by the fusion community. The scope and progress of work will be reviewed by a small subcommittee of the IFRC consisting of IFRC-nominated experts and the chairman of INDC or his nominee.

V.2. FUTURE IAEA PROGRAMME ON ATOMIC AND MOLECULAR DATA FOR FUSION

A. Lorenz, J.J. Schmidt, K. Katsonis, J. Rumble
IAEA, Nuclear Data Section

The detailed considerations and recommendations of the International Fusion Research Council (IFRC) of the IAEA, as well as various national and international meetings of fusion and atomic scientists in the past five years have shown that the fusion research community has a primary need for a world-wide computerized A+M data centre service. As a consequence, the IAEA has been requested and has agreed to coordinate this data centre service activity through its Nuclear Data Section.

The last three years have seen the development and final establishment of the Agency's activity in the form of the A+M Data Unit within the IAEA Nuclear Data Section. The over-all objective of this activity is the establishment of an international data centre service to provide the fusion research community with evaluated A+M data of adequate and uniform quality and acceptable accuracy. This objective is proposed to be achieved by an international co-operative effort with the participation of national and regional A+M data centres and research groups in various laboratories and universities. As co-ordinating centre, the A+M Data Unit of the IAEA plans to convene meetings of the Data Centre Network once a year for the organization, implementation and maintenance of this international programme.

To review the planning and execution of the Agency's A+M data programme, the IAEA has formed a small Subcommittee of the IFRC on A+M Data for Fusion consisting of five fusion and atomic scientists, nominated by the IFRC, and including the chairman of the International Nuclear Data Committee or his nominee. The Subcommittee is planned to be convened every two years.

Based on recommendations from the fusion community, and on the experience gained by the NDS during its 15-years existence as a data centre the following programme is proposed as a basis for the future IAEA A+M data centre activity.

Programme Outline

A. Assessment of data requirement and status

1. Continue to review the A+M data requirements for fusion, as well as the status and availability of the required data through specialist meetings convened at appropriate intervals, in order to maintain current awareness.

B. Bibliographic Data

1. Continue to publish the International Bulletin on Atomic and Molecular Data for Fusion at quarterly intervals as a current communication medium between atomic and fusion scientists.
2. Maintain and update the computer master file of the computerized index to the literature on atomic and molecular collision data relevant to fusion research (CIAMDA), and publish future issues of this index as required.

C. Numerical Data

1. Coordination of the compilation, evaluation and dissemination of A+M Collision Data
   a) Assemble, sort and organize existing numerical data relevant to fusion, initiating this activity with collision data;
   b) Support by research contracts and agreements with the Agency the evaluation of specific data types of high priority by atomic physics research groups;
   c) Combine the independently evaluated data into an international evaluated A+M collision data file;
   d) Disseminate the evaluated A+M collision data in the required form to the fusion community.
2. Coordination of the compilation, evaluation and dissemination of other A+M data.

D. Coordination of Data Production

1. Collate and disseminate periodically a list of A+M data required by fusion researchers which need to be measured, calculated or evaluated.
2. Support the measurement and calculation of selected important data through research contracts and agreements with pertinent atomic physics research groups, with due consideration of possible contributions by developing countries.

Programme Description

A. Assessment of Data Requirement and Status

1. Review of A+M Data Requirements for Fusion

In order that the proposed effort is kept relevant to the actual developments in fusion research, the A+M Data Unit must keep pace with the A+M data requirements of this fast moving field.

The effort to identify the A+M data that are required in fusion research was initiated on an international level by the IAEA Nuclear Data Section before the start of its own A+M data programme in 1975 [Ref. 1]. The subject of A+M data needs for fusion was subsequently addressed thoroughly at the IAEA Meeting at the UKAEA Culham Laboratory in November 1976 [Ref. 2], and again at this year's Technical Committee Meeting at Fontenay-aux-Roses.

Therefore in order to maintain a current awareness of the A+M data requirements for fusion it is proposed to

(i) begin a series of smaller international specialist meetings on specific aspects of A+M data for fusion, such as electron data for plasma modelling codes, charge exchange, etc..., which could be convened at a frequency of one or two meetings per year,

(ii) continue convening larger international A+M data for fusion meetings of the Culham or Fontenay-aux-Roses type on a less frequent basis, say every four or five years, and

(iii) publicize the results of these meetings in the form of concise reports to the A+M physics and fusion communities.

B. Bibliographic Data

1. Publication of the International Bulletin on A+M Data for Fusion

As of May 1980, 12 issues of this Bulletin will have been published and distributed cost-free to approximately 750 scientists, laboratories or libraries.

The periodic publication of the Bulletin, which was started in 1977, will be continued. Aside from providing a current awareness information source to the A+M physics and fusion communities, that part of the Bulletin which deals with A+M collision data, provides a continuous up-date to the A+M Collision Data Index (CIAMDA) master file (see B2 below). It is planned to maintain the quality of the Bulletin, to increase its effectiveness as a current communication medium between atomic and fusion scientists, and to improve the part of the Bulletin devoted to plasma surface interaction data.

2. Publication of the Computerized Index to Atomic and Molecular Collision Data (CIAMDA)

The preparation of the computerized Index to Atomic and Molecular Collision Data (CIAMDA) relevant to fusion research was completed by the end of 1979, and submitted for publication in March 1980. The Index contains about 13,000 references and over 40,000 indexation lines covering published references to measured or calculated atomic collision reaction data from 1950 to 1979. The nominal price of the Index is about US $ 30.-, with a 50 % reduction if purchased through the Member States' Missions to the IAEA.

The entire preparation of CIAMDA was computer based, and extensive use was made of the programme that prepare the International Bulletin on A+M Data for Fusion. The CIAMDA file now exists in a format, identical to that of the Bulletin, and may be used as an index to the data which is proposed to be compiled in the numerical A+M data files (see section C). Depending upon the rate of growth of the CIAMDA master file, it is planned to publish updated volumes of this index at appropriate intervals in the future.

C. Numerical Data

As stated in the introduction, the principal objective of the IAEA A+M data programme is the establishment of an international data centre service to provide evaluated A+M data to the fusion research community. The coordination of the compilation, evaluation and dissemination of A+M data is therefore the area which will receive the greatest emphasis in

the future A+M programme of the IAEA. The A+M data which need to be addressed with the highest priority are the A+M collision data, the scope of which has already been identified and used in the selection of fusion-relevant references for the International Bulletin and CIAMDA [Ref. 3].

The A+M collision data base is proposed to consist of two separate files:

- A file of unevaluated data consisting of existing measured or calculated data, designated AMCO/UDF (A+M Collision/Unevaluated Data File)
- A file of evaluated data consisting of evaluated A+M collision data, designated AMCO/VDF (A+M Collision/Evaluated Data File).

A flow diagramme showing the process of compilation, evaluation and dissemination of A+M collision data is shown in attached Figure.

1. Compilation of A+M Collision Data

The principal steps to be taken by the Agency's A+M Data Unit in establishing an international A+M collision data base are:

a) Assess the existence of data compilations. This survey is currently under way.

b) Collect from other data centres and groups and from publications selected data compilations pertinent to fusion.

c) Include the data received into AMCO/UDF in a unique format, associate each selected data set with the corresponding CIAMDA index entry, and transfer any previously evaluated data sets into a preliminary version of the AMCO/VDF (see C.2 below).

d) Maintain AMCO/UDF up-to-date. It is proposed to establish an agreement with members of the A+M Data Centre Network to supply to the A+M Data Unit newly measured or calculated data for input into AMCO/UDF, in an exchange format which will be developed in the future between the members of the A+M Data Centre Network.

2. Evaluation of A+M Collision Data

As the build-up of a sizable evaluated collision data file will take a considerable amount of time, it is proposed to set up initially a provisional evaluated data file consisting of the presently available "best" measured or calculated data set for fusion-relevant atomic species and reaction types, selected from the AMCO/UDF file (see C.1 above), and of existing published evaluated collision data publications.

This file will be replenished gradually, replacing old evaluations with new evaluations proposed to be performed within the framework of the Agency's A+M data programme. These evaluations could be performed by individual experienced research groups under contract with the IAEA, preferably as part of an IAEA coordinated research programme in which several research groups (each under contract with the IAEA) co-operate in the evaluation of specific data required for fusion. To help with these evaluations, the A+M Data Unit could supply the appropriate existing data from the data files to the evaluators. At the conclusion of a given evaluation, the evaluated data would be entered into the AMCO/VDF and indexed in CIAMDA.

3. Creation of the evaluated AMCO/VDF

The AMCO/VDF evaluated collision data file will be composed preferably of one unique data set in a defined format (consisting of energy/cross-section pairs over the energy range pertinent to fusion with uncertainties if possible) for each atomic species and reaction type of interest to fusion, which would be recommended as "best data" to be used by the fusion community. The AMCO/VDF master file would be maintained at IAEA on magnetic tape. With the advent of newly measured or calculated data it will be necessary to arrange re-evaluations of the data in the AMCO/VDF file and update the file whenever necessary.

4. Dissemination of Numerical Data

All data files held by the IAEA A+M Data Unit, including AMCO/UDF and AMCO/VDF, will be available free of charge to anyone on request. To maximize its utility, the evaluated collision data file, AMCO/VDF, could be made available in a variety of ways, depending on demand and cost considerations:

a) Evaluated cross-section data on magnetic tape in a computation format or in the form of "people readable" computer print-out;

b) Evaluated cross-section data transformed to temperature-dependent reaction rate coefficients, where the conversion could be performed by the A+M Data Unit;

c) Small format publications, each comprising an evaluation of a specific data type for the fusion-relevant atomic species (such publications would have to be re-issued with every update of the pertinent part of the file);

d) In computer-produced graphical and/or tabular form.

In addition to the data themselves, the A+M Data Unit will also distribute the evaluation reports documenting each of the evaluations performed in the framework of this international co-operative effort.

In general, the A+M Data Unit could serve as an A+M report distribution centre, where A+M data reports pertinent to fusion would be provided to the A+M Data Unit in Vienna through members of the A+M Data Centre Network for distribution to a specific number of recipients. The scope of this service and the identification of the report recipients would have to be decided in accordance with the IFRC Subcommittee on A+M Data and in cooperation with the A+M Data Centre Network.

D. Coordination of Data Production

1. Request List for Required A+M Data

A request list to communicate requirements for A+M data in fusion research would be published periodically and distributed to the A+M physics and fusion research communities by the IAEA. The request list, containing specific data requirements (e.g. atomic or molecular species, reaction, energy range, accuracy, specific purpose) which are not met by the data base accessible to fusion research scientists, would be published periodically and distributed to the A+M physics and fusion research communities by the IAEA. These lists would be used to guide, support and coordinate measurements, calculations and evaluations of required A+M data.

2. Data Measurement and Calculation

Although the actual measurement or calculation of A+M data is outside the scope of the A+M data programme of the Agency, it is possible for the IAEA to be instrumental in encouraging the generation of some of the data required in fusion research. In support of such work, the Agency has the possibility to conclude contracts with selected groups. Priority would be given to measurements, calculations or evaluation of data specified in the "Request List". However, in view of the limited funds available for research contracts and because of the urgency to provide the existing A+M data to the fusion community, it is suggested to assign initially higher priority to the evaluation of such A+M data which are already in existence.

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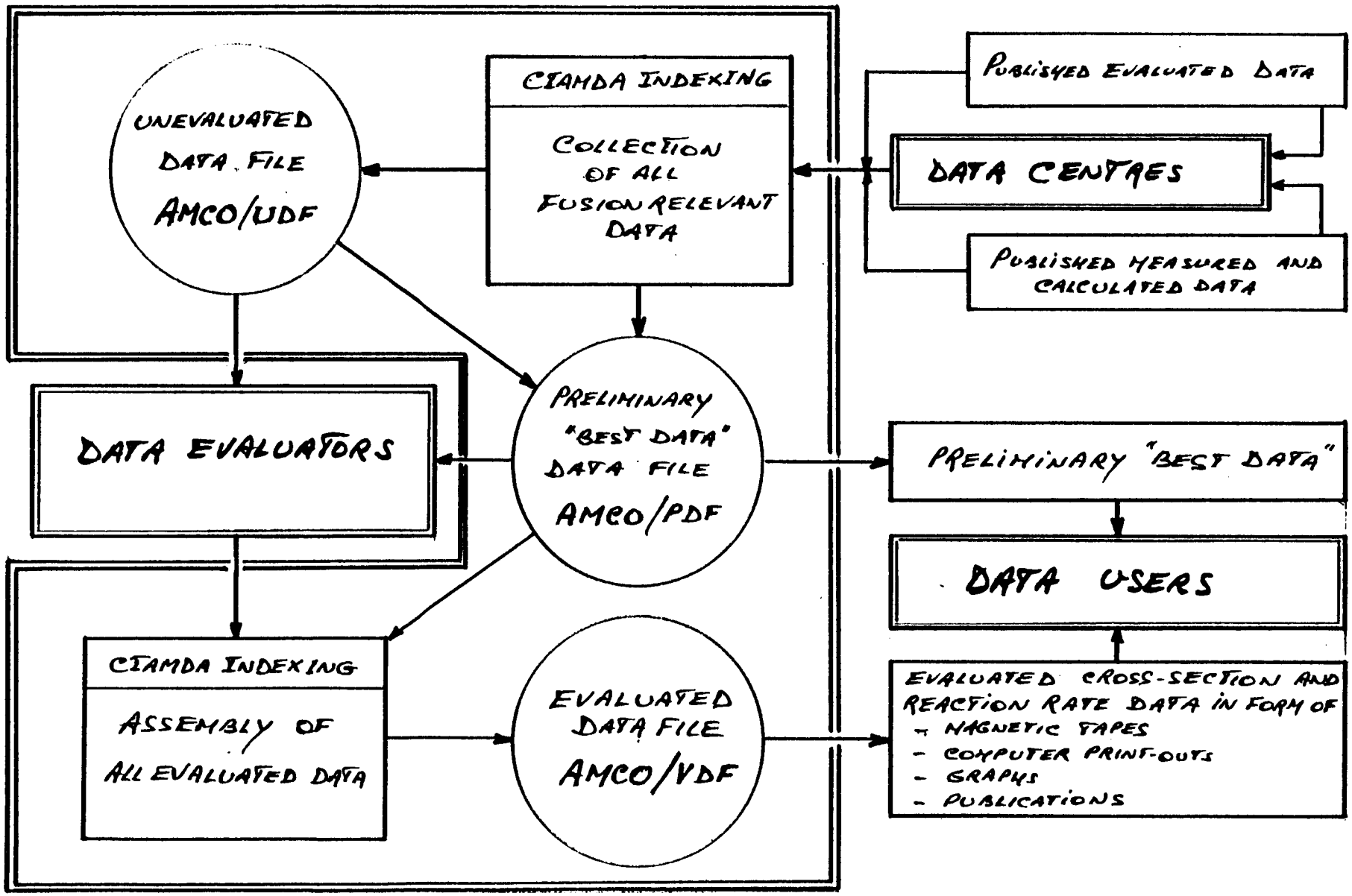
3. The International Programme of Atomic and Molecular Data for Fusion, K. Katsonis and F.J. Smith, in Proc. Nagoya Seminar on Atomic Processes in Fusion Plasmas, Nagoya, 1979 (Institute of Plasma Physics, Nagoya University), Rept. IPPJ-AM-13.

FLOW DIAGRAM FOR THE COMPILATION, EVALUATION AND DISSEMINATION OF A+M COLLISION DATA



V.3. CLASSIFICATION SCHEME FOR INTERACTION OF PLASMA WITH SURFACES

(submitted by Dr. V.A. Abramov, Institut Atomnoi Energii
I.V. Kurchatova, Moscow, USSR)

1. Sputtering
2. Reflection of ions
3. Penetration, pathways and changes of composition of structure upon penetration
4. Blistering
5. Chemical reactions at the surface
6. Inelastic processes: ion-electron and secondary-electron emission; study of changes in the charge state
7. Desorption and emission of gas under the effect of ions, electrons and photons; condition of the surface
8. General aspects of plasma-surface interaction

V.4. DATABASE AND RETRIEVAL-DISPLAY SYSTEM OF ATOMIC DATA FOR FUSION

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1. INTRODUCTION

An effort to compile atomic and molecular data has been made for several years by the Working Groups of the Research Information Center at the Institute of Plasma Physics (IPP)[1)~5)]. To computerize A+M numerical data has been one of the important problems in data compilation. We have constructed under the collaboration with the Computer Center of IPP, a computerized database and a retrieval-display system for the data on electron-atom (ion) collisions. This system makes it possible to store and retrieve the collected data on an on-line interactive basis and to display numerical data on graphic terminal with relevant biliographical information. We call this system as AMRDS (Atomic and Molecular Retrieval Display System).

2. DATABASE

Our database is composed of ionization and excitation cross sections of atomic ions ($Z \geq 2$) by electron impact. For ionization, stored are experimental data obtained by beam method (54 sets) and theoretical results for C,N,-O-like ions(19). Excitation cross sections measured by beam method (30) and calculated by the close-coupling (86) and the Coulomb-Born methods (355) are also stored in the computer at present. About 4000 data sets produced by the Coulomb-Born and the similar calculations have been already collected and are in preparation to computerize.

Each data set includes the following information: 1) process (ionization or excitation), 2) method (experiment or theory), 3) type of experiment (or theory), 4) name of element, 5) atomic

number, 6) number of electrons, 7) initial state, 8) final state, 9) numerical data in x-axis (energy in eV), 10) numerical data in y-axis (cross section in cm^2), 11) literature and 12) comment. The standard units of energy (eV) and cross section (cm^2) are adopted in order to simplify the system. The information of the units used in the original paper is also stored. In future, we plan, numerical data in their original units will be stored and a conversion of unit will be made at the output, when required. The details of the information stored in computer are listed in Table I along tag numbers. We use a tag number system which is similar to the INSPEC Database so as to utilize the FACOM Advanced Information Retrieval System (FAIRS).

3. DATA FORMAT AND FILE FORMAT

Each data element is placed after the directory part of the tag number shown in Table I. Tag format has two part; the first one character indicates the broad category of the data field and the rest the sub-category specifying more detailed description of the data. With the use of this format data are easy to be transformed into other type of format.

One of the problems in dealing with atomic data is how to express in a computer the processes like N^{+4} 2s $^2S_{1/2} \rightarrow 2p\ ^2P_{1/2}$ and the special symbols such as Δ, δ, π, Ω, ω, Å. In our system, the symblos $\wedge$ and $\backslash$ are used to denote superscript and subscript, respectively, and ` is placed at the end of the superscript or subscript. For example, the excitation process shown above is written as

$$N\wedge + 4` \quad 2s\wedge 2` S\backslash 1/2` \longrightarrow 2p\wedge 2` P\backslash 1/2`$$

In principle, a combination of printable characters is used in order to express special symbols. A transformation to any other format is easy. An example of expressions for special symbols is listed in Table III.

4. DATA INPUT

Numerical data with references are stored in computer file through TSS (Time Sharing System) terminal by the use of interactive program. This system sends messages to a key operator on which kind of data to enter next or correct, if necessary, according to

the list of the information stored (Table I). Thus the system makes it easy to input data and reduces the number of possible errors during input. In Table II, an example of input messages is shown. The operator keys in each data after the corresponding messages (e.g. No. of data point, Ionization energy...). When one set of data are finished to be entered, they are displayed on a terminal again with the tag numbers, and if there are input errors, they are corrected by restoring the correct data.

5. RETRIEVAL AND DISPLAY SYSTEM

Atomic data stored in the computer can be retrieved in terms of any items listed in Table I. In most cases we search data by i) processes (ionization or excitation)(PR) ii) theory or experiment (TE), iii) name of element (EL), iv) ionic stage (IS), v) initial state(IN), vi) final state (FI)(The abbreviated codes in parentheses indicate the corresponding items and are used in the retrieval). The FACOM Advanced Information Retrieval System (FAIRS) is used to retrieve the data. The FAIRS has been already employed in IPP for the retrieval system of the literature information based on the INSPEC database.

When you get the data which you want, the numerical values can be obtained in a graphical form on a graphic display terminal (An output device for the graphic display can be chosen among Sony Tektronix, Calcomp, and Versatec). First you have a list of information of each data set (data number, process, theory or experiment, transition, author's name, year of publication) as shown in Fig.1(a). Then you have a graph of the data (Fig.1(b)) with the names of authors corresponding to each symbol. To display a graph as widely as possible the explanation of the graph is output separately. The position of the author's name can be transferred to any place, if desired. When you get two or more data sets, you can display all of them in a graph or some of them in a separate graph. Figs. 1(c) and 1(d) are ,respectively, the experimental and theoretical data selected from the data sets shown in Fig.1(b). You can also get a complete list of information about each data set. The standard output of the information is listed in Fig.1(e) for the data shown in Fig.1(b). Items to be

output can be chosen from those of Table I. The numerical valus are available also in a tabular form. An example of tabuler output, corresponding to Fig.1(c), is shown in Table IV. With this format, it is easy to read out data by FORTRAN Language from a MT or a file.

you can change output format from the standard one like Fig.1 (b). Fig.2(a) shows a "request form" on TSS. For the scale of axis you can select a linear or a log arithmetic one. As for the unit of energy (X axis) available are, 1) eV, 2) Rydberg, 3) atomic unit, 4) $x=E/\Delta E$ (ΔE: transition energy) 5) E x C(C: constant), and as for the unit of cross section (y-axis) 1) cm^2, 2) πa_0^2, 3) collision strength (Ω), 4) Q x C. The necessary conversion of units are made automatically by the computer. The regions of energies and cross sections displayed can be altered by an input of the values of X_{max}, X_{min}, Y_{max}, and Y_{min}. Fig.2(b) gives the resulting output according to the directions indicated in Fig.2(a). In Fig.3(a) the ionization cross sections for carbon ions are shown in a standard form at linear-log scale, while the scale is changed to log-log in Fig.3(b).

6. EVALUATION AND FUTURE PLAN

At present only raw data are stored in our system. Evaluated data are necessary for plasma physicists who are not familiar with atomic and molecular physics. Data evaluation is under planning at the Research Information Center, IPP. We expect that this retrieval-display system is very useful to evaluate atomic data, when added more functions such as curve fitting of discrete data.

With the use of the present system, we are making a critical comparison of empirical formula for the cross section eventually to derive a more reliable and tractable formula. In Fig.4 the empirical formulas for ionization by proposed by Lotz [6),7)] and Golden and Sampson [8)~11)] are compared with experimental data. You can see clearly which formula is better in this case. A reliable empirical formula ,once found, will be used to produce data for the processes and/or species for which no data are available at present.

This system is planned to be extended to ion-atom (ion) collisions, as numerical data for this processes are also collected by a Working Group in our institute.

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1) Cross Sections for Atomic Processes. Vol. 1,(H) IPPJ-DT-48(1975) English Version (1978)

2) Cross Sections for Atomic Processes. Vol. 2.(He) IPPJ-DT-50 (1976)

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4) H. Sūzuki,. Report at the 1st Meeting of the Atomic and Molecular Data Center Network, INDC(NDS)-88 (1977)

5) Y. Itikawa, Report at the 2nd Meeting of the Atomic and Molecular Data Center Network (1980)

6) W. Lotz, Z. Phys. 216 (1968) 241

7) W. Lotz, Z. Phys. 220 (1969) 466

8) L.B. Golden and D.H. Sampson, J. Phys. B 10 (1977) 2229

9) L.B. Golden, D.H. Sampson and K. Omidvar, J. Phys. B 11 (1978)

10) D.L. Moores, L.B. Golden and D.H. Sampson, J. Phys. B 13 (1980)

11) L.B. Golden and D.H. Sampson, Submitted to J. Phys. B

FIGURE CAPTIONS

Fig. 1(a) Explanation of the data sets for Be^{+} 2s $^2S \rightarrow$ 2p ^2P

〃 1(b) Standard output in a graphical form for the data shown in Fig.1(a)

〃 1(c) Experimental data selected from the data sets shown in Fig.1(a)

〃 1(d) Theoretical data selected from the data sets shown in Fig.1(a)

〃 1(e) Standared output for bibliographical Information

Fig. 2(a) Request form for a graphic display

〃 2(b) A graph displayed according to the request shown in Fig.2 (a) for the data in Fig 1(b). (linear-linear scale, energy region; 0~20eV)

Fig. 3(a) Ionization data for carbon ions ($C^{+1} \rightarrow C^{+4}$) in a standard form at (linear - log scale)

〃 3(b) The same data as in Fig.3(a) shown in log-log scale

Fig. 4 Examples of comparison of empirical formulas for by Lotz[6)~7)] (solid line) and Golden and Sampson[8)~11)] (dashed line) with experimental data.

(a) $C^{+2} \longrightarrow C^{+3}$

(b) $C^{+3} \longrightarrow C^{+4}$

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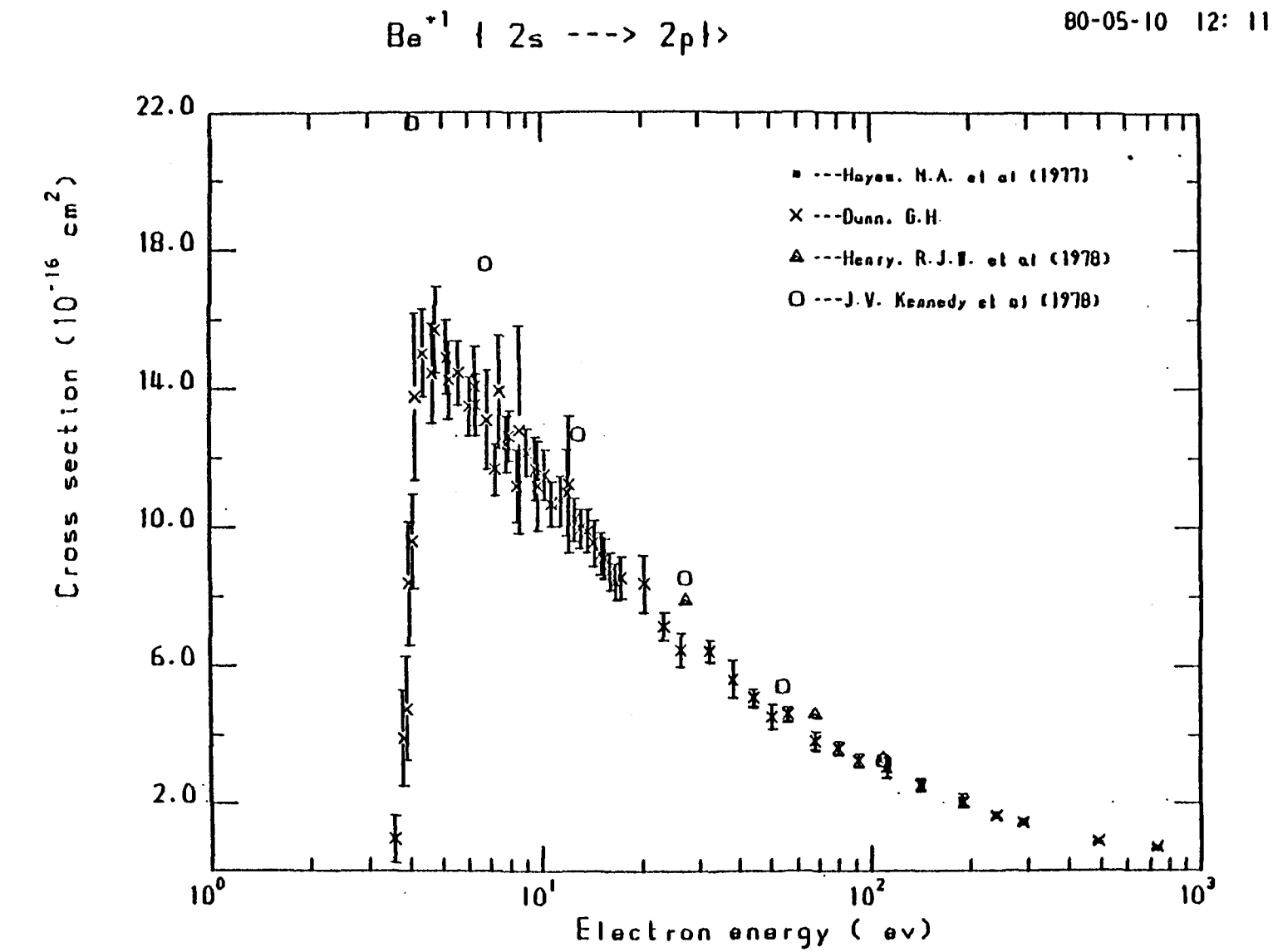
Figure Caption

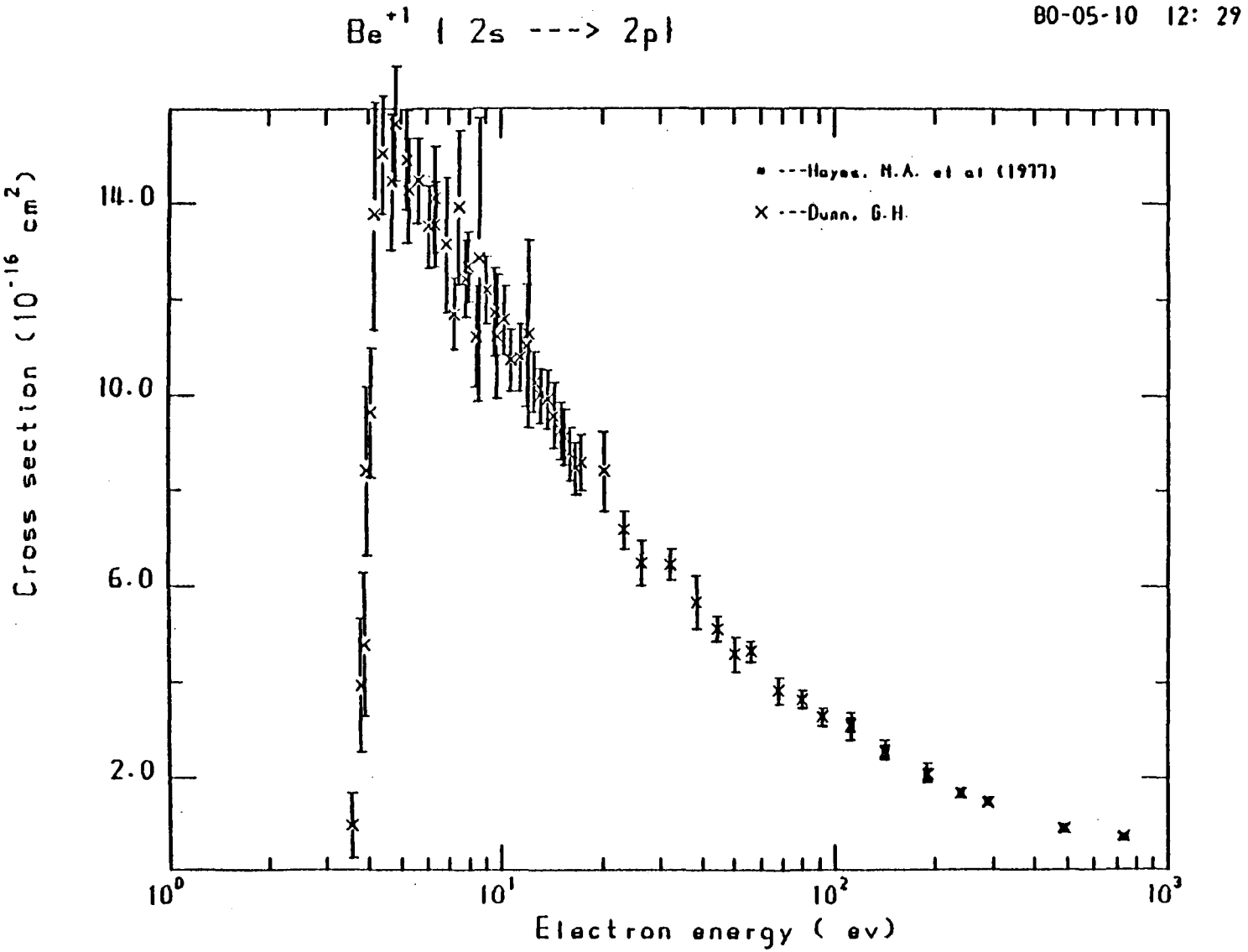
Data NO.	Process	<T>heary or <E>xperiment	Transition	Author (Date)
1----•	Excitation	E	Be^{+1} I 2s ---> 2pI	Hayes. M.A. et al (1977)
2---x	〃	〃	〃	Dunn. G.H. et al
3---▲	〃	T	Be^{+1} I 2s ^2S ---> 2p ^2PI	Henry. R.J.W. et al (1978)
4---o	〃	〃	Be^{+1} I 2s ---> 2pI	J.V. Kennedy et al (1978)

After local conv. kpw in (1) ?

Fig.1(b)

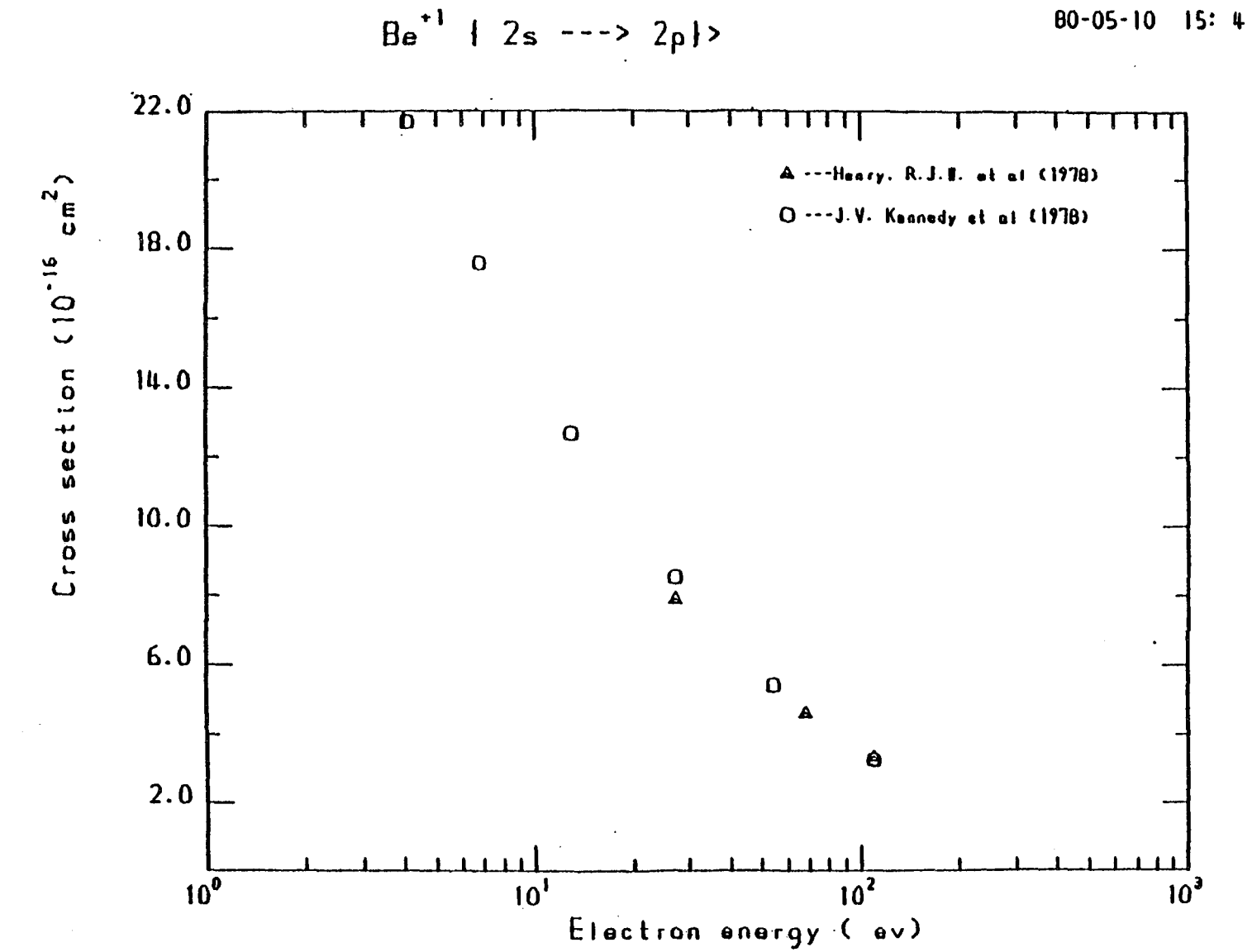


key in 1 (1=1(END),2(DISPLAY),3(KOSEI),4(COPY)(1)= ?



key in I (I=1(END),2(DISPLAY),3(KOSEI),4(COPY)(I1)= ?

Fig.1(d)



key in I (I=1(END),2(DISPLAY),3(KOSEI),4(COPY)(I1)= ?

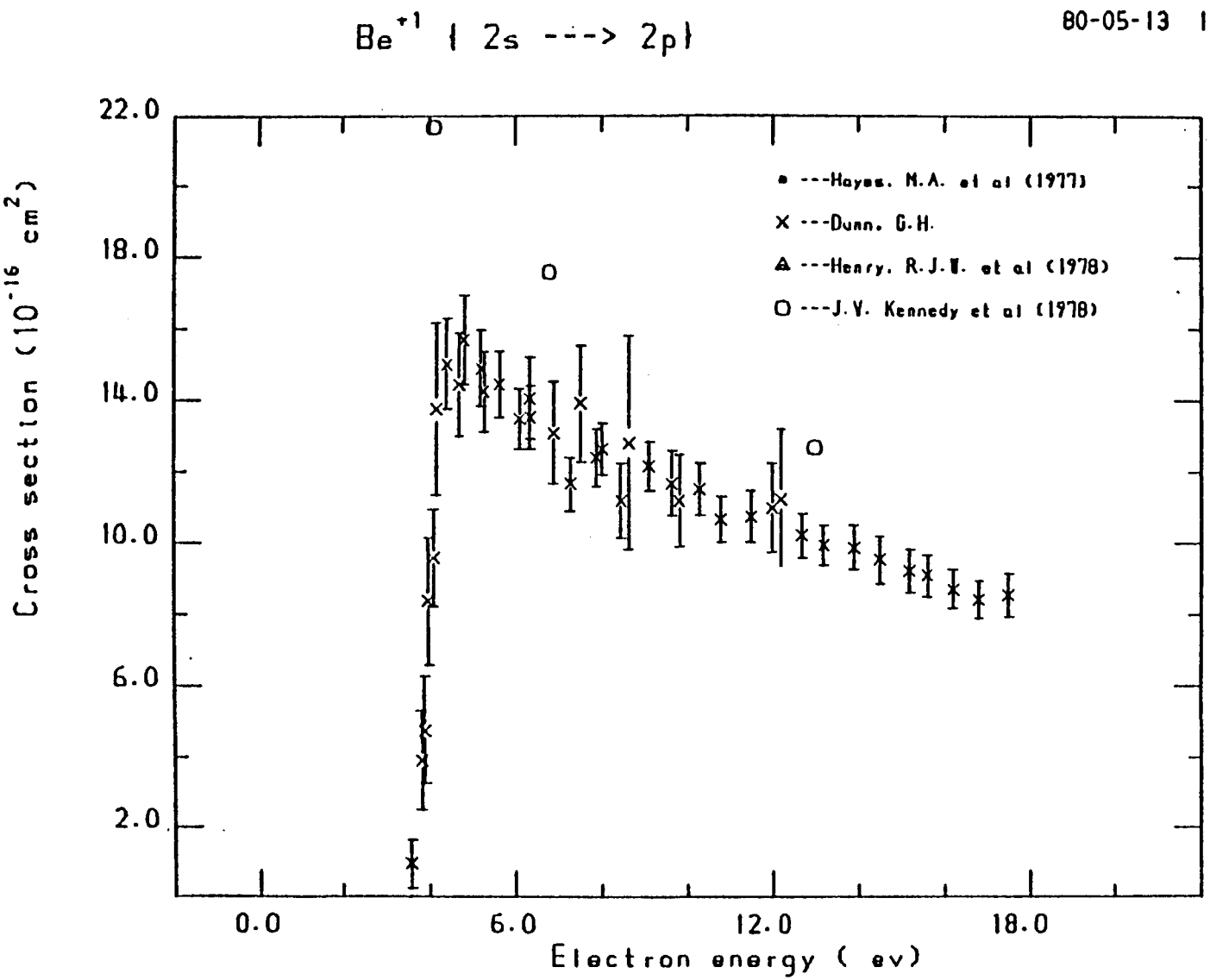
#1	PROCESS	EXC
	THEORY OR EXPERIMENT	E
	METHOD	Born approximation/Beam
	ATOMIC NUMBER	4
	ELEMENT	Be
	STATE	+1
	# OF ELECTRONS	3
	INITIAL STATE	2s
	FINAL STATE	2p
	MEANING OF X-AXIS	Electron energy
	MEANING OF Y-AXIS	Cross-section
	MAX ENERGY	727
	MIN ENERGY	112
	X-AXIS NORM. CONST	0
	Y-AXIS NORM. CONST	-16
	# OF DATA POINTS	7
	AUTHOR(S)	Hayes. M.A.
		Nararass. W.D.
		Hann. J.B.
		Robb. W.D.
	TITLE OF RECORD	Electron impact excitation of Be^+ : a benchmark study
	JOURNAL NAME	J. Phys. B
	VOLUME NUMBER	10
	PAGE NUMBERS	LA29
	DATE OF PUBLICATION	1977
	COMMENT	Small figure. Experiment by Taylor et al(1977: private communication)
#2	PROCESS	EXC
	THEORY OR EXPERIMENT	E
	METHOD	Born approximation/Beam
	ATOMIC NUMBER	4
	ELEMENT	Be
	STATE	+1
	# OF ELECTRONS	3
	INITIAL STATE	2s
	FINAL STATE	2p
	MEANING OF X-AXIS	Electron energy
	MEANING OF Y-AXIS	Cross-section
	MAX ENERGY	737

	MIN ENERGY	3.57
	X-AXIS NORM. CONST	0
	Y-AXIS NORM. CONST	-16
	# OF DATA POINTS	57
	AUTHOR(S)	Dunn, G.H.
	TITLE OF RECORD	Private communication
	COMMENT	Private communication
#3	PROCESS	EXC
	THEORY OR EXPERIMENT	T
	METHOD	Close-Coupling approximation
	ATOMIC NUMBER	4
	ELEMENT	Be
	STATE	+1
	# OF ELECTRONS	3
	INITIAL STATE	$2s\ ^2S$
	FINAL STATE	$2p\ ^2P$
	MEANING OF X-AXIS	Electron energy
	MEANING OF Y-AXIS	Cross-section
	MAX ENERGY	108.8
	MIN ENERGY	27.2
	X-AXIS NORM. CONST	0
	Y-AXIS NORM. CONST	-16
	# OF DATA POINTS	3
	AUTHOR(S)	Henry, R.J.W. van Wyngaarden, W.L. Matese, J.J.
	TITLE OF RECORD	Excitation of Be^+ by electron impact
	JOURNAL NAME	Phys. Rev. A
	VOLUME NUMBER	17
	PAGE NUMBERS	798
	DATE OF PUBLICATION	1978
#4	PROCESS	EXC
	THEORY OR EXPERIMENT	T
	METHOD	Unitarized distorted wave polarized orbital II
	ATOMIC NUMBER	4
	ELEMENT	Be
	STATE	+1

# OF ELECTRONS	3
INITIAL STATE	$2s$
FINAL STATE	$2p$
MEANING OF X-AXIS	Electron energy
MEANING OF Y-AXIS	Cross-section
MAX ENERGY	108.8
MIN ENERGY	4.08
X-AXIS NORM. CONST	0
Y-AXIS NORM. CONST	-16
# OF DATA POINTS	6
AUTHOR(S)	J.V. Kennedy V.P. Myerscough M.R.C. McDowell
JOURNAL NAME	J. Phys. B
VOLUME NUMBER	11
PAGE NUMBERS	1303
DATE OF PUBLICATION	1978

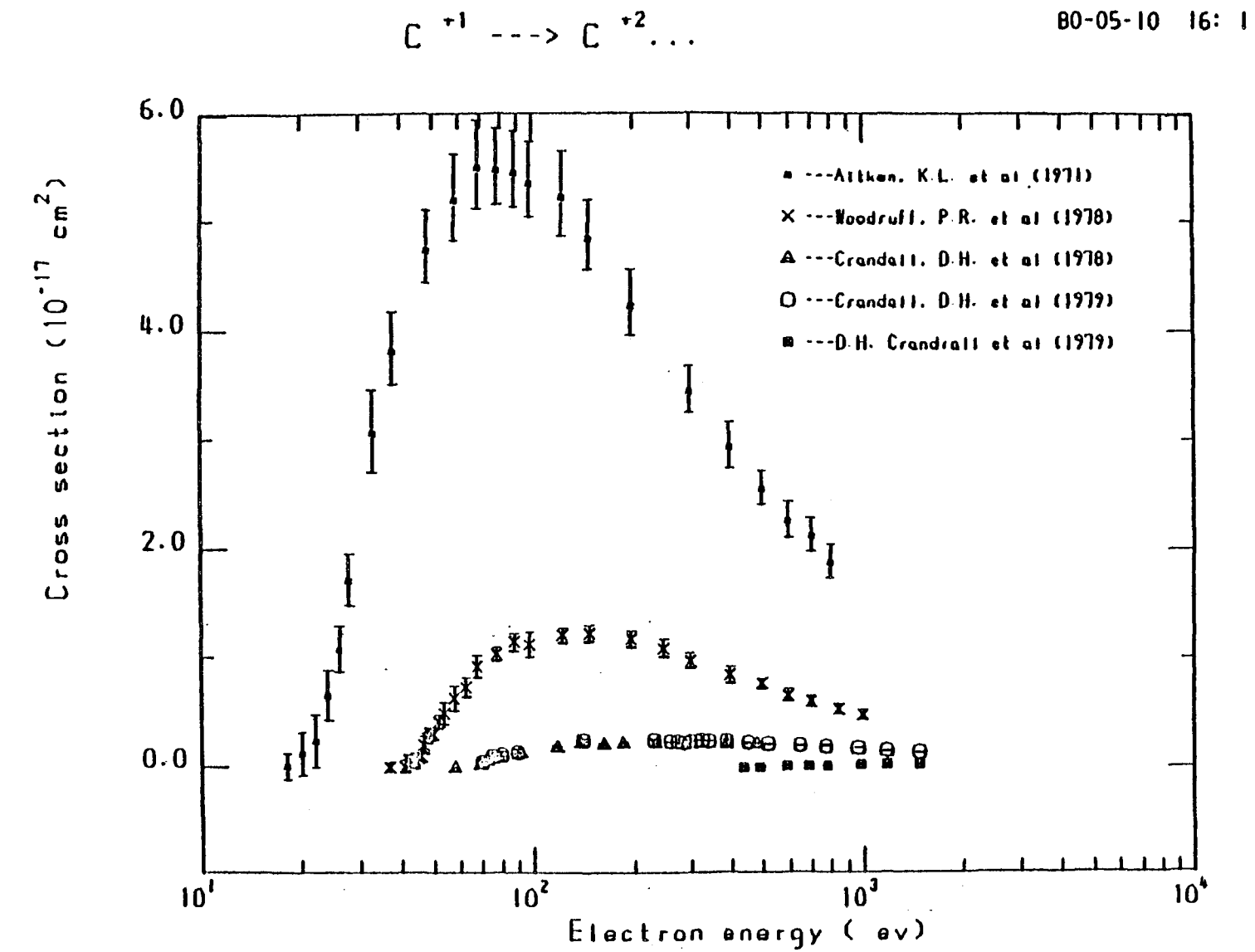
```
          Request Output Parameters
                  Parm. No.
standard      0.............Log-Lin.E(ev).Q(cm²).original-range
scale         11.12.13.14.....Lin-Lin.Log-Lin.Lin-Log.Log-Log
unit-X        21.22.23.24.25..E(ev).E(Ry).E(au).E/ΔE.E*Factor
unit-Y        31.32.33.34.....Q(cm²).Q(na0²).Q.Q*Factor
range         41.42.43.44.....Input(Xmin.Xmax).Input(Ymin.Ymax).
                              X-original range. Y-original range
end of Input   9  ........

key in  Parm. No. (I)= ?   11
key in  Parm. No. (I)= ?   41
key in  Xmin,Xmax(E-range) (E)= ?   0,20
key in  Parm. No. (I)= ?   9
NEW          scale=11  unit(21.31)  Range-X.Y=(0.000E 00.0.200E 02)
                                              (Original.Original)
key in K(K=1(input again),0(display)(I)= ?
```

Fig.2(b)



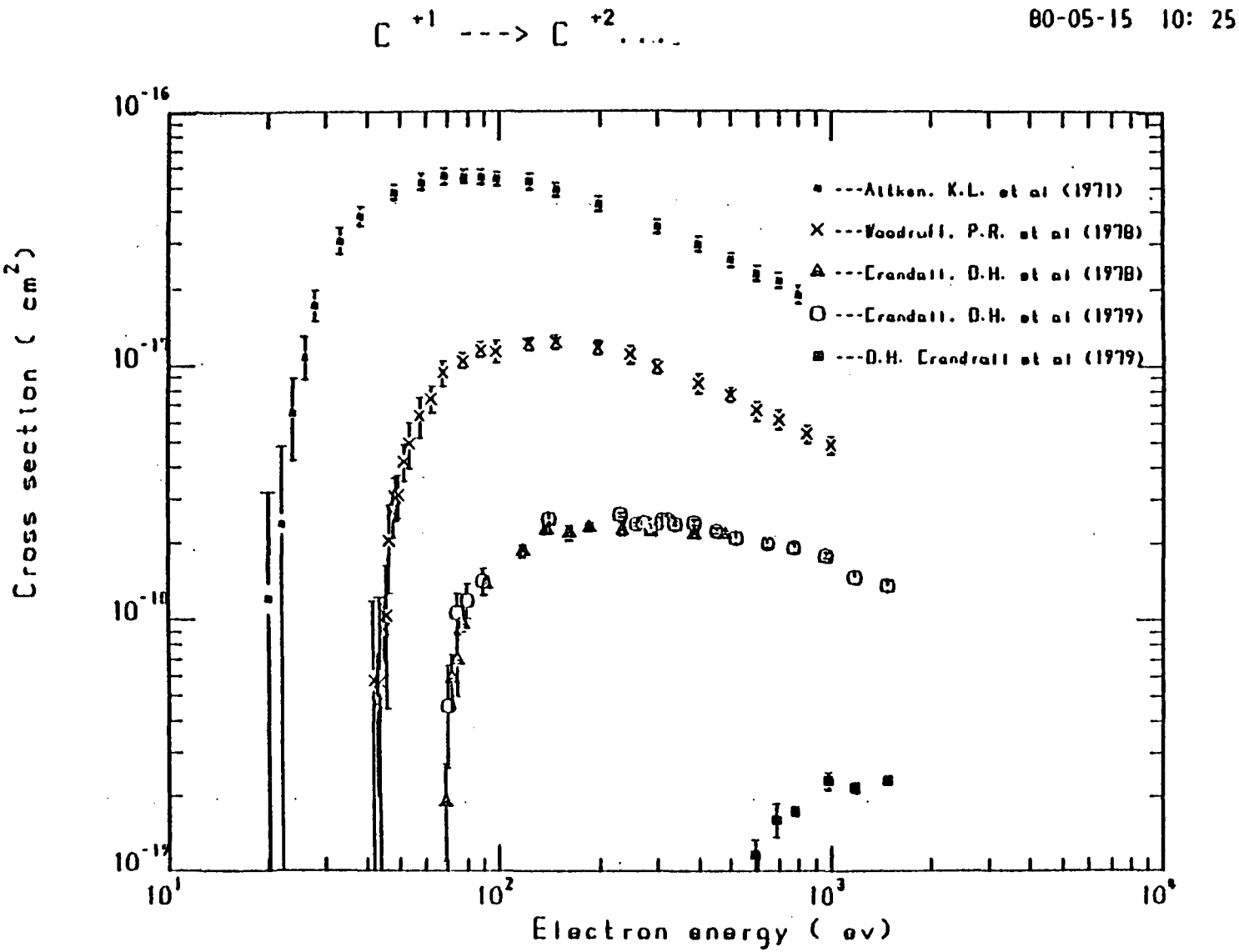
key in I (I=1<END>,2<DISPLAY>,3<KOSEI>,4<COPY>(I1)= ?

Fig.3(a)



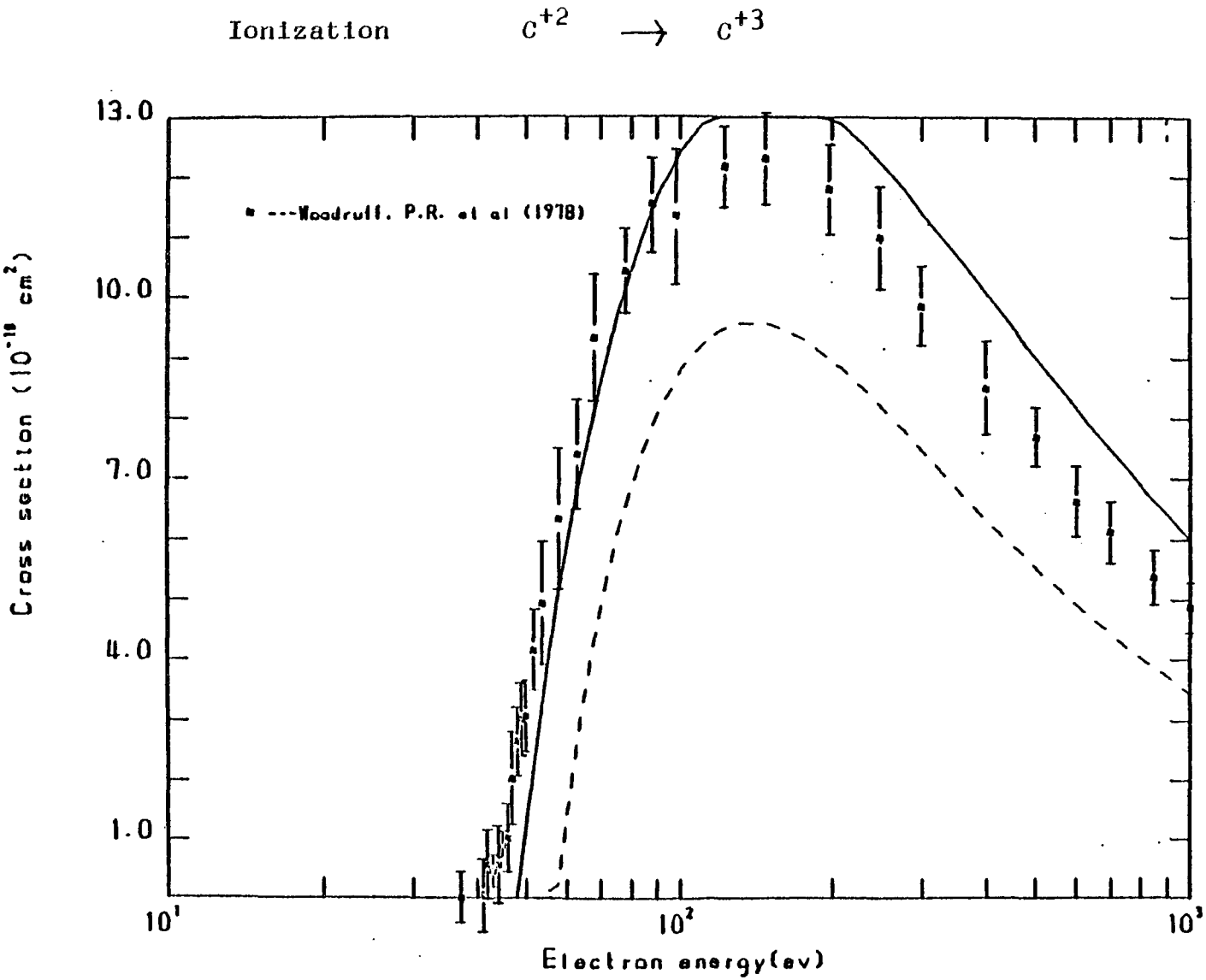
key in I (I=1<END>,2<DISPLAY>,3<KOSEI>,4<COPY>(I1)= ?

Fig.3(b)



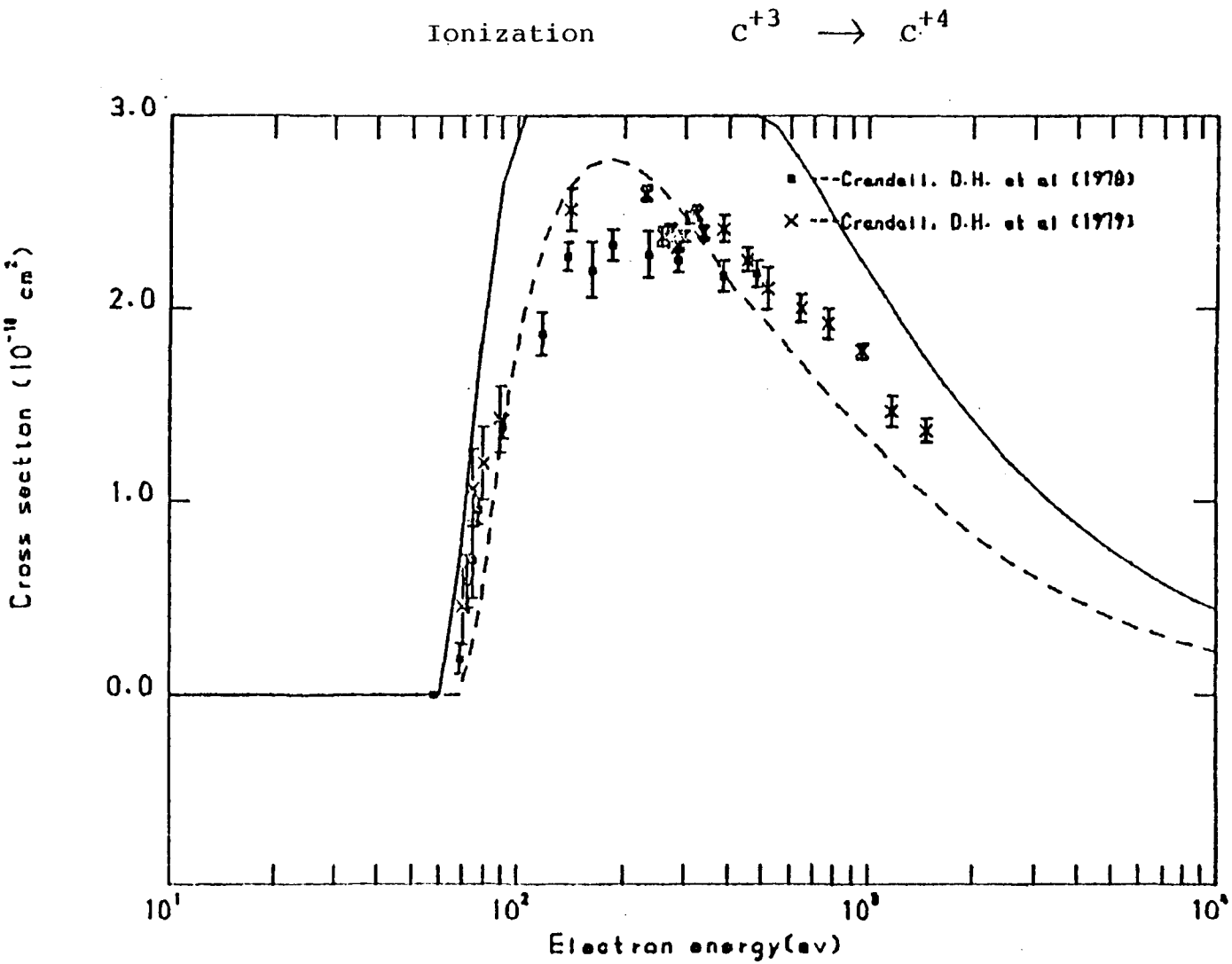
key in I (I=1(END),2(DISPLAY),3(KOSEI),4(COPY)(I1)= ?

Fig.4(a)



key in 1(END), 2(REVIEW), 3(REVIEW,KOSEI),4(COPY)(I1)- ?

Fig.4(b)



key in 1<END>, 2<REVIEW>, 3<REVIEW,KOSEI>,4<COPY>(I1)= ?

Table I TAG LIST

MAIN CATEGORY 00 (control fields)

001	control number
010	record, control number
020*	update, corrected

MAIN CATEGORY 1 (objective field)

100	process
110	theory or experiment
120	type of theory or experiment (abbreviation)
130	type of theory or experiment (full)

MAIN CATEGORY 2 (atomic process data field)

200	atomic number
210	element
220	ionic state (charge number)
225	number of electron
230	initial state
240	final state
250	unit of x-axis
251	title of x-axis
260	unit of y-axis
261	title of y-axis

MAIN CATEGORY 3 (numerical data field)

300	threshold energy (ev)
310	maximum energy
311	minimum energy
320	oscillator strength

TAG LIST (continued)

	330	data for x-axis
	340	data for y-axis
	350	error data for y-axis (absolute value)
	351*	error data for y-axis (% expression)
	360	error data for x-axis
	361*	error data for x-axis (% expression)
	370	normalization constant of x-axis
	380	normalization constant of y-axis
4	(extracted data field)	
	400	maximum of x-axis
	401	minimum of x-axis
	410	maximum of y-axis
	411	minimum of y-axis
	420	number of data points
	430*	error rate calculated for x-axis
	440*	error rate calculated for y-axis
5	(field for future usage)	
6	(original data specification field)	
	600	energy (symbolic expression)
	601	energy (literal expression)
	610	cross section (symbolic expression)
	611	cross section (literal expression)
	620*	normalization constant for x-axis
	630*	normalization constant for y-axis
	640*	continuous data or discrete data

TAG LIST (continued)

650* linear or log for x-axis
660* linear or log for y-axis

7 (reference record field)
700 reference number (numeric)
710 author(s)
720 title of record
730 name of journal (abbreviation)
731 name of journal (full)
740 volume and issue number
750 page number
760 data of publication

8 (comment field)
800 comment

9 (file description)
900 collected by
910 tabulated by
920 in put by
930 date input

Table II

Example of Input Procedure

```
KEQ56650I TIME-07:55:04 CPU-00:00:08 SESSION-00:36:29 MAY 8,1980
Data from file? (Y or N(=Return.))
@
Your name?
@Y. Kanada
Generating number?
@3000
Start of data input
TAG 001(Record number) =
@1190
TAG 700(Reference #(Numeric)) =
@1400
TAG 100(Process) =
@ion
TAG 200(Atomic number) =
@8
TAG 210(Element) =
@O
TAG 220(Ionic state(Charge #)) =
@+1
TAG 225(Number of electrons) =
@7
TAG 230(Initial state) =
@O+1
TAG 240(Final state) =
@O+2
TAG 110(Theory or experiment) =
@e
TAG 120(Type of theory(Exp)(Abb)) =
@cb
TAG 300(Ionization energy(ev)) =
@
TAG 320(Oscillator strength) =
@
TAG 600(Energy(Symbolic)) =
@4
TAG 610(Cross section(Symbolic)) =
@d
TAG 800(Comment) =
@Test data input
TAG 420(# of data points) =
@2
TAG 370(X-axis normalize to 10**) =
@0
TAG 310(Energy region(Max)) =
@430.
TAG 311(Energy region(Min)) =
@371.
TAG 380(Y-axis normalize to 10**) =
@-20
TAG 312(Cross section(Max)) =
@2.950
TAG 313(Cross section(Min)) =
@2.647
TAG 330(Data points for X-axis) =
@371.,430.
TAG 340(Data points for Y-axis) =
@2.647,2.950
TAG 360(X-axis error data(value)) =
@
TAG 350(Y-axis error data(value)) =
@
End of data input
Data ok?
@
```

Table II (continued)

```
Data manipulation end
TAG001 = 1190
TAG010 = 3000
TAG100 = ION
TAG110 = E
TAG120 = CB
TAG130 = Coulomb-Born approximation
TAG200 = 8
TAG210 = O
TAG220 = +1
TAG225 = 7
TAG230 = O+1
TAG240 = O+2
TAG250 = ev
TAG251 = Electron energy
TAG260 = cm^2`
TAG261 = Cross-section
TAG310 = 430.
TAG311 = 371.
TAG312 = 2.950
TAG313 = 2.647
TAG330 = 371.,430.
TAG340 = 2.647,2.950
TAG370 = 0
TAG380 = -20
TAG400 = 430.
TAG401 = 371.
TAG410 = 2.950
TAG411 = 2.647
TAG420 = 2
TAG421 = 2
TAG600 = 4

TAG601 = X(E/~gDE)
TAG610 = D
TAG611 = ~gW(collision strength)
TAG700 = 1400
TAG800 = Test data input
TAG900 = Y. Ichikawa
TAG910 = Y. Kanada
TAG920 = Y. Kanada
TAG930 = 8 MAY 80

File out ok?
@n
Edit?
@y
Tag no?
@700
Value?
@69t1
Tag no?
@
Data manipulation end
TAG001 = 1190
TAG010 = 3001
TAG100 = ION
TAG110 = E
TAG120 = CB
TAG130 = Coulomb-Born approximation
TAG200 = 8
TAG210 = O
TAG220 = +1
TAG225 = 7
TAG230 = O+1
TAG240 = O+2
TAG250 = ev
TAG251 = Electron energy
TAG260 = cm^2`
TAG261 = Cross-section
TAG310 = 430.
TAG311 = 371.
TAG312 = 2.950
TAG313 = 2.647
TAG330 = 371.,430.
TAG340 = 2.647,2.950
TAG370 = 0
TAG380 = -20
TAG400 = 430.
TAG401 = 371.
TAG410 = 2.950
TAG411 = 2.647
TAG420 = 2
TAG421 = 2
```

Table II (continued)

```
TAG600 = 4
TAG601 = X(E/~gDE)
TAG610 = D
TAG611 = ~gW(collision strength)
TAG700 = 69Tl
TAG710 = O. Bely
         S.B. Schwartz
TAG720 = Ionization of highly charged positive ions.
TAG730 = AA
TAG731 = Astron. Astrophys.
TAG740 = 1
TAG750 = 281
TAG760 = 1969
TAG800 = Test data input
TAG900 = Y. Ichikawa
TAG910 = Y. Kanada
TAG920 = Y. Kanada
TAG930 = 8 MAY 80
File out ok?
@
Edit?
@n
Start of data input
TAG 001(Record number) =
@/*
KEQ56650I TIME-08:02:23 CPU-00:00:09 SESSION-00:43:47 MAY 8,1980
READY
```

Table III Expressions for special symbols

superscript	^
subscript	\
return	`
△	∿GD
δ	∿Gd
π	∿Gp
Ω	∿GW
ω	∿Gw
±	∿?+
Å	∿?A
∞	∿?0
λ	∿Gl
ℓ(Italic)	∿Il
→	∿?-
≤	∿SL
≥	∿SG
é	∿Fe
ü	∿Du
ã	∿?-a
ǐ	∿"i

Table IV

Example of Tabular Output of Numerical Data

```
%  Numerical values for cross-section  DATE 80-05-12 TIME 18:41:41 # of data  4
#  1   Hayes, M.A. et al (1977)
Maximum X-axis =  7.2700E+02 Minimum X-axis =  1.1200E+02 X-axis Norm = 10**  0
Maximum Y-axis =  3.1000E+00 Minimum Y-axis =  7.2000E-01 Y-axis Norm = 10**-16
Excitation energy =              Oscillator strength =
Atomic number =  4 Number of electrons =  3 Number of data points =  7
Element name     = Be
Charge number    = +1
Initial state    = 2s
Final state      = 2p
Method           = Born approximation/Beam

  #   Energy(ev)  Cs(cm**2)          +- Energy              +- Cs

  1   1.1200E+02 3.1000E+00 ( 0.0       , 0.0       )( 3.0000E-01,-3.0000E-01)
  2   1.4200E+02 2.6000E+00 ( 0.0       , 0.0       )( 2.0000E-01,-2.0000E-01)
  3   1.8900E+02 2.1000E+00 ( 0.0       , 0.0       )( 2.0000E-01,-2.0000E-01)
  4   2.4000E+02 1.7000E+00 ( 0.0       , 0.0       )( 1.0000E-01,-1.0000E-01)
  5   2.8800E+02 1.5000E+00 ( 0.0       , 0.0       )( 1.0000E-01,-1.0000E-01)
  6   4.8500E+02 9.2000E-01 ( 0.0       , 0.0       )( 8.0000E-02,-8.0000E-02)
  7   7.2700E+02 7.2000E-01 ( 0.0       , 0.0       )( 7.0000E-02,-7.0000E-02)


#  2   No data on author(s) Dunn, G.H.
Maximum X-axis =  7.3700E+02 Minimum X-axis =  3.5700E+00 X-axis Norm = 10**  0
Maximum Y-axis =  1.5700E+01 Minimum Y-axis =  7.4000E-01 Y-axis Norm = 10**-16
Excitation energy =              Oscillator strength =
Atomic number =  4 Number of electrons =  3 Number of data points = 57
Element name     = Be
Charge number    = +1
Initial state    = 2s
Final state      = 2p
Method           = Born approximation/Beam

  #   Energy(ev)  Cs(cm**2)          +- Energy              +- Cs

  1   3.5700E+00 9.6600E-01 ( 0.0       , 0.0       )( 6.9600E-01,-6.9600E-01)
  2   3.8200E+00 3.9400E+00 ( 0.0       , 0.0       )( 1.4000E+00,-1.4000E+00)
  3   3.9000E+00 4.7900E+00 ( 0.0       , 0.0       )( 1.5000E+00,-1.5000E+00)
  4   4.0000E+00 8.4100E+00 ( 0.0       , 0.0       )( 1.7700E+00,-1.7700E+00)
  5   4.1100E+00 9.6300E+00 ( 0.0       , 0.0       )( 1.3500E+00,-1.3500E+00)
  6   4.1800E+00 1.3770E+01 ( 0.0       , 0.0       )( 2.4000E+00,-2.4000E+00)
  7   4.4300E+00 1.5040E+01 ( 0.0       , 0.0       )( 1.2600E+00,-1.2600E+00)
  8   4.7100E+00 1.4460E+01 ( 0.0       , 0.0       )( 1.4500E+00,-1.4500E+00)
  9   4.8300E+00 1.5700E+01 ( 0.0       , 0.0       )( 1.2400E+00,-1.2400E+00)
 10   5.2200E+00 1.4920E+01 ( 0.0       , 0.0       )( 1.0700E+00,-1.0700E+00)
 11   5.2900E+00 1.4270E+01 ( 0.0       , 0.0       )( 1.1100E+00,-1.1100E+00)
 12   5.6500E+00 1.4470E+01 ( 0.0       , 0.0       )( 9.1000E-01,-9.1000E-01)
 13   6.1200E+00 1.3500E+01 ( 0.0       , 0.0       )( 8.5000E-01,-8.5000E-01)
 14   6.3600E+00 1.4080E+01 ( 0.0       , 0.0       )( 1.1300E+00,-1.1300E+00)
 15   6.3700E+00 1.3550E+01 ( 0.0       , 0.0       )( 8.8000E-01,-8.8000E-01)
 16   6.9000E+00 1.3120E+01 ( 0.0       , 0.0       )( 1.4200E+00,-1.4200E+00)
 17   7.3000E+00 1.1690E+01 ( 0.0       , 0.0       )( 7.4000E-01,-7.4000E-01)
 18   7.5400E+00 1.3930E+01 ( 0.0       , 0.0       )( 1.6300E+00,-1.6300E+00)
 19   7.9000E+00 1.2420E+01 ( 0.0       , 0.0       )( 8.0000E-01,-8.0000E-01)
 20   8.0400E+00 1.2670E+01 ( 0.0       , 0.0       )( 7.2000E-01,-7.2000E-01)
 21   8.4700E+00 1.1210E+01 ( 0.0       , 0.0       )( 1.0400E+00,-1.0400E+00)
 22   8.6500E+00 1.2840E+01 ( 0.0       , 0.0       )( 2.9700E+00,-2.9700E+00)
 23   9.1200E+00 1.2180E+01 ( 0.0       , 0.0       )( 6.9000E-01,-6.9000E-01)
 24   9.6500E+00 1.1720E+01 ( 0.0       , 0.0       )( 9.1000E-01,-9.1000E-01)
 25   9.8200E+00 1.1210E+01 ( 0.0       , 0.0       )( 1.2800E+00,-1.2800E+00)
 26   1.0300E+01 1.1550E+01 ( 0.0       , 0.0       )( 7.2000E-01,-7.2000E-01)
 27   1.0800E+01 1.0710E+01 ( 0.0       , 0.0       )( 6.4000E-01,-6.4000E-01)
 28   1.1500E+01 1.0780E+01 ( 0.0       , 0.0       )( 7.1000E-01,-7.1000E-01)
 29   1.2000E+01 1.1020E+01 ( 0.0       , 0.0       )( 1.2600E+00,-1.2600E+00)
 30   1.2200E+01 1.1270E+01 ( 0.0       , 0.0       )( 1.9500E+00,-1.9500E+00)
 31   1.2700E+01 1.0260E+01 ( 0.0       , 0.0       )( 6.2000E-01,-6.2000E-01)
 32   1.3200E+01 9.9800E+00 ( 0.0       , 0.0       )( 5.7000E-01,-5.7000E-01)
 33   1.3900E+01 9.9100E+00 ( 0.0       , 0.0       )( 6.2000E-01,-6.2000E-01)
 34   1.4500E+01 9.5700E+00 ( 0.0       , 0.0       )( 6.7000E-01,-6.7000E-01)
 35   1.5200E+01 9.2600E+00 ( 0.0       , 0.0       )( 6.0000E-01,-6.0000E-01)
```

APPENDIX VI

REPORTS FROM THE A+M DATA CENTRES

May 198o

THE FACHINFORMATIONSZENTRUM ENERGIE, PHYSIK, MATHEMATIK GMBH KARLSRUHE, FEDERAL REPUBLIC OF GERMANY.

G. Ebel

1. Organization and information services

The Fachinformationszentrum Energie, Physik, Mathematik, founded in 1977 as a company of the Bund and the Länder of the Federal Republic of Germany, has the task of providing scientific and technical information services in the fields of:

- energy, nuclear research and technology
- aeronautics and astronautics, space research
- physics
- mathematics
- astronomy and astrophysics,

by making this information available and carrying out all related activities.

The following former institutions have been merged into the Fachinformationszentrum:

- Zentralstelle für Atomkernenergie-Dokumentation (ZAED), Karlsruhe
- Zentralstelle für Luft- und Raumfahrtdokumentation und -information (ZLDI), Munich
- Physikalische Berichte (PB), editorial department, Brunswick
- Zentralblatt für Mathematik (ZfM), editorial department, Berlin
- Zentralblatt für Didaktik der Mathematik (ZDM), editorial department, Karlsruhe.

The Fachinformationszentrum has a staff of about 24o people, one third of them being scientists from different fields of science and technology, as well as a large technical staff.

All activities are supported by modern information technologies which provide comprehensive and efficient information services.

To meet the various information needs, the Fachinformationszentrum offers a wide range of information services on technical literature, data, and conference dates as well as nonconventional literature supply. Information services on on-going research and development projects are in preparation.

At present the following information services are offered:

- Literature information: retrospective searches, SDI profiles, standard profiles, scientific-technical information, interactive on-line retrieval services, magnetic tape services, printed information services: abstract journals, indexes, bibliographies.
- Physics data information: printed data compilations, magnetic tape services, searches.
- Factual information on patent families: on-line retrieval service, searches
- Conference information: conference calendar, information, searches, SDI profiles
- Technical advice, special services: advice to users concerning problems of information supply, advice on how to set up in-house information systems, special services in the fields of information and documentation systems, computer operation, library services
- Literature supply (emphasis on nonconventional literature): loan, referral services.

The basis of these information services are machine-readable data bases. Appropriate storage in the data processing system (complex memory organisation) mechanical scratch file) turns these data bases into machine-readable data banks. The Fachinformationszentrum disposes of bibliographic and numerical data bases in its special subject fields and will provide further data bases if the problems posed by the users make this necessary. These data bases have been established either by the Fachinformationszentrum itself or in international cooperation; some of them are obtained from other organisations.

Since the beginning of 1979 the data bases of the Fachinformationszentrum are on-line accessible via the public telephon network and since January 1980 via EURONET. This network, set up by the member countries of the European Community, transmits information using the latest packet-switching technologies. Together with the Fachinformationszentrum the most important European on-line information centres are connected as host within EURONET and offer their interactive retrieval services.

2. Information on numerical data

The Fachinformationszentrum takes into account the rising demand for selected and evaluated data by gradually expanding data documentation and information. The centre's own documentation activities are focused on the following special subjects:

- High energy physics
- Atomic and molecular physics
- Crystallography
- Nuclear physics
- Solid state physics

Data documentation in other fields of physics as well as on properties of materials is being prepared. Expansion into the energy research sector is in a preparatory stage.

Critical selection, evaluation and compilation of data is carried out in close cooperation with research groups at universities, research centres, at Max-Planck institutes, etc. There is also cooperation with national and international data centres.

Information services in all fields of physics are offered using data bases and data compilations elaborated by the Fachinformationszentrum itself or in cooperation with others or using external data banks and compilations.
The following data bases are available for informations services at the moment:

- Data compilations in the field of physics and energy (INKA-DATACOMP)
- Cambridge Crystallographic Data Files (CCDF) (territorial rights; not available for enquiries from abroad)
- Evaluated Nuclear Structure Data File (ENSDF)
- Karlsruhe Charged Particle Group File (Kachapag)

The Fachinformationszentrum also has a reference library of data compilations in physics on a worldwide basis.

The following services are offered:

- Printed information
- SDI profiles and retrospective searches ,
- Magnetic tapes

On-line services are planned for the near future.

The Fachinformationszentrum offers the following publications in the Physikdaten/ Physics Data series:

- Data compilations in selected fields of physics
- Bibliographies of existing data compilations in physics on a worldwide basis.

The data compilations are published in single issues which are either constantly brought up to date or else replaced by new editions. Reference is always made to the source of data. Up to now 3o issues have been published in the Physikdaten/ Physics Data series.

The activities of the Fachinformationszentrum in the field of atomic and molecular data have been described already at the first meeting of this group.
In the first place the "Surface and Vacuum Physics Index" should be mentioned which is compiled at the Max-Planck-Institut für Plasmaphysik in Garching and published by the Fachinformationszentrum. It is aimed at the prompt dissemination of the latest results in surface and vacuum physics research and comprises a bibliography, an author index and an alphabetical subject index. Each issue covers all new laboratory reports and publications for that particular month. Besides the usual information, the bibliographic part contains keywords or combinations thereof that indicate the subject matter of an article. A distinction is made between primary and secondary keywords. The primary keywords are accepted terms in surface and vacuum physics. They are arranged alphabetically in the subject index, followed by the titles of relevant works. The secondary keywords are used to describe important details, thus combining with the primary keywords and title to give a good idea of the content. Unlike primary keywords, they are not included in the subject index.
Both the bibliographic part and the indexes are compiled by computer. The language used is English. Titles in other languages are translated into English, the original being added in slashes. A literature retrieval service by computer is provided when required. In 1979 about 26oo documents were covered.

In 1978 the "Surface and Vacuum Physics Index" was extended to a bibliographic index for surface interaction data following the recommendations at the IAEA Advisory Group Meeting on Atomic and Molecular Data for Fusion at Culham 1976. This has been done in the following way:

All papers containing numerical data are given a special treatment in addition to the usual procedure for compiling the Surface and Vacuum Physics Index. They are indexed with additional keywords on a formatted worksheet specifying the type of data contained in the papers. These keywords give information on the following items:

Interaction process
Reaction bombarding particle and target
Energy range of bombarding particle
Measured quantities
Measuring method
Comments (if necessary)

All information is stored in a computer in the same way as for the "Surface and Vacuum Physics Index". This allows the generation of different types of indices, arranged e.g. by reactions, measured quantities or measuring methods.

In addition, the Fachinformationszentrum is willing to cooperate in the field of atomic and molecular data in a similar way as it already does so in the field of nuclear data. It will support and coordinate activities in data compilation and evaluation within the Federal Republic of Germany and act as the German partner in the international data center network.

DATA CENTER ACTIVITIES OF THE RESEARCH INFORMATION CENTER, IPP/NAGOYA

Y. Itikawa

The Research Information Center was established officially in 1977. Its objectives are (1) compilation, evaluation and dissemination of scientific information required for fusion research and (2) analysis and investigation of problems arising in the course of development of fusion reactors. The activity of the Atomic Data Study Group, IPP/Nagoya, has been succeeded and extended by the Center. The Center is still in its building-up stage. The major activities, including some future plans, are described below.

1. Compilation, evaluation and dissemination of atomic data for fusion research and related fields

Most of the activity of data compilation is supported by Working Groups which are organized by the participation of scientists belonging to various institutions in Japan on a collaboration basis. Names of the members are shown in Appendix A. They survey literature, collect numerical data and evaluate them. They make also an analysis of problems to be encountered in fusion research. The results of the Working Group activities are published in a form of the Center report (mostly in IPPJ-AM series). The list of publications relevant to A & M data is given in the Appendix B. The collected numerical data are stored in a computer to form a computerized data base. In 1980, two Working Groups are active in the field of atomic data.

(1) Working Group on Atomic Processes in Plasmas

The main emphasis is now placed on impurity ions. The major activities are being performed by the following subgroups.

(a) electron-ion collisions

Collection of excitation and ionization cross sections (both theoretical and experimental) are under way. Based on the data collected, a computerized data base is being produced. To handle the data, a retrieval and display system has been developed (see the next section).

(b) collisions between H, He and their ions and impurities

As a first step, data collection is being made for the process

$$H + A^{q+} \longrightarrow H^{+} + A^{(q-1)+} \qquad (A = \text{impurity atom})$$

Other relevant processes will be dealt with in the future. To make a computerized data base is under planning.

(c) recombination

A workshop on the role of multiply excited ions in plasmas has been held under the leadership of this subgroup. A very extensive discussion was made there about the dielectronic recombination. Some joint research programs on dielectronic recombination have been started on the stimulation by the discussion at the workshop.

(d) spectroscopic data of multiply-charged ions

This subgroup has just begun to work. They plan to make a data collection on Ti and Ni ions. Also they have a plan to survey the availability of computer code for the calculation of the spectroscopic data.

One of the final goals of the working Group is to provide an evaluated numerical data base for all the atomic processes taking place in plasmas. As a first step to the goal, a small workshop was held last February to discuss how to evaluate atomic data. Although there was an extensive discussion, no definite conclusion has yet been drawn. Another meeting will be held this year to continue the discussion.

(2) Working Group on Plasma-Wall Interactions

Plasma-wall interaction involves a wide variety of problems, some of which are difficult even to define clearly. This Working Group has started by choosing the elementary processes which are rather easily tractable. Subgroups are organized for each of them.

(a) ion sputtering

Experimental data on ion-sputtering yield have been collected for all the elements (both for projectiles and for targets) and over a wide range of incident energies. On the basis of the evaluation of the collected data, a semiempirical formula useful in the fusion research has been derived. The compilation will be published soon, while a computerized data base of sputtering yield is now under

development. The data collection will be extended to include dependences of the sputtering yield on incident angles, energy and angular distributions of sputtered particles, and other properties.

(b) blistering

To understand the phenomena of blistering and its relation to fusion research, a workshop was held. This subgroup is planning to publish a critical review on blistering after having several workshops.

(c) reflection/desorption

This subgroup has been organized in 1980. A compilation of reflection coefficients and related quantities for ion impacts has been started. Desorption is more complicated to handle than reflection. This subgroup is now discussing how they can make a data compilation on desorption.

2. Computer retrieval of literature and numerical data

Under the collaboration of the Computer Center of IPP, a computer retrieval system of literature information has been developed. This system is based on INSPEC data base, which contains bibliographical information, including abstracts, taken from over 2000 journals all over the world. One can make a literature survey by any word in titles and abstracts so that a key word system is unnecessary. This system will be adapted to the use of CIAMDA and other existing data base on bibliography.

As is mentioned in the previous section, the numerical data collected by the Working Groups are stored in a computer. A system is being developed to retrieve and display those data. The details of the system (called AMRDS) are shown in another report. At present, this system can handle only the electron-ion cross section. In the future it will be modified to include other data such as charge-transfer cross section.

The above two systems (for literature and numerical data) are open to public. Through TSS, any scientist in IPP or those who participate in the collaborating research program of IPP can access the system to get information they want.

3. Promotion of collaboration between atomic physics community and fusion research community

Once or twice a year the Center organizes a workshop on the problem of mutual interest to both the communities. The subjects already taken are "The role of multiply excited ions in plasmas" and "Atomic processes in laser-produced plasmas". This year the latter topic will be discussed again and another workshop is planned to be held on "Charge transfer collisions in tokamak plasmas". Proceedings of each workshop is published in Japanese. It is hoped that a joint research program is started from such a kind of meeting.

In September, 1979, the Center organized Nagoya Seminar on Atomic Processes in Fusion Plasmas as a satellite meeting to the XI ICPEAC. Over 80 participants came from 13 countries and discussed various problems related to atomic processes in high-temperature plasmas. The proceedings of the Seminar has been published as a report of the Center (IPPJ-AM-13).

The Center has a plan to publish review articles written by experts in respective fields to bring contemporary achievements and their evaluation in specific subjects to the community of fusion research. Those reviews will appear in English.

4. International cooperation

Collaboration among data centers and groups is essential to establish comprehensive data compilations and distribute them to fusion people. The Center has already contributed and will continue to contribute to the activity at IAEA through sending information about the relevant works done in Japan and through other possible means.

To promote the world-wide collaboration in the field of atomic data, each local effort is also important. Collaboration program is now starting between the U.S. and Japan data centers as a part of the U.S.-Japan collaboration program in fusion research. Our Center is willing to cooperate with any other centers and groups.

Members of Working Group on Atomic Processes in Plasmas

Kazuo Takayanagi (Chairman)	Inst. of Space and Aeronautical Science University of Tokyo
Tatsuo Arikawa	Faculty of Technology Tokyo Univ. of Agriculture & Technology
Takashi Fujimoto	Faculty of Engineering Kyoto University
Junji Fujita	Institute of Plasma Physics Nagoya University
Yukikazu Itikawa	Institute of Plasma Physics Nagoya University
Tsuruji Iwai	Dept. Liberal Arts Kansai Medical University
Yozaburo Kaneko	Faculty of Science Tokyo Metropolitan University
Takako Kato	Institute of Plasma Physics Nagoya University
Takaichi Kawamura	Institute of Plasma Physics Nagoya University
Michio Matsuzawa	University of Electro-Communications
Kazuo Mori	The Institute of Physical and Chemical Research
Hajime Narumi	Faculty of Science Hiroshima University
Shunsuke Ohtani	Institute of Plasma Physics Nagoya University
Kazuhiko Okuno	Faculaty of Science Tokyo Metropolitan University
Masamoto Otsuka	Institute of Plasma Physics Nagoya University
Hiroshi Ryufuku	Japan Atomic Energy Research Institute
Hiroshi Suzuki	Faculty of Science and Technology Sophia University
Hiroyuki Tawara	Faculty of Engineering Kyushu University
Tsutomu Watanabe	Faculty of Engineering University of Tokyo

Members of Working Group on Plasma-Wall Interactions

Noriaki Ito (Chairman)	Faculty of Engineering Nagoya University
Kenya Akaishi	Institute of Plasma Physics Nagoya University
Genichi Horikoshi	National Laboratory for High Energy Physics
Yukio Ishibe	The Institute of Physics and Chemical Research
Hajime Ishimaru	National Laboratory for High Energy Physics
Yukikazu Itikawa	Institute of Plasma Physics Nagoya University
Koji Kamata	Institute of Plasma Physics Nagoya University
Takako Kato	Institute of Plasma Physics Nagoya University
Takaichi Kawamura	Institute of Plasma Physics Nagoya University
Takao Kino	Laboratory of Crystal Physics Hiroshima University
Kazunori Kitajima	Research Institute of Applied Mechanics Kyushu University
Masanori Kobayashi	National Laboratory for High Energy Physics
Atsushi Koma	The University of Tsukuba
Soji Miyagawa	Government Industrial Research Institute Nagoya
Akira Miyahara	Institute of Plasma Physics Nagoya University
Kenro Miyamoto	Faculty of Science University of Tokyo
Kenji Morita	Faculty of Engineering Nagoya University
Yoshimasa Murata	Institute of Solid State Physics University of Tokyo

Kosuke Okamoto	ULVAC Corporation
Jun Okano	College of General Education Osaka University
Kunio Ozawa	Japan Atomic Energy Research Institute
Ryuichi Shimizu	Faculty of Engineering Osaka University
Haruki Shiraishi	National Research Institute for Metals
Tatsuo Tabata	Radiation Center of Osaka Prefecture
Teruhiko Tajima	Institute of Plasma Physics Nagoya University
Yasunori Yamamura	Faculty of Applied Physics Okayama University of Science

List of publications on atomic data for fusion

(1) K. Takayanagi and H. Suzuki, ed., "Cross Sections for Atomic Processes. Vol.1, Processes Involving Hydrogen Isotopes, Their Ions, Electrons and Photons" IPPJ-DT-48 (1976) [in Japanese] (English edition has been published in 1979)

(2) K. Takayanagi, H. Suzuki and S. Ohtani, ed., "Cross Sections for Atomic Processes. Vol.2, Processes Involving Helium, Hydrogen Atoms and Molecules, Their Ions, Electrons and Photons" IPPJ-DT-50 (1977) [in Japanese]

(3) H. Tawara, "Cross Sections for Charge Transfer of Hydrogen Beams in Gases and Vapors in the Energy Range 10 eV - 10 keV" IPPJ-AM-1 (1977)

(4) T. Kato, "Ionization and Excitation of Ions by Electron Impact - Review of Empirical Formulae - " IPPJ-AM-2 (1977)

(5) K. Mori, M. Otsuka and T. Kato, "Grotrian Diagrams of Highly Ionized Iron Fe VIII - Fe XXVI" IPPJ-AM-3 (1977)

(6) T. Kato, "Atomic Processes in Hot Plasmas and X-Ráy Emission" IPPJ-AM-4 (1978)

(7) S. Hiraide, Y. Kigoshi and M. Matsuzawa, "Charge Transfer between a Proton and a Heavy Metal Atom" IPPJ-AM-5 (1978)

(8) T. Kato and H. Narumi, "Free-Free Transition in a Plasma - Review of Cross Sections and Spectra -" IPPJ-AM-6 (1978)

(9) K. Takayanagi and T. Iwai, "Bibliography on Electron Collisions with Atomic Positive Ions: 1940 through 1977" IPPJ-AM-7 (1978)

(10) T. Fujimoto, "Semi-Empirical Cross Sections and Rate Coefficients for Excitation and Ionization by Electron Collision and Photoionization of Helium" IPPJ-AM-8 (1978)

(11) K. Okuno, "Charge Changing Cross Sections for Heavy-Particle Collisions in the Energy Range from 0.1 eV to 10 MeV. I. Incidence of He, Li, Be, B and their Ions" IPPJ-AM-9 (1978)

(12) K. Okuno, "Charge Changing Cross Sections for Heavy-Particle Collisions in the Energy Range from 0.1 eV to 10 MeV. II. Incidence of C, N, O and their Ions" IPPJ-AM-10 (1978)

(13) K. Okuno, "Charge Changing Cross Sections for Heavy-Particle Collisions in the Energy Range from 0.1 eV to 10 MeV. III. Incidence of F, Ne, Na and their Ions" IPPJ-AM-11 (1978).

(14) S. Nakazaki and T. Hashino, "Electron Impact Excitation of Positive Ions Calculated in the Coulomb-Born Approximation -A data list and comparative study" IPPJ-AM-12 (1979)

(15) ed. Y. Itikawa and T. Kato, "Atomic Processes in Fusion Plasmas. Proceedings of the Nagoya Seminar" IPPJ-AM-13 (1979)

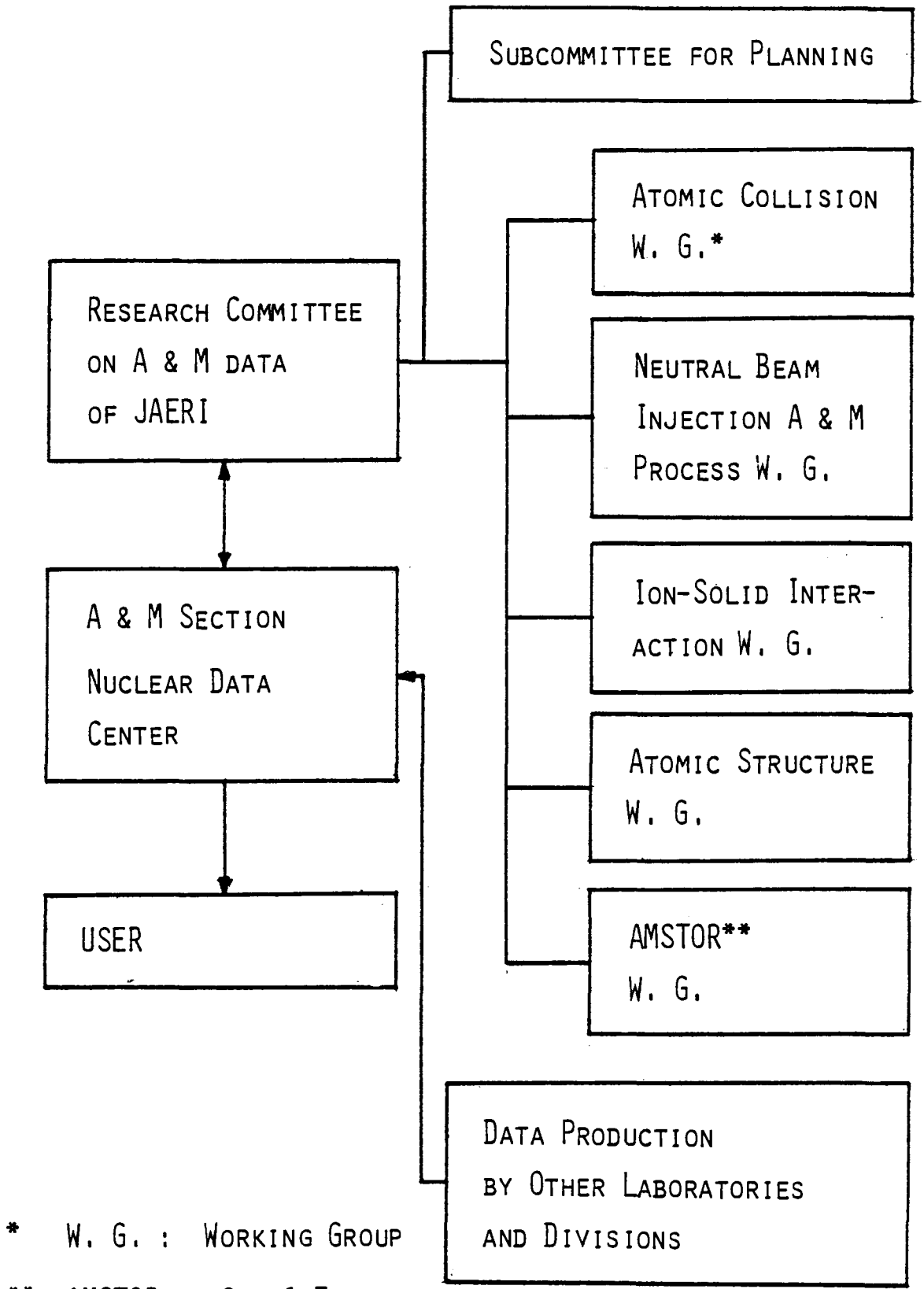
Recent Activities and Programs on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute

Yohta Nakai

Nuclear Data Center,
Japan Atomic Energy Research Institute,
Tokai-mura, Ibaraki-ken, Japan

May 1980

Organization for A & M Activities in JAERI



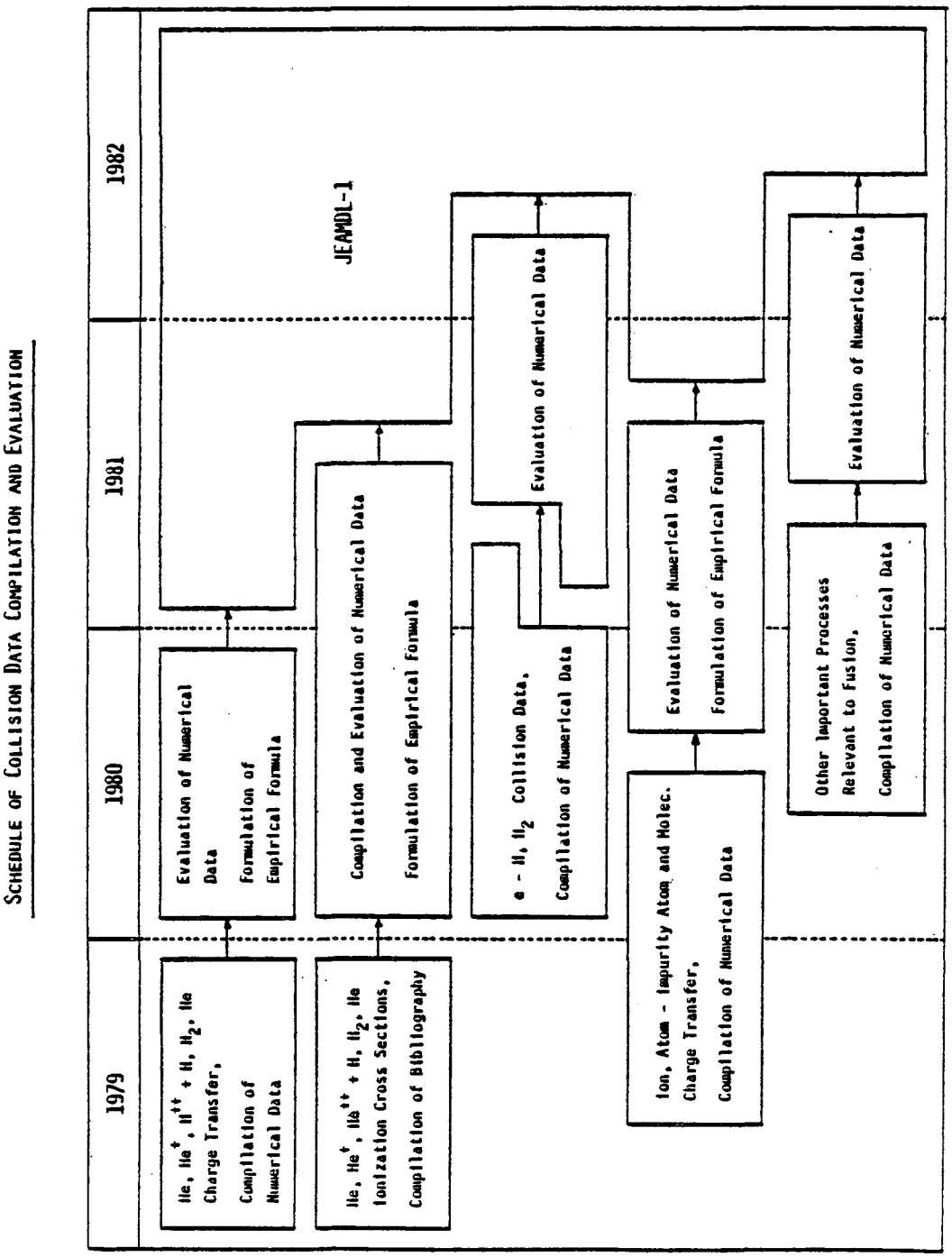
* W. G. : Working Group

** AMSTOR : See 1.3

1. Data Compilation and Evaluation[1-3]

1.1 Japanese Evaluated A & M Library, 1st Edition (JEAMDL-1) Program

Schedule of collision data compilation and evaluation



1.2 Data on Radiation Blistering

A. Literature survey; 1963 - 1979

B. Physical parameters employed in this compilation

(a) Energy dependence

(b) Temperature dependence

(c) Dose dependence

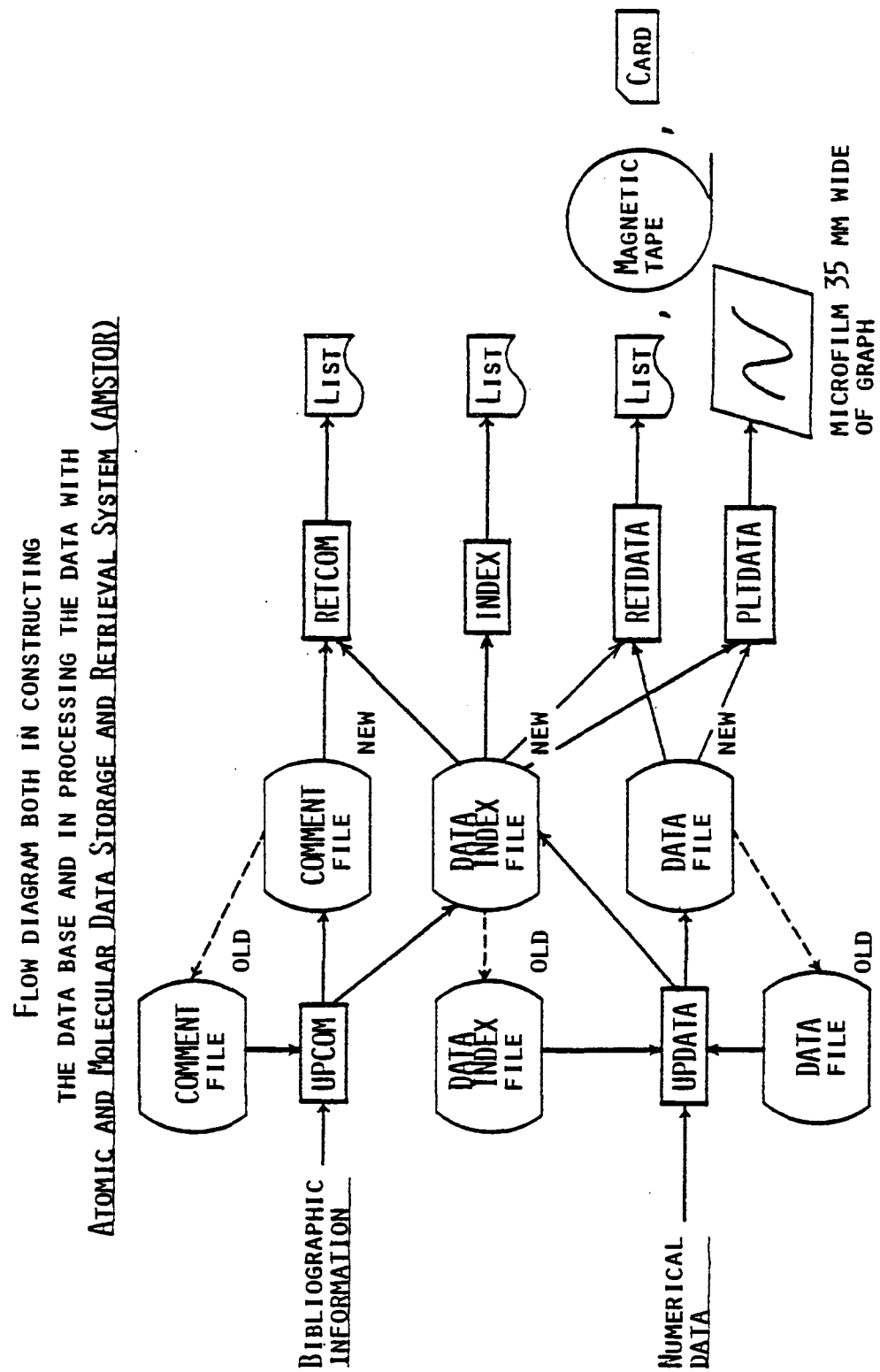
(d) Diameter dependence

(e) Size distribution

(f) Dose-rate dependence

(g) Incident angle dependence

1.3 A & M Data Storage and Retrieval System (AMSTOR) Program



Flow diagram both in constructing the data base and in processing the data with Atomic and Molecular Data Storage and Retrieval System (AMSTOR)

2. Studies on Atomic Collisions in Gases

2.1 Measurements of Total Charge Transfer Cross Sections[4]

(1) Ne^+, Ne^{++} + He, Ne, Ar — 0.4 ~ 0.9 MeV; 0.8 ~ 3.0 MeV

Measured cross section:

for Ne^+ incidence — σ_{10}, σ_{12}, σ_{13}

Ne^{++} — σ_{21}, σ_{20}, σ_{23}

(2) Ne^+ + CO, CO_2, CH_4, O_2 — 0.4 ~ 0.9 MeV

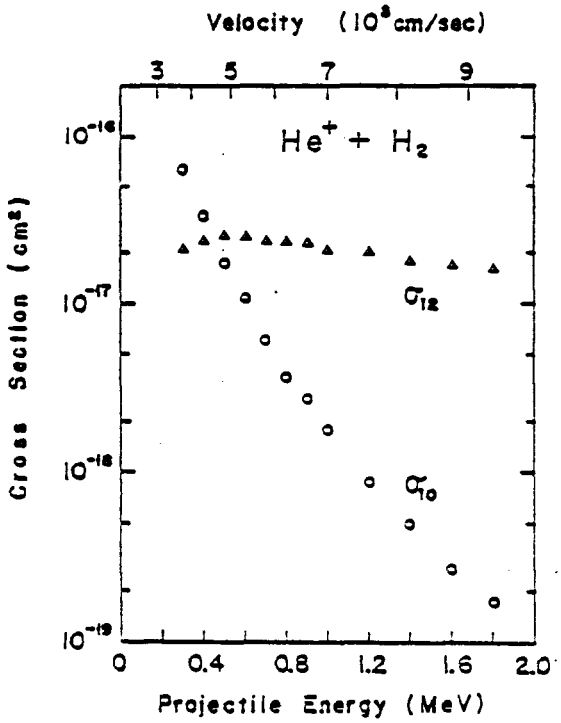
Measured cross section: σ_{10}, σ_{12}, σ_{13}

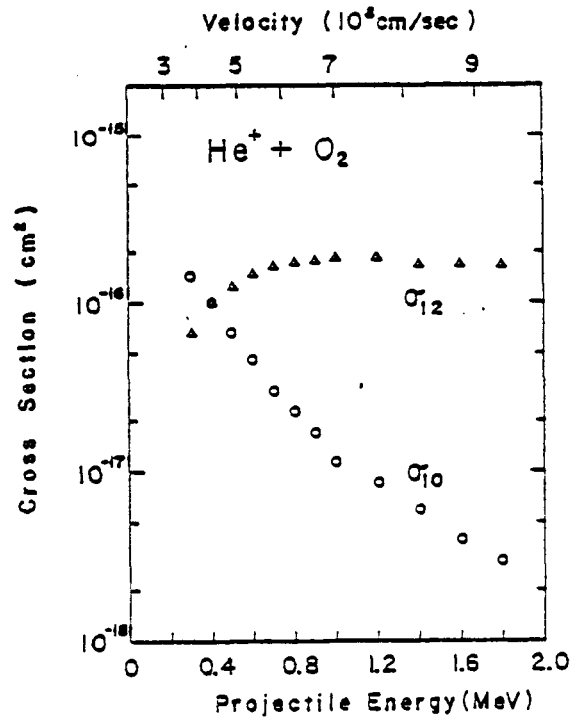
(3) He^+ + H_2, O_2, CO, CO_2, CH_4 — 0.3 ~ 1.9 MeV

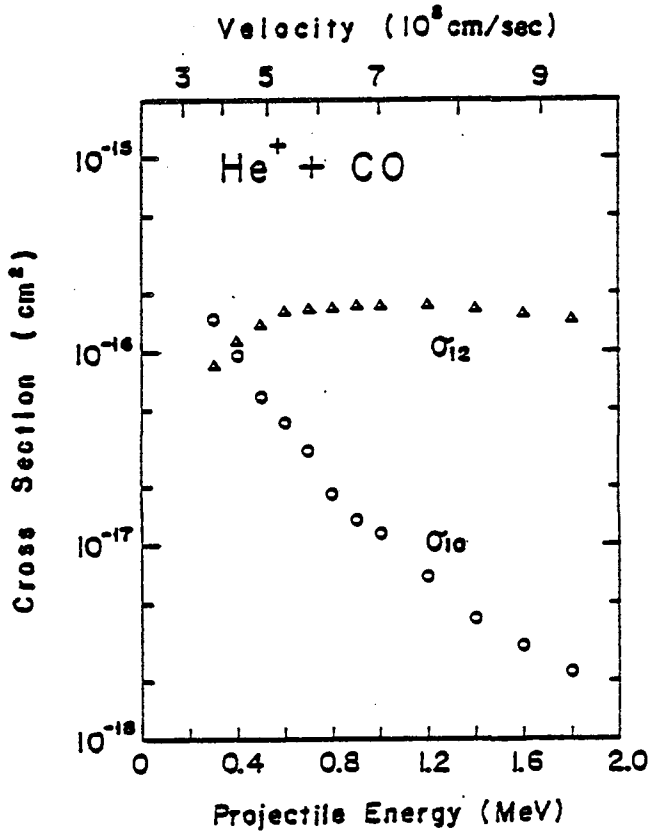
Measured cross section: σ_{10}, σ_{12}

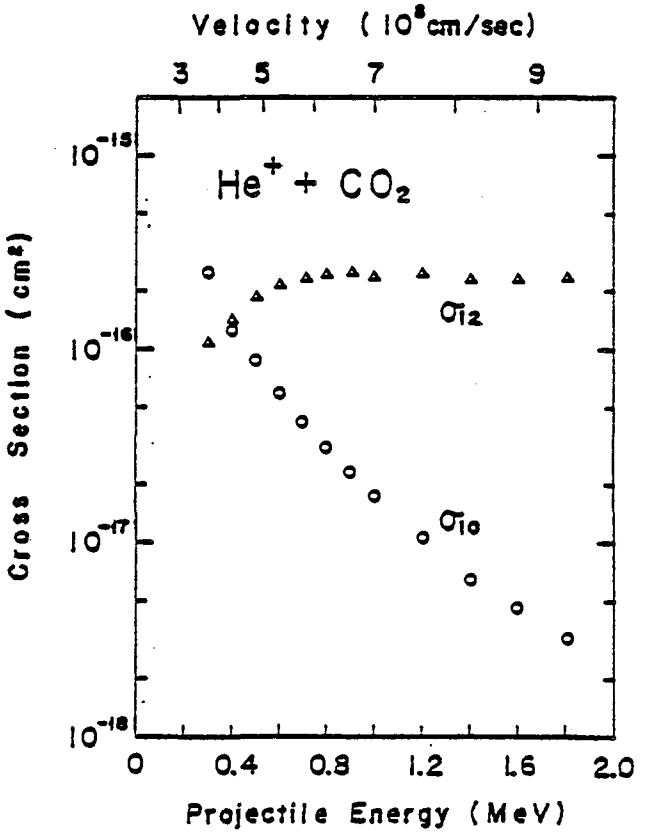
(4) He + H_2, O_2, CO, CO_2, CH_4 — 0.3 ~ 1.9 MeV

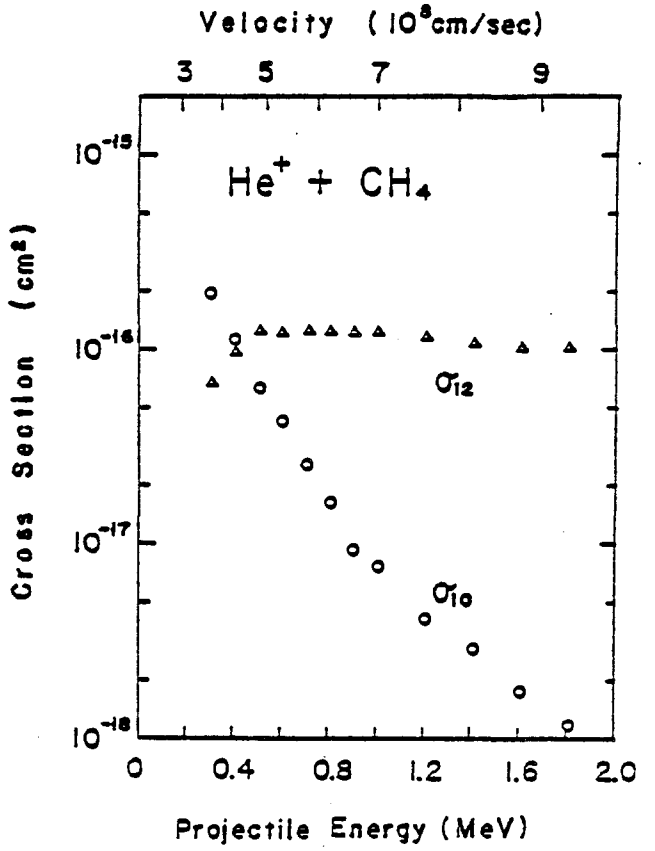
Measured cross section: σ_{01}, σ_{02}

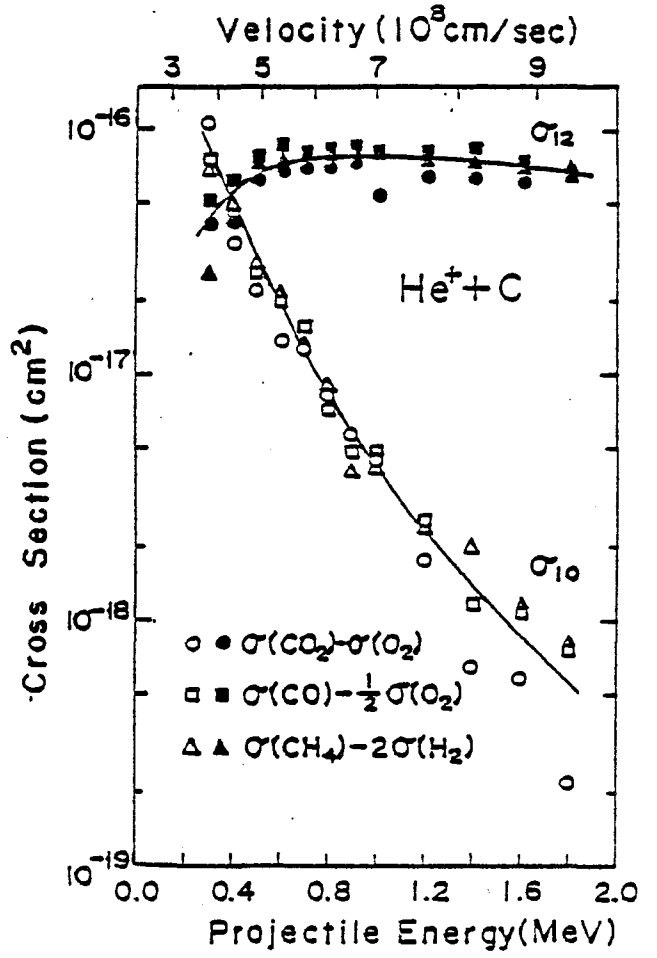





Velocity (10^8cm/sec)
3 5 7 9
$He^+ + CO$
σ_{12}
σ_{10}
Cross Section (cm^2)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
0 0.4 0.8 1.2 1.6 2.0
Projectile Energy (MeV)


Velocity (10^8cm/sec)
3 5 7 9
$He^+ + CO_2$
σ_{12}
σ_{10}
Cross Section (cm^2)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
0 0.4 0.8 1.2 1.6 2.0
Projectile Energy (MeV)

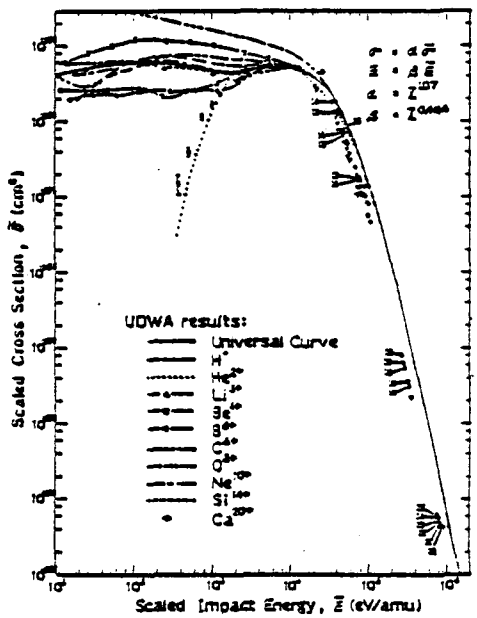

Velocity (10^8cm/sec)
3 5 7 9
$He^+ + CH_4$
σ_{12}
σ_{10}
Cross Section (cm^2)
10^{-15}
10^{-16}
10^{-17}
10^{-18}
0 0.4 0.8 1.2 1.6 2.0
Projectile Energy (MeV)


Velocity (10^8cm/sec)
3 5 7 9
$He^+ + C$
σ_{12}
σ_{10}
$\circ \bullet \sigma(CO_2)-\sigma(O_2)$
$\square \blacksquare \sigma(CO)-\frac{1}{2}\sigma(O_2)$
$\triangle \blacktriangle \sigma(CH_4)-2\sigma(H_2)$
Cross Section (cm^2)
10^{-16}
10^{-17}
10^{-18}
10^{-19}
0.0 0.4 0.8 1.2 1.6 2.0
Projectile Energy(MeV)

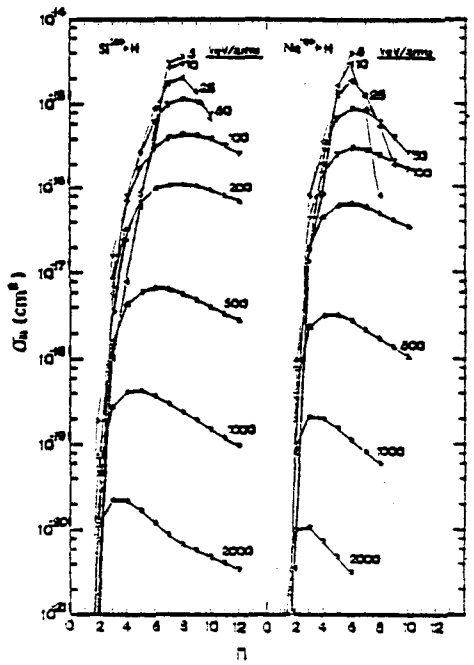
2.2 Total and Partial Cross Sections for Charge Transfer of Fully Stripped Ions in H^5 :

$$A^{Z+} + H(1s) \longrightarrow A^{(Z-1)+} + H^+, \quad \text{where } Z = 1 \sim 14.$$

A. Scaled total cross sections

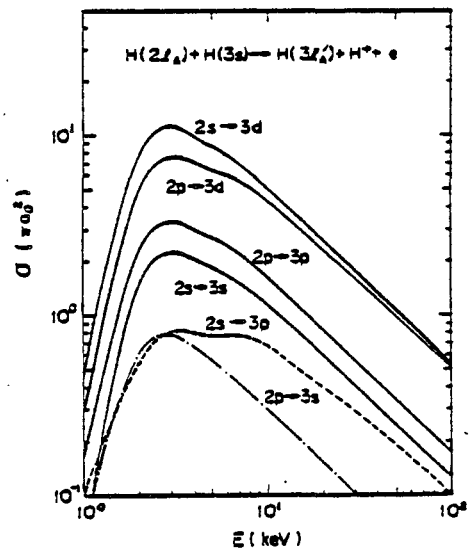


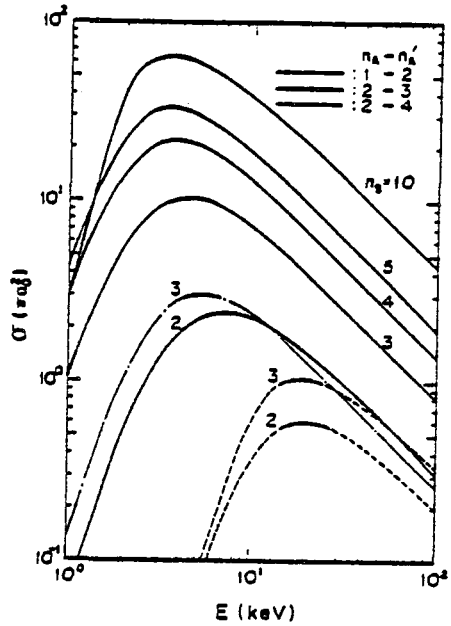
B. Dependence of the partial cross sections on the principal quantum number

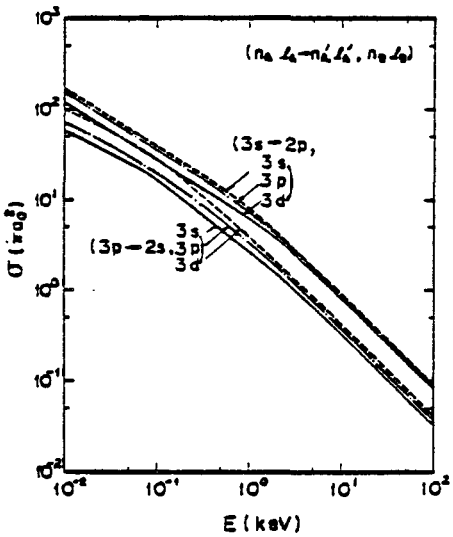


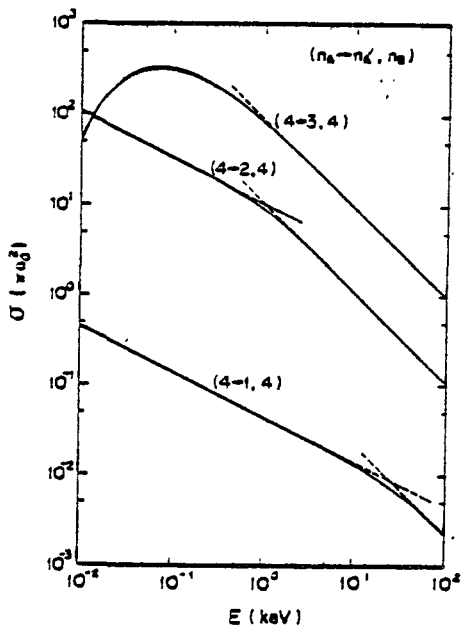
2.3 Energy dependence of the cross sections for ionization collisions between two excited hydrogen atoms:

$$H_A(N_A\ell_A) + H_B(N_B\ell_B) \rightarrow H_A(N'_A\ell'_A) + H_B^+ + E \quad N_A \leq N_B.$$





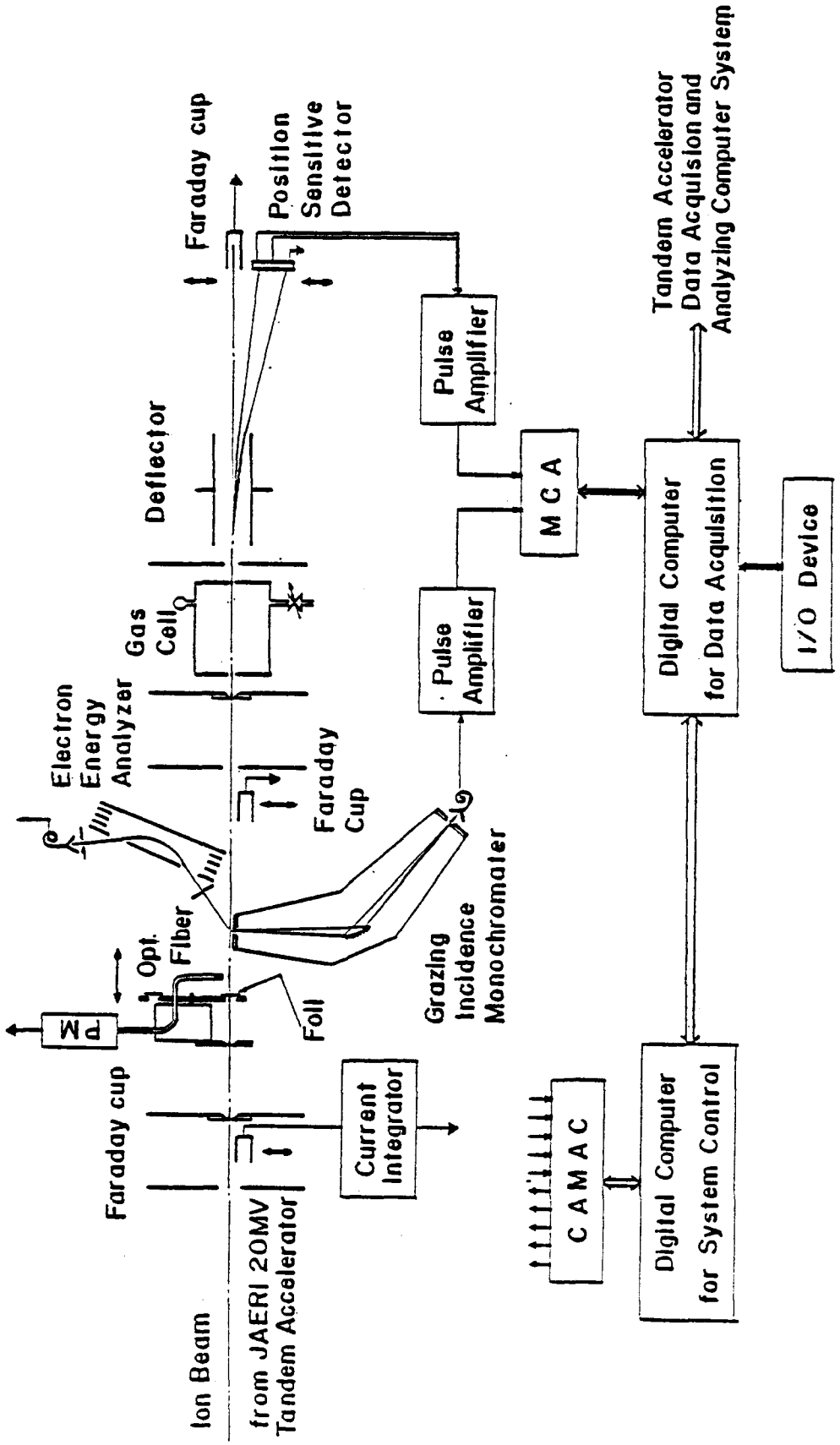




For the general ionization collisions in the contributed paper, it is shown in ref. 6 that the cross sections can easily be estimated by using the quantities calculated in the case of the collisions between two excited hydrogen atoms.

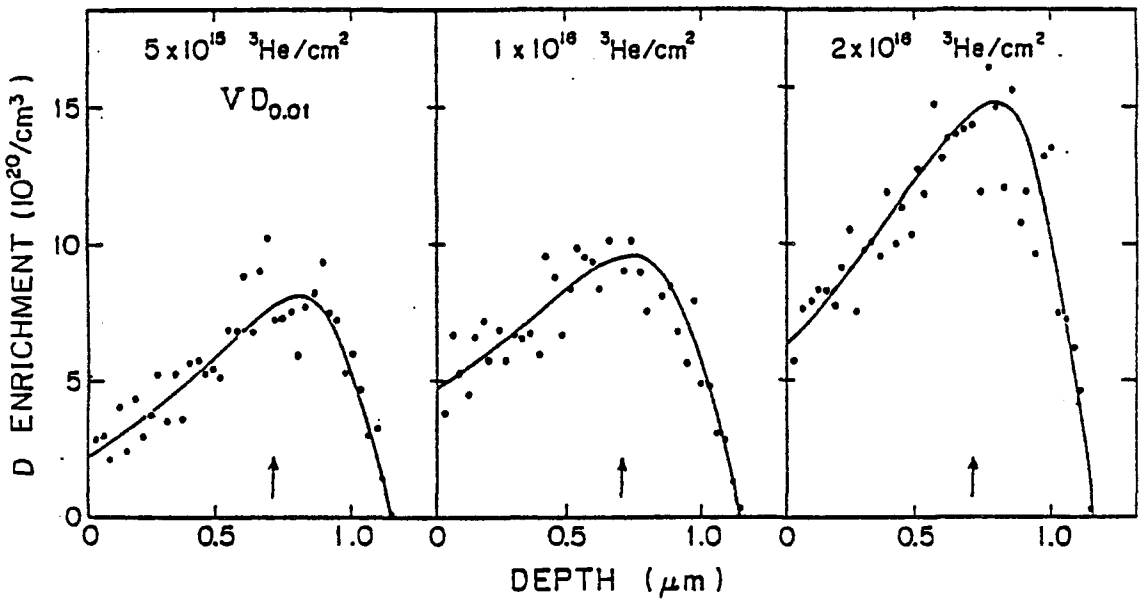
3. Studies on Heavy Ion Collisions

Schematic diagram of apparatus for beam foil and charge transfer experiments



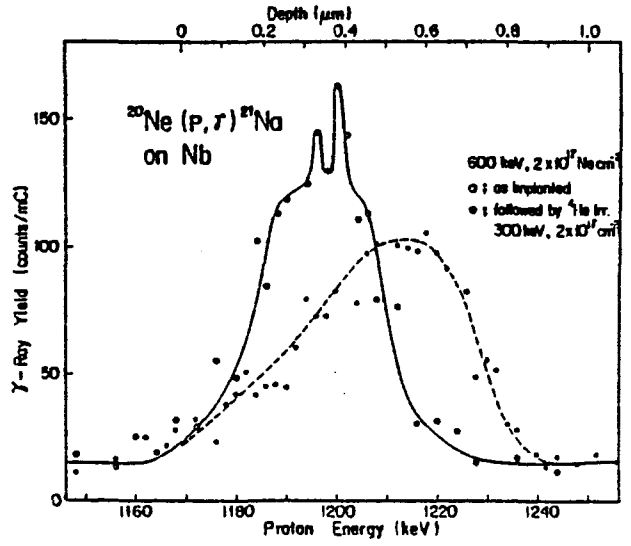
4. Studies on Atomic Collision in Solids[7,8]

(1) Deutron enrichment during ion bombardment in VD alloys



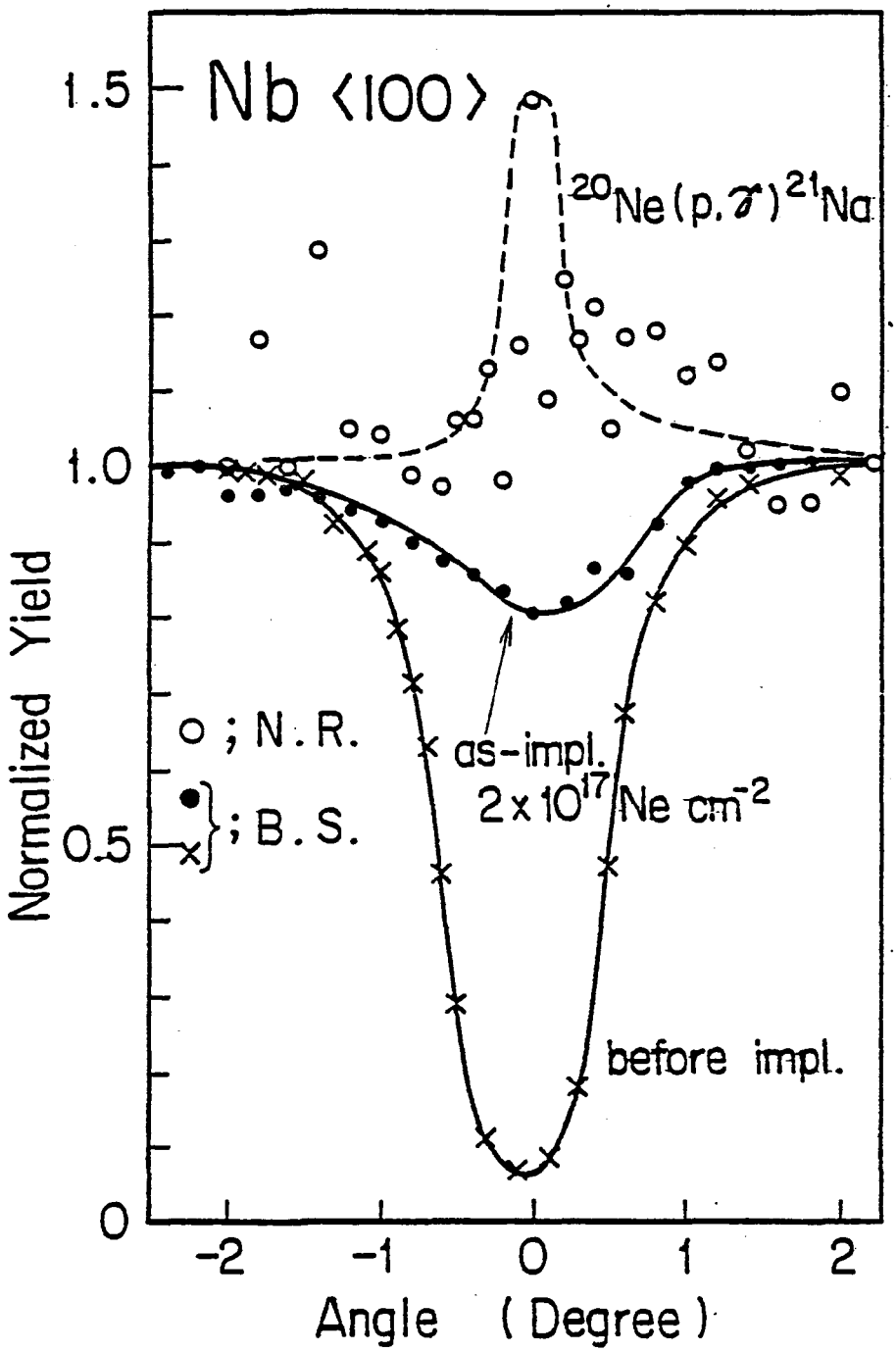
(2) Depth-profiling and location of Ne atoms implanted onto Nb

A. Depth-profiling of Ne atoms using $^{20}Ne(p,\gamma)^{21}Na$ resonant nuclear reaction



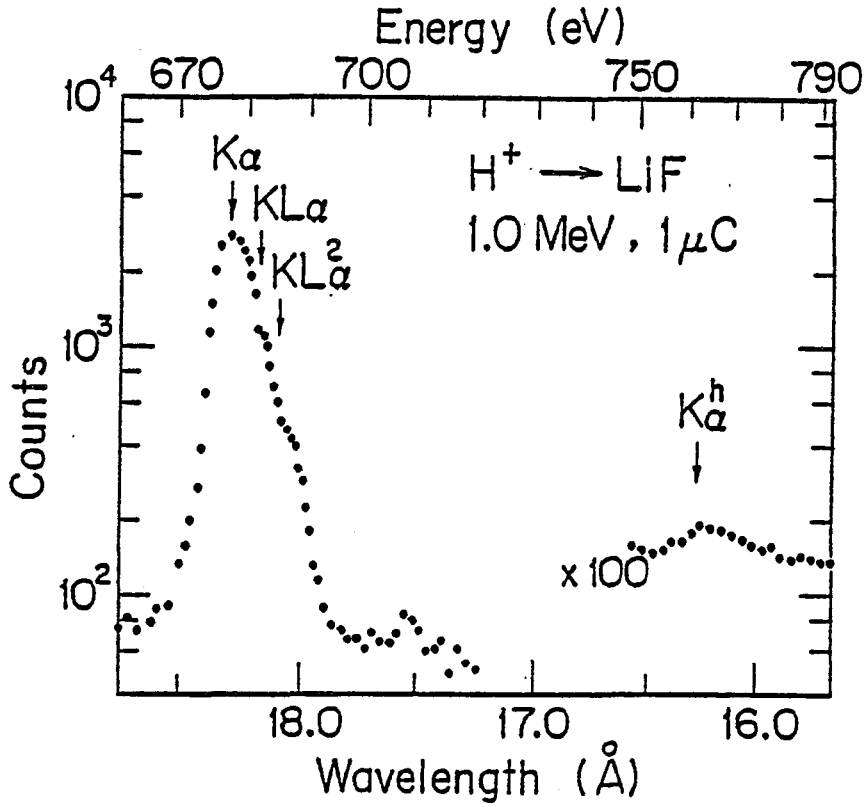
* DASHED LINE SHOWS THE EFFECT OF POST IRRADIATION BY He

B. LOCATION OF Ne ATOMS USING CHANNELING EXPERIMENT

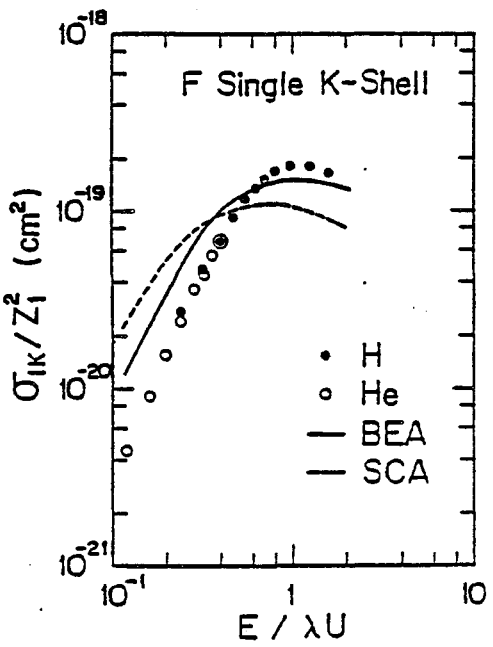


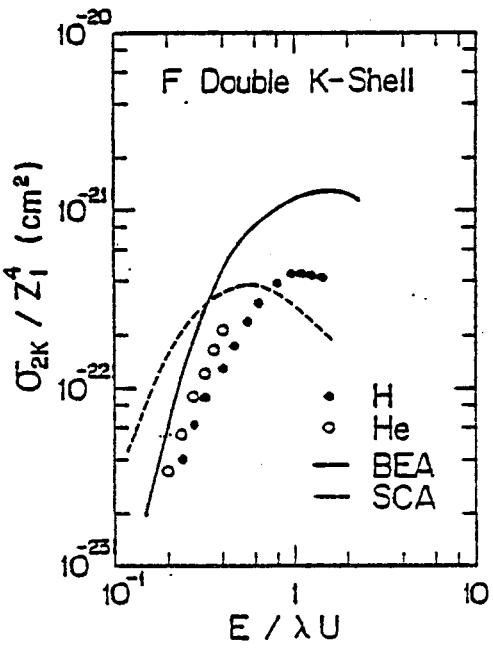
5. Studies on Inner-Shell Excitation[9-11]

A. Fluorine K-Xray spectra from bombardment of LiF with H^+ using crystal monochrometer



B. Single K(σ_{1K}) - and double K(σ_{2K}) - shell ionization cross sections



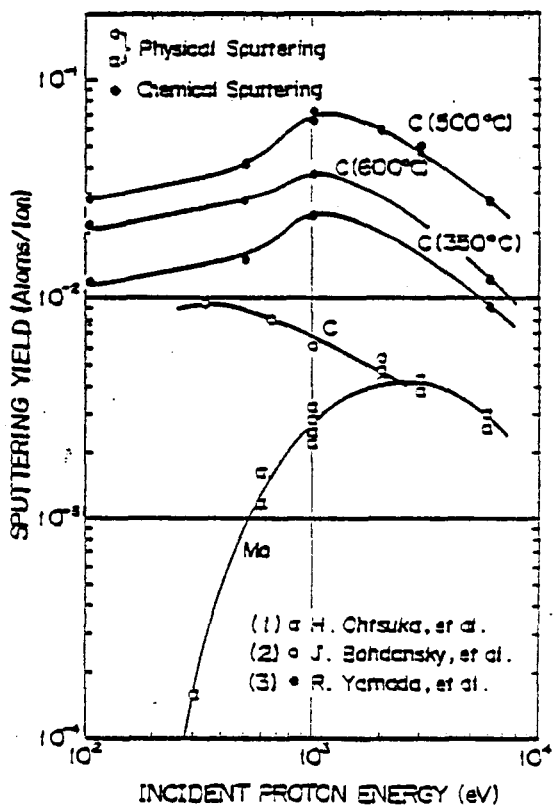


6. Studies on Plasma-Material Interaction

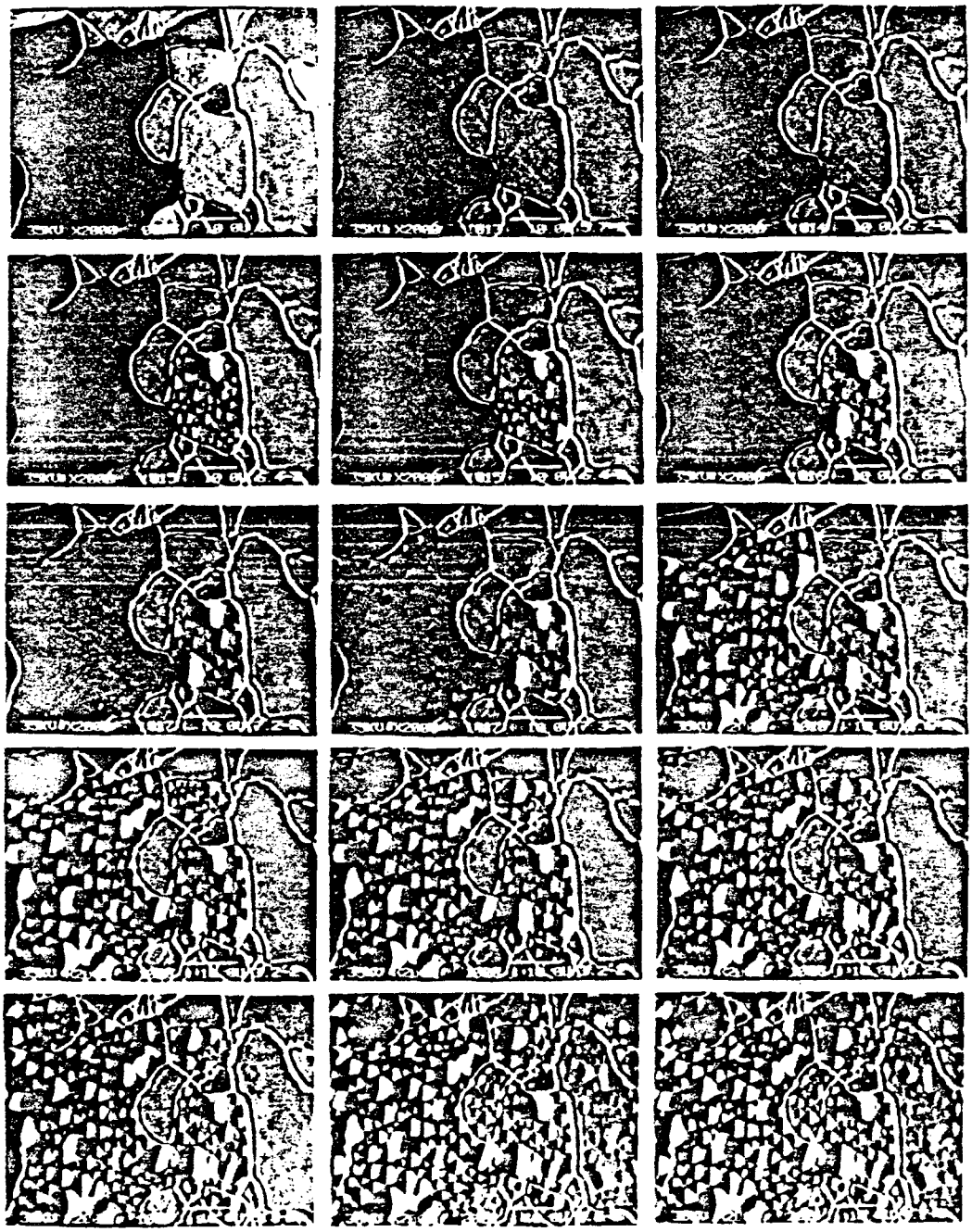
(1) List of experiments on sputtering in JAERI

Target Material	Incident Particle	Angle of Incidence	Energy (keV)	Dose and Dose Rate* (cm^{-2} and $cm^{-2} \cdot s^{-1}$*)	Temperature (°C)	Notes
Mo (Polycrystalline)	H^+	Normal	0.1 - 6		RT	Energy dependence
	Ne^+	Normal	2	1.5×10^{19}	RT	Dose effect
		Normal, 45°	0.6, 1.5	2×10^{19}	RT	Angular distribution of sputtered atoms
	Ar^+	~Normal	~1		RT	Honeycomb structure
	Ar^+, O^+	45	0.5 - 5	$2\text{-}6 \times 10^{15}$*	RT - 1500	Secondary ion emission
C (Pyrolytic, isotropic, glassy, and vacuum deposited)	H^+	Normal	0.1 - 6	$3\text{-}7 \times 10^{14}$*	RT - 650	Chemical sputtering (Energy and temperature dependence)
	H^0	Random	Thermal	$10^{13} - 10^{14}$*	RT - 900	Surface conditioning
SiC (Ion-plated)	H^+	Normal	1.5	2×10^{20}, 2.5×10^{15}*	500	Total erosion, Chemical composition dependence

(2) Sputtering yield of molybdenum and pyrolytic graphite by proton



(3) "IN SITU" SEM OBSERVATION ON Mo SURFACE WITH 100 KeV He^+ BOMBARDMENT



References

1 Y. Nakai, M. Sataka, and T. Shirai, JAERI-M 8849 (1980).

2 K. Kamada and M. Saidoh, JAERI-memo 8794 (1980) (unpublished).

3 T. Shirai, Y. Kazumata, T. Aruga, and H. Ryufuku, JAERI-memo 8789 (1980) (unpublished).

4 Y. Nakai, M. Kase, K. Ozawa, T. Shirai, and A. Kikuchi, Abstracts of the 6th ICRR, 86 (1979).

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JILA ATOMIC COLLISIONS INFORMATION CENTER

May 15, 1980

The general objective of the JILA Information Center is the review and evaluation of selected atomic collisions data. The central part of the data of concern is low energy collision of electrons and photons with atoms and simple molecules. Other data concern collisions of excited atoms or molecules with other atoms or molecules with a transfer of internal energy. The scope of data includes low energy electron swarm data.

The published literature is regularly reviewed to identify the selected data and an index prepared. Bibliographies indexed according to data characteristics are published as special reports. Current titles are:

Kieffer, Lee J., Bibliography of Low Energy Electron and Photon Cross Section Data (through December 1974), Nat. Bur. Stand. (U.S.), Spec. Publ. 426, 219 pages (March 1976).

Gallagher, J. W., Rumble, Jr., J. R., Beaty, E. C., Bibliography of Low Energy Electron and Photon Cross Section Data (January 1975 through December 1977), Nat. Bur. Stand. (U.S.), Spec. Publ. 426, Suppl. 1, 115 pages (June 1979).

Gallagher, J. W., Beaty, E. C., Bibliography of Low Energy Electron and Photon Cross Section Data (1978), JILA Information Center Report 18, 142 pages (January 1980).

Beaty, E. C., Dutton, J., Pitchford, L. C., A Bibliography of Electron Swarm Data, JILA Information Center Report 20, 240 pages (December 1979).

Eberly, J. H., Gallagher, J. W., Beaty, E. C., Multiphoton Bibliography 1977, University of Colorado, University of Rochester, Nat. Bur. Stand. (U.S.), Publ. LP-92, 60 pages (April 1979).

Eberly, J. H., Gallagher, J. W., Beaty, E. C., Multiphoton Bibliography 1978, University of Colorado, University of Rochester, Nat. Bur. Stand. (U.S.), Publ. LP-92, Suppl. 1, 60 pages (August 1979).

Gallagher, J. W., Energy Transfer Collisions of Atoms and Molecules, JILA Information Center Newsletter, published quarterly.

Numerical data is compiled on an irregular basis. Generally this effort is in support of a specialized review program. An effort is made to insure that the data recorded is an accurate representation of the data in the original publication. Original units are preserved. This data bank is not yet complete enough nor error-free enough for general release.

Activities concerning data reviews have been at a low ebb for the past several years. A more intense level of effort is underway. Data fields currently under review include: excitation of ions, excitation of alkali atoms, elastic scattering by atoms, and vibrational excitation. As these projects are completed, the results will be published as an appropriate article. Also, we expect to have reviewed and corrected the computer data bank and will release it to anyone who is interested. A general objective of each of these reviews is to generate a set of "recommended" data.

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Translated from Russian

I.V. Kurchatov Institute of Atomic Energy

THE WORK OF THE ATOMIC AND MOLECULAR (A + M) DATA CENTRE AT THE KURCHATOV INSTITUTE

V.A. Abramov and Yu.V. Martynenko

Moscow 1980

As already announced at a meeting of representatives of centres for the collection of atomic and molecular (A + M) data for nuclear fusion, the Kurchatov Institute is carrying out work on the collection of such data for the purpose stated.

At present, the staff of the Centre consists of one specialist working full time and three working part time. The technical operations are carried out by the central services of the Institute. In addition, for writing reviews containing data evaluation, highly qualified experts on the subject covered by the review in question are employed.

At present, work is going on continuously on the collection of bibliographical data for the quarterly publication "International Bulletin on Atomic and Molecular Data for Fusion", issued by the IAEA's Nuclear Data Section (Editor Dr. K. Katsonis). The bibliographic data are collected from Soviet publications including preprints and the proceedings of All-Union conferences and seminars. The bibliographical material thus collected is communicated to the IAEA's Nuclear Data Section each quarter. Certain reports by Soviet authors containing specific data for publication in the "Numerical Data" section of the Bulletin are also provided. It should be observed that this work on the collection of A + M data has been very much appreciated by the IAEA's Nuclear Data Section.

Work is continuing on the collection of numerical A + M data. Owing to the fairly large volume of information now available on various subjects, particular attention is at present being paid to the evaluation of substantive data by highly qualified experts. Recently preprints have been issued on the subject of charge exchange of hydrogen atoms on impurities - V.A. Abramov, F.F. Baryshnikov and V.C. Lisits: "Charge exchange of hydrogen atoms on multiply-charged impurity ions in a hot plasma" (preprint IAE-3121) - and of excitation (ionization) of multiply-charged ions by electrons - V.A. Bazylev and M.N. Chibisov: "The excitation and ionization of multiply-charged ions by electrons. General theory. Hydrogen-like ions" (preprint IAE-3125); also V.A. Bazylev and M.N. Chibisov: "Excitation and ionization of multiply-charged ions by electrons. Helium-like and more complex ions" (preprint IAE-3152). Of great value and interest is the material included in preprint IAE-3147 by V.S. Marchenko and S.I. Yakovlenko: "Problems of impurity ion diagnostics in thermonuclear facilities. Theoretical questions of passive diagnostics". It is planned to prepare similar reviews on other subjects.

Until recently the information collected was stored in the form of a data library. Work is at present in progress on transferring the material to machine use in FORTRAN. For information storage and search use is made of an EC-1040 computer. Since the supplementing of data is a continuous process, we believe that primary importance attaches to the development of a unified and convenient international recording format and a system permitting sufficiently rapid retrieval of the data required.

The data bank collected by the Centre enables us as far as possible to meet the demands of staff in various sections of the Plasma Physics Division at the Kurchatov Institute researching on nuclear fusion.

We greatly value international co-operation on the collection of A + M data and the issue of the international quarterly Bulletin; we believe that only on the basis of international co-operation is it possible to establish complete banks of data capable of meeting our requirements and purposes.

ASSESSED NUMERICAL DATA ON ATOMIC AND MOLECULAR COLLISIONS

J.G. Hughes and F.J. Smith

The Queen's University of Belfast

Background

The School of Physics and Mathematical Sciences at Queen's University, Belfast, is collecting atomic and molecular numerical data relevant to fusion in three different areas:

1. Interatomic Potentials and Elastic Collisions
2. Electron Excitation
3. Assessed Electron Ionization and Charge Transfer Data.

Work on the first area, Interatomic Potentials and Elastic Collisions, was reported at the Culham Conference in 1977.

The second collection, electron excitation data, is being collected under the supervision of Dr A.E. Kingston and Dr K.A. Berrington at Queen's University with the co-operation of the Daresbury Laboratory. Much of this data is obtained directly from large computer codes.

This report is mainly concerned with the third area: the collection of assessed numerical data on atomic and molecular collisions, initially electron ionization and charge transfer.

Aim

The aim is (i) to determine for which atomic collision processes, data is most needed for fusion, (ii) to evaluate the numerical data; (some of which has already been extracted from the literature elsewhere), (iii) to produce recommended "best" data (sometimes outside the range of the original data), (iv) to estimate its reliability, and (v) to produce it in the form needed by the user scientist. All of these steps will be taken only on the advice of consultants who are experts on fusion or on a particular collision process. The work is supported by The United Kingdom Atomic Energy Authority through the Culham Laboratory.

We will rely mainly on the IAEA CIAMDA index and on the IAEA Bulletin on Atomic and Molecular Data Relevant to Fusion for references and, where possible, we hope to receive raw data from other data centres when it has already been collected. Our aim, of what we hope will become a co-operative project, is to produce data of high quality and highest possible reliability rather than quantity.

First Data

On the advice of Culham the first sets of numerical data we are studying are on electron ionization of the light atoms and ions. Later, subject to the advice of our consultants, we intend to extend the data to charge transfer cross sections and rate coefficients of relevant atoms and ions.

Because electron impact ionization of C and O^{++} are both important to Fusion research we have started our collection of ionization data with these two. They are part of the same isoelectronic sequence with N^{+}. We have therefore looked for data for all three in this sequence and using both experimental and theoretical results and the scaling laws for ionization of ions in such a sequence we hope to obtain a better assessment of their accuracy and thus produce more reliable "best" recommended data for all three. At high energies, outside the range of current data, extrapolation has used the Bethe approximation:

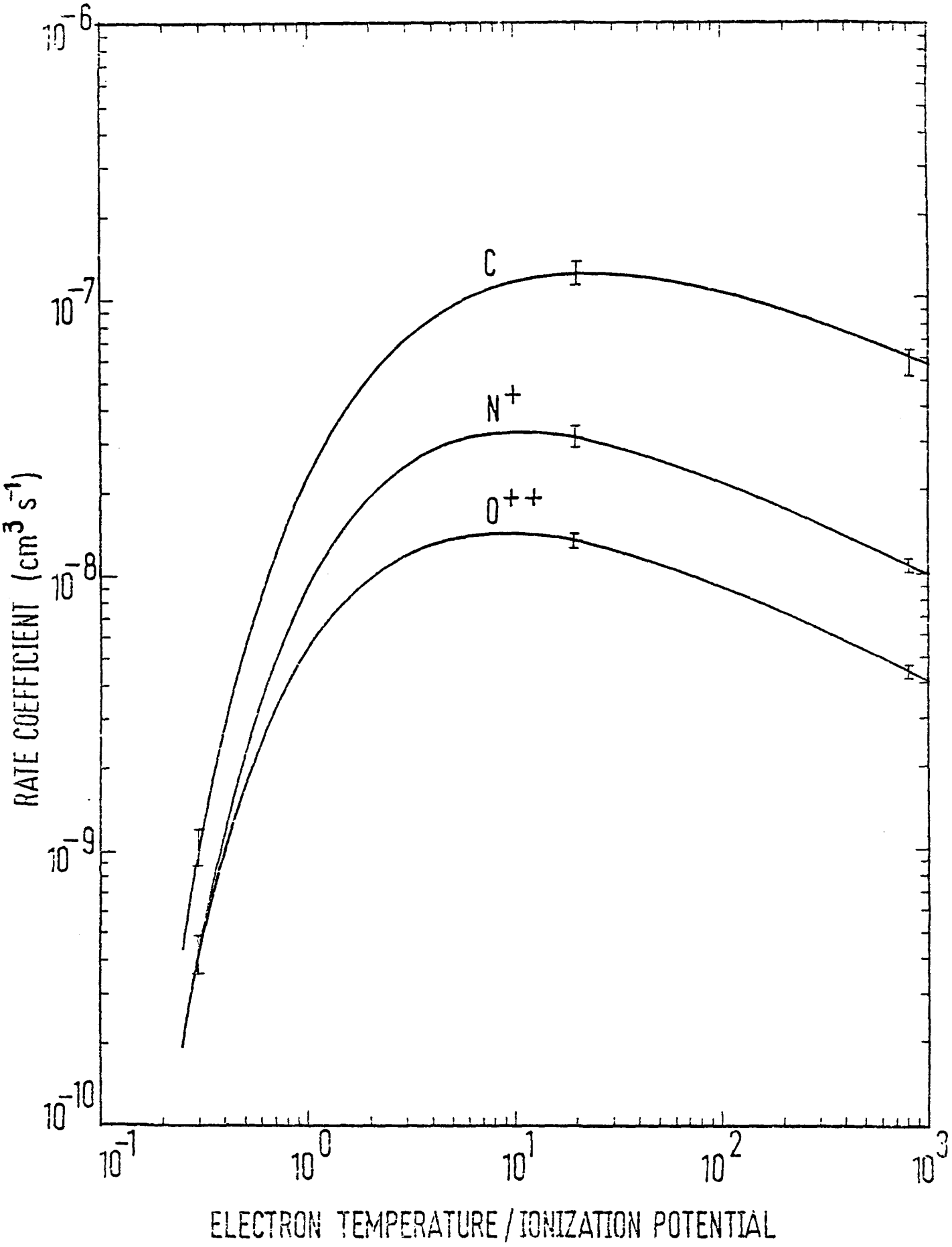
$$Q = A \frac{\ln E}{E} + \frac{B}{E}$$

and Bethe's relation of the constant A with the Photoionization cross section has been checked in the case of carbon.

Recommended cross sections for this Carbon sequence and also for the Boron, Nitrogen and Oxygen sequences are already available on request.

Because Fusion scientists need rate coefficients rather than cross sections we have therefore computed the rate coefficients over a wide temperature range, as in the following figure. Data for C, N^{+} and O^{++} are shown with estimated error bars.

Finally, we have generated a FORTRAN subroutine which the Fusion physicist may use to obtain the rate coefficient at any temperature. Thus we will present our "best" recommended data in three forms: (1) tables of values, (2) graphs, and (3) subroutines.


ELECTRON IONIZATION OF C-LIKE IONS
RATE COEFFICIENT (cm^3 s^{-1})
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
C
N^+
O^{++}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
ELECTRON TEMPERATURE / IONIZATION POTENTIAL

ACTIVITIES OF THE CONTROLLED FUSION ATOMIC DATA CENTER (CFADC) AT OAK RIDGE NATIONAL LABORATORY

The activities of the data center include categorizing of bibliography of atomic collisions (including collisions with photons) and of particle collisions with surfaces from a total of about 140 journals and the compilation and evaluation of cross sections and rates for these collision processes.

The bibliography for atomic collisions is comprehensive in that all reactants (except molecules of more than 4 atoms), all processes, and all energies are categorized into 8 major categories and 114 minor categories. The collected bibliography for collisions of particles on surface are an integrated part of this categorization of atomic collisions but in the case of surfaces we categorize only those papers believed to be of fusion interest and which provide quantitative data on surface changes resulting from particle impact. This bibliography has been collected back to 1950 but has not been generally published. We have published the bibliographic compilations in 4 specific categories of fusion interest and in 1978 for the whole bibliography. We hope to publish the whole bibliography each year from now on (1979 is ready to print) and believe it will be primarily of use to atomic and molecular physicists. It is available from the National Technical Information Services (NTIS), 5285 Port Royal Road, Springfield, Virginia, 22161, USA., Document # DOE/ER-0044 at $13.25.

The data center has published several compilations of "evaluated" numerical data most recently in a two volume set. This set was published in 1977 and an updated compilation on surfaces data was printed in 1979. Currently we are planning a third volume on cross sections and rates for impurity ions and have begun this work but have encountered some delays and difficulties for example in determining how to "evaluate" theoretical results when there are

no experimental data. We may collaborate with other data centers in some future compilation-evaluation activities and in this connection we will participate in a workshop involving U. S. and Japanese data centers in October 1980 which will define specific collaborative activities.

For the immediate future, we expect to continue to publish the newsletter "Atomic Data for Fusion" in collaboration with the National Bureau of Standards Atomic Structure Data Center (W. Wiese). This newsletter will contain bibliographic listing of recent papers of direct interest to fusion in areas of atomic structure, atomic collisions, collisions of atomic particles with surfaces, and uses of atomic data in plasma diagnostics. In addition the newsletter contains a section for new (unpublished) numerical data and formulas. This section is intended to deliver particularly useful results to the fusion community before, but not in place of, standard journal publication.

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APPENDIX VII

DATA BASE SURVEY

TABLE I. Scientific Areas Covered in Various Data Centres
Preliminary Result of the Data Base Survey Prepared by Dr. J. Rumble Jr.

	Collisions			Spectra		
Definition	Electron	Photons	Heavy Particles	Trans. Prob.	Line Broad.	Other
JPN/PPN	Excit. Ion. Positive Ions		Charge Exchange			Sputtering of Elements
US/JILA	Ion. Excit., Elastic Total, Dissociation					Electron Transport Properties
UK/QUB	Ion & Excit. Light Atoms & Ions		(Charge Transfer) Elastic Scattering			Interatomic Potentials
US/ORNL	Elastic, Total, Excit. Ion., Diss. Attach Recom.	Absorp., Ion. Diss. Detach.	Elastic, Excitation, Dissociat., Electron capture, Ionizat. Stopping x-sec, Interchange			Sputtering, Second. Elect. Emission, Reflection Trapping, Electron Ion Transfer
UK/DARESB	Excit. Ioniz. Atoms & Ions	Ionization				
UK/CULHAM	Ion & Excit. Rate of Li, Be LiBe Ions					
US/PRINC	Ions, Recomb., Excit. Multiply charged Ions Rad. Cooling Rates					
US/LLL		Photo Electron & Fluorescence x-sec				
US/LASL	Excit.			Oscillator Strength		Structure Levels
JPN/JAERI			Charge Transfer, Ion with He, Ne			(Surface) (Structure)
USSR/IAE	Excitation-Ionization		Charge Transfer		Line Broad.	Surface
US/NBS-AT					Transition Probabilities & Lifetimes	
US/NBS-AT					Line Shapes & Shifts	

Table II. General Information

	JPN/PPN	US/JILA	UK/QUB	US/ORNL	UKDARESBUK	CULHAM	USPRINC	US/LLL	US/LASL	JPNJAERI	USSRIAE	USNBS-AT	USNBS-AT
Compilation													
Data Selected from													
Journals	x	x	x	x		x	x			x	x	x	x
Reports	x	x		x		x	x			x	x	x	x
Thesis		x				x				x	x	x	x
Unpublished work	x	x			x	x	x		x	x		x	x
Other Data Centers			x		x	x	x				x		
Other					x	x					x	x	
Translation of Graphical Information to Numbers	(Hand)	Machine	Hand Machine		Hand Machine		Hand			Author G. Tab		Read Curve	Read Curve
Storage Information													
How are Data Stored?	Computer	Mini Computer	Computer		Paper Computer	Computer	Paper	Computer Output		Computer	Computer	Paper	Paper
Computers used, if any	FACOM M-200	Iex4051 CDC6600	ICL1904A 1906S IBM 370/ 168		PDP 10 IBM360	IBM 370/165		PDP 10 CDC 7600 CRAY-1		FACOM 230-75 M-200	EC 1040		
Computer Language(s) used													
Fortran		x	x	x	x		x			x	x		
Cobol													
PL/I											x		
Assembler Basic (Pascal)											x		
What Bibliographic and Descriptive Information are Stored													
Author	x	x	x	x	x	x				x	x	x	x
Article Title	x		x	x	x	x				x	x	x	x
Citation (Journal, etc.)	x	x	x	x	x	x				x	x	x	x

Table II (continued)

	JPN/PPN	US/JILA	UK/QUB	US/ORNL	UKDARESBU	KCULHAM	USPRINC	US/LLL	US/LASL	JPNJAERI	USSRIAE	USNBS-A	TUSNBS-AT
Figure Number		x				x							
Curve Number		x				x							
Caption						x				x			
Process/Property	x	x	x	x	x	x				x	x		
Reactants	x	x	x	x	x	x				x	x	x	
State of Reactants	x	x	x		x	x				x	x	x	
Method	x	x	x		x	x				x	x	x	
Key Words						x				x			
ID Number	x	x	x		x	x				x		x	
Error Limits	x		x		x	x							
Evaluation			x	x	x	x							
For which of the following may the Data Base be searched?													
Author	x	x	x	x						x	x		
Citation (Journal, etc.)	x	x	x	x						x	x		
Process/Property	x	x	x	x	x					x	x		
Reactants	x	x	x	x	x					x	x		
State of Reactants	x	x	x							x	x		
Method	x	x	x							x	x		
Other Key Words										x			
Are Consistent Units used? If so, what are they?	Yes cm2 ev	No Original	a.u.	cm2 ev	a.u.	Yes Mixed	Yes cgs			No	No	Yes Mixed	A
Are Original Significant figures maintained and how?	No	Yes	No	No	Yes Generated	Yes					No	No	No
Size of the Data Base? (How many Individual Tables or Graphs?)	500	4500	3000	(1500+)	10 files 1.2 M words each	Small	47 Elements			CT 200 Ion 200	1000	4300	2300 Article
How up to date is the Data Base?				1 Year									
How far back does the Data Base cover?	1960	1974	1940	1950	1978		1977			1960-1979	1975-1980	1914-1980	1959-1980

Table II (continued)

	JPN/PPN	US/JILA	UK/QUB	US/ORNL	UKDARESBUK	CULHAM	USPRINC	US/LLL	US/LASL	JPNJAERI	USSRIAE	USNBS-AT	USNBS-AT
Evaluation													
Is any evaluation of individual Data records done? By whom?	No	No	Outside	Outside	Author	Author	Yes	Outside Yes		Later	No		Yes in & out
Are separate files of "Evaluated" Data maintained?	No	No	Yes	Yes	Yes	No	No	Only	No	Not Now	No		No
Are copies of the Data sources (Articles, etc.) kept?	No	Yes	Yes	Yes	No	Yes	Yes	No	No	Yes	No		Yes
Has the Data Base been used as a resource for critical reviews and/or published Data compilations?	No	Yes	No	Yes	Soon	No	Yes	Yes	No	No	Yes		Yes
Dissemination of Data													
Data Distributed by													
Books				x				x				x	
Mongraphs	x	x	(x)							x	x	x	x
Reprints	x		(x)		x		x		x		x		
Computer Tapes	x	x		(x)	x		x	x			x		
Computer Cards					x						x	x	x
Photocopies					x	x		x				Handbook	
Other		Reviews			x								
Form of Data Distribution													
Tables	x	x	x	x	x	x	x	x	x	x	x	x	x
Graphs	x	x	x	x	x	x	x	x		x		x	x
Others			Sub-Routine				Formula			Micro Film		Formulas	
Do you have an external format?	No	Yes	No		Yes			Yes		No	Yes	No	No
Is the Data Base on-line? If so, do outside users access it?	Yes Yes	No	Yes No	No	Yes Yes		Yes Yes	Yes No	No	No	No	No	No
How frequent are individual Data requests?	-	10-20/ YR	-	25-40/ YR		Not in Data Bank Business	12/yr	2-3/yr		-	20/yr	150/yr	100/yr