

INTERNATIONAL NUCLEAR DATA COMMITTEE

First Meeting of the

Atomic and Molecular Data Centre Network

Vienna, 9-13 May 1977

SUMMARY REPORT

Edited by A. Lorenz and R.E. Seamon Nuclear Data Section International Atomic Energy Agency

August 1977

IAEA NUCLEAR DATA SECTION, KARNTNER RING 11, A-1010 VIENNA

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Edited by A. Lorenz and R.E. Seamon Nuclear Data Section International Atomic Energy Agency Kaerntnerring 11-13 P.O. Box 590 A-1011 Vienna, Austria

August 1977

Summary

The IAEA Nuclear Data Section convened the first meeting of the Atomic and Molecular (A+M) Data Centre Network at IAEA Headquarters in Vienna from 9 - 13 May 1977. The meeting was held on the recommendation of the IAEA Advisory Group Meeting on A+M Data for Fusion held at the Culham Laboratory in the UK in November 1976 and supported by the Joint IFRC/INDC (International Fusion Research Council/International Nuclear Data Committee) Subcommittee on A+M Data for Fusion. The meeting was attended by 18 participants representing ten existing or planned atomic and molecular data centres, two nuclear data centres, and three international organizations.

The general objective of the effort started at this meeting is the formation of an internationally coordinated network of centres and groups for the systematic world-wide compilation, evaluation, exchange and dissemination of bibliographic and numerical A+M data required by the fusion community.

The specific accomplishments of this meeting were the establishment of agreements for the cooperation between existing A+M data centres and groups and the IAEA Nuclear Data Section/A+M Data Unit with regard to the Quarterly Bulletin on Atomic and Molecular Data for Fusion, the Bibliographic Index to Atomic Collision Data, and the exchange of evaluated atomic collision data.

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 K. Katsonis and A. Lorenz
- Activities of the ZAED in the field of data information and documentation. G. Ebel
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- 12. Activities and Programme on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute. T. Fuketa
- Reviews of the Recent Activities on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute (JAERI). Y. Obata, Y. Nakai, T. Shirai, M. Kase
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List of Abbreviations

Atomic and Molecular A+M Centre de Compilation de Données Neutroniques of the CCDN Organization for Economic Cooperation and Development at Saclay, France. CINDA Computerized Index of Neutron Data, a specialized bibliography and data index on neutron nuclear data. FRG/ZAED Zentralstelle fuer Atomkernenergie-Dokumentation of the Federal Republic of Germany. FR/Orsay Laboratoire Physique des Plasmas of the University of Paris in Orsay. CAPHYOR GAz-PHYsique-ORsay, a computerized retrieval system on properties of atoms, molecules and gases. IAEA International Atomic Energy Agency IFRC International Fusion Research Council INDC International Nuclear Data Committee INIS International Nuclear Information System JAP/JAERI Japan Atomic Energy Research Institute JAP/Nagoya Institute of Plasma Physics, Nagoya, Japan NDS Nuclear Data Section of the International Atomic Energy Agency UK/Belfast 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 of the United States US/ORNL Oak Ridge National Laboratory of the United States

Summary of the Meeting

A. Introduction

The First Meeting of the Atomic and Molecular Data Centre Network was held in order to convene representatives of data centres and groups interested in participating in the coordinated international management of atomic and molecular data pertinent to fusion research and technology. The meeting was held on the recommendation of the 1976 Advisory Group Meeting on Atomic and Molecular Data for Fusion and supported by the Joint IFRC/INDC (International Fusion Research Council/International Nuclear Data Committee) Subcommittee on Atomic and Molecular Data for Fusion.

The meeting was attended by 18 participants representing ten existing or planned atomic and molecular data centres, two nuclear data centres, and three international organizations. The list of participants is given in Appendix 1.

B. Objectives

The general objective of the effort started at this meeting is the formation of an internationally coordinated network of centres and groups for the systematic world-wide compilation, evaluation, exchange and dissemination of bibliographic and numerical atomic and molecular data required by the fusion community.

The specific objectives of this meeting were the establishment of agreements for the cooperation between the existing A+M data centres and groups and the IAEA/NDS A+M Data Unit, and the initial formulation and adoption of common operational procedures for the implementation of this international effort.

The Adopted Agenda is given in <u>Appendix 2</u> and the list of papers presented to the meeting by the participants is given in <u>Appendix 3</u>.

C. Conclusions

The Conclusions listed below summarize the agreements between the participating centres and groups and the IAEA A+M Data Unit for the publication of a Quarterly International Bulletin on A+M Data for Fusion, the formulation and publication of an A+M collision data index, and the development of a format for the exchange of A+M collision data. Specific "actions" on meeting participants which detail the results of the agreements reached are listed in Appendix 4. 1. International Bulletin on A+M Data for Fusion

Following the recommendation of the November 1976 Culham Meeting, the NDS A+M Data Unit will publish a Quarterly International Bulletin on Atomic and Molecular Data for Fusion. This bulletin is to provide scientists and engineers working on fusion research and technology with recently determined and unpublished A+M data, and is to serve as a link between them and atomic physicists working on atomic data for fusion.

The bulletin will be compiled from original contributions provided directly from investigators or through existing A+M data centers and groups, and will be patterned after the US "Atomic Data for Fusion" newsletter circulated by the ORNL Controlled Fusion Center and the US National Bureau of Standards.

The following conclusions were reached at the meeting:

- a. During the trial period of the NDS/A+M Data Unit the publication of the ORNL and IAEA newsletters will be carried on simultaneously: and during that period, contributors should send duplicate copies of their contributions to ORNL and IAEA.
- b. As "pre-publication" of data in the A+M Data Bulletin may preclude subsequent publication in an established journal, distribution of the Bulletin should be restricted to the A+M and fusion communities. The Bulletin is not to be used as a substitute for data publication.

It was reiterated that if "pre-publication" of certain data in the Bulletin would force their rejection by an established journal, IAEA/NDS should not include the data in the Bulletin.

- c. The Bulletin should be a collection of timely information reflecting work in progress as well as recently published work. The source of information for the Bulletin should include "unconventional" literature, including laboratory reports, conference proceedings, theses, preprints, private communications and unpublished data tabulations. The content of the Bulletin should be closely related to fusion research; the exact decision as to its "physics scope" is to be left to the NDS/A+M Data Unit.
- d. It was agreed that information on work in progress in Japan, references to unconventional literature and other pertinent publications in Japanese will be provided to the NDS/A+M Data Unit in English. Communication between Japanese researchers and the NDS/A+M Data Unit should proceed directly or through the existing centres in Japan. Additional names of A+M data researchers in Japan will be provided by the Japanese centres to the NDS/A+M Data Unit.

- e. Information on work in progress in the Soviet Union will be sent to the NDS/A+M Data Unit by Dr. Martynenko (Kurchatov Institute). The Soviet contributions will include work taken from the conventional literature published in Russian (including conference proceedings, preprints, and others). Distribution of the Bulletin in the USSR will be done by the Kurchatov Institute; twenty five copies of each Bulletin issue are to be sent to Dr. Martynenko. The names of Soviet researchers currently on the (K) distribution in the NDS files for the distribution of the Bulletin should be removed.
- f. The first issue of the Bulletin is to include all suggestions which were given by the meeting participants, and is to be submitted for publication (effective cut-off date) on 1 July 1977. Contributions to the second issue of the Bulletin must be received by the NDS/A+M Data Unit in Vienna not later than 1 August, so as to issue it around 1 October (allowing one month of collation of the information, and one month of printing).

Subsequent deadlines for contributions will follow at 3-month intervals (i.e. 1 November, 1 February, 1 May etc.). This schedule is to be maintained until the A+M Data Centre Network meets again and reviews the situation.

2. Bibliographic A+M Collision Data Index

One of the first and foremost tasks assigned to IAEA/NDS is the creation of an international computerized index of references to A+M collision data and its publication by the end of 1978.

This index should contain references to all publications on data measurements, calculations, evaluations and reviews of reactions between atoms, selected molecules, ions, electrons and photons, expressed in terms of cross sections and reaction rates. Excluded from the index would be plasma-solid interactions (except in the few cases where these phenomena give information about single binary collisions) and atomic and molecular structure data, as these data would require a more sophisticated format.

The format of the index to A+M collision data should integrate as far as possible the formats and information of existing A+M bibliographies, namely those of Dr. C.F. Barnett (US/ORNL), Prof. J.L. Delcroix (FR/Orsay), Dr. E.C. Beaty (US/NBS-JILA) and Prof. K. Takayanagi (JAP/ Nagoya) and take advantage of the experience gained by these groups. The experience and the methods used in the development of the CINDA index on neutron reaction data should also be used.

The following conclusions were reached at the meeting:

a. The information content of the Bibliographic A+M Collision Data Index (referred to as the Index below) was agreed upon on the basis of the proposal put forth by IAEA/NDS (see Appendix 14). The information content of the Index, given in Annex B, consists of 14 information items, divided into seven <u>obligatory</u> items (which are necessary to define a specific data reference) and seven <u>optional</u> items (desirable supplementary information). Contributions provided to the NDS/A+M Data Unit should comply to the agreed information content as far as possible.

- b. The physics scope of the Index was discussed in context of the overall classification scheme of A+M data pertinent to fusion. The general classification scheme, agreed upon by the meeting participants, is given in Annex C. The Atomic and Molecular Collision part of the classification scheme was agreed to form the basis for the physics scope of the Index.
- c. The energy range of the collision data included in the Index is to be such that the data can be (unequivocally) considered to be part of atomic physics, unless the data are clearly outside the interest of fusion researchers. It was also suggested to improve the energy identification in the Index by allowing an identification of six broad energy categories (i.e. thermal, <100 eV, <10 KeV, <100 KeV, <1 MeV, and >1 MeV).
- d. Six existing (or potential) A+M Data Centros have agreed to contribute to the Agency's international Bibliographic A+M Collision Data Index: FR/Orsay, JAP/Nagoya, UK/Belfast, US/NBS-JILA, US/ ORNL-CTR and USSR/Kurchatov. For data published before 1 Jan. 1976, information will be supplied by US/ORNL-CTR and US/NBS-JILA in computerized form and will form the basis of the Index data base. For data references originating after 1 January 1976, the data base will be supplemented by input from Japan and the Soviet Union, and France. The data base from UK/Belfast will be used to check completeness over the whole time span. The time schedule for contributions to the Index from the six centres is shown in Annex D.
- e. Four aspects of the Index were not agreed upon by the meeting: the time covered by the published index, whether to include reference titles in the published version or not, which molecular species to include in the index, and whether to limit the scope to data pertinent to magnetically confined systems. All questions were referred for consideration by the Joint IFRC/INDC Subcommittee.
 - (i) With regard to time period to be covered, the subsequent meeting of this subcommittee recommended not to make a truncation in time of the data base.
 - (ii) With regard to titles, the subcommittee recommended not to exclude titles from the data base of the index, but not to include titles in the first (1978) issue of the Index.
 - (iii) With regard to the inclusion of molecular species the subcommittee recommended that data for molecules should be excluded unless clearly pertinent to fusion.

- (iv) The subcommittee felt that although it may be necessary to limit the scope of the data considered by the A+M Data Unit, in view of the limited manpower, the initial priority given to magnetic confinement devices was accepted only with the understanding that the requirements of inertial confinement devices would be taken into account as the programme matures.
- 3. A+M Collision Data Exchange Format

A lengthy discussion was pursued concerning the development of a format for the exchange of evaluated A+M collision data. By "evaluated" is meant that for a given quantity within a certain argument range only one value is recommended. Such data would be used by fusion researchers or by those who prepare data for use in fusion calculations. The results of the discussion are summarized in "Actions" 36-42 (See Appendix 4).

4. Next meeting

The network concluded that it should meet again in Vienna in May 1978.

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Centre Code	Address	Head of Project or Centre
FR/Orsay	Laboratoire Physique des Plasmas Faculte des Sciences d'Orsay Batiment 212 F-91400 Orsay	Prof. J.L. Delcroix
FRG/ZAED	Zentralstelle fuer Atomkern- energie-Dokumentation Kernforschungszentrum D-7514 Eggenstein-Leopoldshafen	Dr. C. Ebel
IAEA/NDS	Nuclear Data Section/A+M Data Unit International Atomic Energy Agency P.O. Box 590 A-1011 Vienna	Dr. J.J. Schmidt
JAP/Nagoya	Atomic Data Study Group Institute for Plasma Physics Nagoya University Nagoya 464, Japan	Prof. H. Suzuki
JAP/JAERI-A+M	Division of Physics Japan Atomic Energy Research Institute Tokai-Mura, Naka-gun Ibaraki-ken 319-11, Japan	Dr. T. Fuketa
UK/Belfast	Computer Centre Queens University Belfast, B17 1NN Northern Ireland, UK	Dr. F.J. Smith
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
us/nbs-el	Atomic Energy Levels Data Center Optical Physics Division National Bureau of Standards Washington, D.C. 20234, USA	Dr. W.C. Martin, Jr.

Members of the A+M Data Centre Network

Centre Code	Address	Head of Project or Centre
US/NBS-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-CTR	Controlled Fusion Atomic Data Center Oak Ridge National Laboratory P.O. Box Y Oak Ridge, Tennessee 37830, USA	Dr. C.F. Barnett
USSR/Kurchatov	Institut Atomnoi Energii I.V. Kurchatova 46 Ulitsa Kurchatova Moscow, D-182, USSR	Dr. Yu.V. Martynenko

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List of Information Items for Inclusion in Bibliographic Index File

for A+M Collision Data

A. Physics Information

1.	Incident particle(s):	identification of the most light-weight of process interactants. For more than one incident particle, list both. Sorted as a function of mass. States of ionization and/or excitation are given by conventional notation (<u>obligatory</u>).
2.	Target (particle):	identification of target particle, atom, ion or molecule. Same convention as for incident particle. In case of undefined target, specific convention can be adopted for individual cases (e.g. for nitrogen plasma, etc.) (<u>obligatory</u>).
3	Reaction process:	defined by adopted classification scheme (<u>obligatory</u>).
4.	Final product:	descriptive information on state and nature of reaction products, if needed (<u>optional</u>).
5•	Energy range:	energy or energy range of the incident particle. Given as E, E_{min} and/or E_{max} , or "larger than" or "smaller than" indicated energy. Also should have option to give temperature instead of energy, and the use of conventional terms, i.e. thermal, maxwellian, etc. (optional).
6.	Type of work:	indication whether referenced data is the result of experiment, theory, evaluation, or deduced from other data (<u>obligatory</u>).
7.	Quantity measured:	cross section, rate coefficient, angular distribution, etc. (<u>optional</u>).
8.	Comment:	Abbreviated commentary relating to the type of experimental or theoretical method used to obtain the referenced data (see CINDA) (<u>optional</u>).

B. Bibliographic Information

1.	Reference type:	indication whether reference is a journal article, a lab report, a book, a conference proceedings, a thesis or a private communi- cation (<u>optional</u>).
2.	Origin of work:	laboratory/institute and country where work was performed (<u>optional</u>).
3.	Reference:	principal part of the bibliographic citation (e.g. name of journal, vol., page, year of publication): can be given in the index proper (as in CINDA), or included in a separate biblio- graphic citation listing as Annex to index, with reference number given in index, or both (obligatory).
4.	Author(s):	All authors are listed in the file for use as part of the full bibliographic citation in the Bulletin, or partially (first author as in CINDA) in the index proper, or both (<u>obligatory</u>).
5.	Title:	Full title is stored in the file for use as part of bibliographic citation which can be given in the index proper or in the biblio- graphic citation listing in the Bulletin (<u>optional</u>).

C. <u>Reference to Data</u>

l. Data:	reference to the existence of the pertinent
	numerical data in a published compilation
	or in the files of a data centre (optional).

1.

Annex C

Classification Scheme for A+M Data

1. Structure and Spectra

- A. Atoms and Ions
 - 1. Energy Levels and Ionization Potentials, Wavelengths, Spectral Identification
 - 2. Wave functions
 - 3. Oscillator Strengths, Lifetimes, Transition Probabilities
 - 4. Differential Oscillator Strengths (see 2.A.4)
 - 5. Line Shapes and Shifts
 - 6. Polarisability
 - 7. Other Properties
- B. Molecules
 - 1. Energy Levels (Electronic, vibrational, rotational), Wavelengths, Spectral Classifications, Dissociation, and Ionization Potentials
 - 2. Interaction Potentials between Two Atoms, Potential Curves of Molecules
 - 3. Wave functions
 - 4. Oscillator Strengths and Lifetimes
 - 5. DifferentialOscillator Strengths (see 2.A.4 and 2.A.7)
 - 6. Line Shapes and Shifts
 - 7. Polarisability
 - 8. Electric Momént's
 - 9. Other Properties

A.	Collisions	Involving	Photons
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- 1. Total Absorption and Scattering
- 2. Elastic Scattering (Thomson, Rayleigh, ...)
- 3. Free-free Transitions (inverse Bremsstrahlung)
- 4. Photoexcitation-deexcitation (See 1.A.4 and 1.B.5)
- 5. Photoionization
- 6. Photodetachment
- 7. Photodissociation
- 8. Multiphoton Processes
- 9. Other Processes
- B. Collisions Involving Electrons
 - 1. Total Scattering and Momentum Transfer
 - 2. Elastic Scattering
 - 3. Excitation
 - 4. Deexcitation
 - 5. Ionization
 - 6. Recombination, particularly Dielectric Recombination
 - 7. Attachment
 - 8. Detachment
 - 9. Dissociation
 - 10. Bremsstrahlung
 - 11. Other Processes

- C. Collisions Between Heavy Particles
 - 1. Total Scattering
 - 2. Elastic Scattering
 - 3. Charge Transfer
 - 4. Excitation
 - 5. Deexcitation
 - 6. Ionization
 - 7. Interchange Reactions
 - 8. Association
 - 9. Dissociation
 - 10. Other Processes

3. Macroscopic Plasma Properties and Plasma Diagnostics

- A. Transport Properties
- B. Thermodynamic Properties
- C. Dielectric Properties
- D. Distribution Functions
- E. Clusters and Pellet Phenomena

4. Particle-Surface Interactions

(not considered at this meeting)

	AGREED SCHEDULE FOR CONTR.	IBUTIONS TO THE A+M COLLISION		
	DATA INDEX DATA BASE FROM	M THE A+M DATA CENTRE NETWORK	Deadline of 1 April 1978 to receive material for first issue	e
1 . 19	Jan. 950	l Jan. 1970	l Jan. l Jan l Jan. 1976 1978 1979	_
FR/Orsay	۲ 	Material on tape: dating back to Jan. in original CAPHYOR format This material to be supplied on tape.	<pre>Apr. 1978 <-materi.l in 70 new GAPHYOR format to be supplied on tape </pre>	
JAP/Nagoya JAP/JAERI	<−-Japanese literature cove	red by US/NBS-JILA and US/ORNL-CTR	Japanese input to be supplied on tape	I
UK/Belfast	Data base in Belfast for for checking completenes	mat (partly overlaps other data bases to be used s)		لی ۱
us/nbs-jila	Data base on electron an to be used as prime sour available	d photon collisions $\sim > 90$ % complete ce for input to Index data base in existing JILA format on tape	_	
us/ornl_ctr	Data base on heavy parti used as prime source for available in existing Oa	cle collisions $\sim > 90$ % complete to be input to Index data base k Ridge format on tape		Am
UESR/Kurchatov	Russian literature parti covered by US centers	ally <	Russian input to be supplied if possible in computerized form	nex D

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Annex D

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Appendices

Appendix 1

First Meeting of the

Atomic and Molecular Data Centre Network

Vienna, 9-13 May 1977

List of Participants

' l.	Barnett, C.F.	Oak Ridge National Laboratory P.O. Box X Oak Ridge, Tennessee 37830, USA
2.	Beaty, E.	Nuclear Data Section/A+M Data Unit IAEA
3.	Delcroix, J.L.	Laboratoire Physique des Plasmas Univ. de Paris XI, B. 212 Rue G. Clemenceau 15 F-91405 Orsay
4.	Drawin, H.W.	Dept. Phys. Plasmas & Fus. Contrl Association Euratom-C.E.A. sur la Fusion Controlée Rue du Panorama, P.O.B. 6 F-92260 Fontenay-aux-Roses
5.	Dunford, C.L.	National Nuclear Data Center Brookhaven National Laboratory Upton, N.Y. 11973, USA
6.	Ebel, G.	Zentralstelle f. Atomkernenergie- dokumentation Kernforschungszentrum D-7514 Eggenstein-Leopoldshafen
7.	Fuketa, T.	Nuclear Data Center, J.A.E.R.I. Tokai-Mura, Naka-Gun Ibaraki-Ken 319-11, Japan
8.	Itikawa, Y.	Institute of Space & Aeronautical Science University of Tokyo 4-6-1 Komaba, Meguro-Ku Tokyo 153, Japan
9.	Johnston, P.	NEA Neutron Data Compilation Centre P.O.B. 9 F-91190 Gif-sur-Yvette
10.	Katsonis, K.	Nuclear Data Section/A+M Data Unit IAEA

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11.	Lorenz, A. (Scientific Secretary)	Nuclear Data Section IAEA
12.	Martynenko, Yu.V.	Institut Atomnoi Energii I.V. Kurchatova 46 Ulitsa Kurchatova Moscow D-182, USSR
13.	Schmidt, J.J. (Chairman)	Nuclear Data Section IAEA
14.	Seamon, R.	Nuclear Data Section/A+M Data Unit IAEA
15.	Smith, F.J.	Computer Centre Queen's University Belfast, Bl7 1NN Northern Ireland, UK
16.	Suzuki, H.	Dept. of Physics Faculty of Science & Technology Sophia University Chiyoda-Ku, Kioicho 7 Tokyo 102, Japan
17.	Wiese, W.L.	Institute of Basic Standards National Bureau of Standards US Department of Commerce Washington, D.C. 20234, USA
18.	Yankov, G.B.	Institut Atomnoi Energii I.V. Kurchatova 46 Ulitsa Kurchatova Moscow D-182, USSR

First Meeting of the

Atomic and Molecular Data Centre Network

Vienna, 9-13 May 1977

(Starred itemswere considered to be of first priority)

Adopted Agenda

- Introductory remarks and election of chairman
- Adoption of agenda and meeting organization

MONDAY

- A. Reports from Data Centres
- 1.* IAEA/Nuclear Data Section (NDS)
- 2.* Presentations by other data centres concerning their current work, centre services and future plans, and initial proposals for future contributions to the data centre network

B. NDS Bulletin on A+M Data for Fusion

- 1.* NDS report on current status
- 2.* Contributions by other data centres to the bulletin

TUESDAY

- C. Scope and Classification of A+M Data
- 1.* Scope and classification of A+M collision data needed for fusion
 research
- 2. Scope and classification of other A+M data of interest to fusion research
 - a. A+M structure data
 - b. A+M plasma/surface interaction data
 - c. Macroscopic data
- D. Bibliographic Index to Atomic Collision Data
- 1.* Scope, content, objective and user community of the index
- 2.* Contributions of A+M data centre network to the index

- 3.* Feeding of computerized input to the bibliographic index, and consideration of common computer exchange standards
- 4.* Publication responsibilities, mode and schedule

WEDNESDAY

E. Bibliographic Indexes to Other A+M Data of Fusion Interest

- 1. A+M structure data
- 2. Plasma interactions with surfaces
- 3. Macroscopic data

F. Data Reviews and Assessment

- 1.* Survey of existing A+M data reviews and evaluations
- 2.* Discussion and summary of A+M data currently required for fusion which need to be evaluated
- 3.* How and by whom should the needed evaluations be performed ?

THURSDAY

G. Compilation and Exchange of A+M Collision Data

- 1.* Survey of existing collision data compilations and current compilation programmes of data centres
- 2.* Discussion of possible inter-centre exchange of computerized numerical A+M collision data and of common computer exchange formats

H. Compilation and Exchange of Other A+M Data

- 1. Structure data
- 2. Surface interaction data
- 3. Macroscopic data

I.* Data Centre Services

FRIDAY

J. Summary of Meeting

- 1. Agreed data centre responsibilities
- 2. List of actions
- 3. Conclusions and recommendations
- A. Next meeting: date, place and suggested agenda items.

List of Papers Presented at the Meeting

Part of the papers presented to this meeting have been included in this Summary Report as Appendices (indicated below); the other part, consisting of the full reproduction or excerpts of reports published or to be published, have not been included in this report.

- CM 1 "A Bibliographic Index for Surface Interaction Data" by G. Ebel and W. Heiland. (included as Appendix 6)
- CM 2 "IAEA Advisory Group Meeting on Atomic and Molecular Data for Fusion", Summary Report, by A. Lorenz. (Published as INDC(NDS)-82/GB)
- CM 3 "The "GAPHYOR" System: A Computerized Retrieval System of the Properties of Atoms, Molecules, Gases and Plasmas", by J.L. Delcroix. (To be published as INDC(FR)-21/GA)
- CM 4 "JILA Atomic Collision Information Center". (included as Appendix 7)
- CM 5 Letter from V.F. Hampel, Data Management Research Project, LLL, to A. Lorenz. (included as Appendix 8)
- CM 6 "The Bibliography of Integral Charged Particle Nuclear Data", by T.W. Burrows and J.S. Burt. (Published as US Report BNL-NCS-50640, March 1977)
- CM 7 "Basis for a General Classification Scheme for A+M Data for Fusion", by K. Katsonis and A. Lorenz. (included as Appendix 9)
- CM 8 "Quarterly International Bulletin on Atomic and Molecular Data for Fusion", Vol. 1, No. 1. (To be published as INDC(NDS)-87/ ABKF)
- CM 9 "Activities of the ZAED in the Field of Data Information and Documentation", by G. Ebel. (included as Appendix 10)
- CM 10 "Memorandum. A Report on Activities of the Atomic Data Study Group, IPP/NAGOYA", by H. Suzuki. (included as Appendix 11)
- CM 11 "Activities and Program on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute", by T. Fuketa. (included as Appendix 12)
- CM 12 "Reviews of the Recent Activities on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute (JAERI)", by Y. Obata, Y. Nakai, T. Shirai and M. Kase. (included as Appendix 13)
- CM 13 "Proposed Framework for a Bibliographic Index for A+M Collision Data for Fusion", by A. Lorenz (included as Appendix 14)
- CM 14 "Tentative Optimization of the Future Bibliographic Index for A+M Collision Data", by J.L. Delcroix. (included as Appendix 15)

- CM 15 Copies of the vu-graphs used by C.F. Barnett in his talk describing the Controlled Fusion Atomic Data Center, ORNL, Physics Division. (included as Appendix 16)
- CM 16 "Ionization and Excitation of Ions by Electron Impact. Review of Empirical Formulae", by T. Kato, Dept. of Physics, Nagoya University. (to be published as INDC report)
- CM 17 "Experiences from an International Cooperation in Data Exchange" (Draft), by H.D. Lemmel, 6 May 1977. (included as Appendix 17)
- CM 18 "A+M Surface interaction data currently required for fusion which need to be evaluated", by W. Heiland. (included as Appendix 18)

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Actions Resulting from

the First Meeting of the Atomic and Molecular Data

Centre Network

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1	NDS/A+M Unit	As a result of the discussion under Agenda Item B.1, the NDS/A+M Unit is asked to pro- duce a more strongly fusion-oriented news- letter.
2	Meeting Participants	To aid NDS/A+M Unit in Action 1, Drs. Wiese, Barnett, Delcroix and Drawin in particular are asked to provide detailed comments on the draft of the first Bulletin by 15 June 1977.
3	Delcroix	Send a letter to French physicists who might possibly contribute to the Bulletin, reminding them of the Bulletin's existence and urging their cooperation.
4	Delcroix	Investigate the possibility of preparing from the GAPHYOR data file a list of authors from all around the world according to the geo- graphical location.
5	Ebel	Send copy of the new directory of research in progress at all German institutions to NDS as soon as it is ready.
6	Ebel	Advertise and distribute the IAEA A+M Bulletin in the Federal Republic of Germany.
7	NDS/A+M Unit	Send ten copies of the first issue of the Bulletin to Dr. Ebel.
8	Ebel	Send information on fusion related A+M data as abstracted from the German literature input to INIS to NDS/A+M Unit for possible inclusion in the Bulletin.
9	NDS/A+M Unit	Send 25 copies of each issue of the Bulletin to Dr. Martynenko at the Kurchatov Institute.
10	NDS/A+M Unit	Publish in the first issue of the Bulletin a short policy statement and state the editorial responsibility assumed.

11	NDS/A+M Unit	Digest the data from all remaining areas of the world (Eastern and Western Europe, Australia, the usual service areas of NDS including de- veloping countries) for use in the Bulletin.
12	NDS/A+M Unit	Send all non-American contributions to JILA, ORNL, and NBS whenever an issue of the Bulletin is ready for press.
13	Ebel	Discuss the classification of particle-surface interactions with surface interaction experts (especially those at Garching) and prepare a proposal for presentation to the participating data centers and groups.
14	Barnett, Delcroix, Drawin, Itikawa and Smith	Send to the NDS/A+M Unit by 15 June 1977 your suggestions for the subdivision of levels in the description of atomic and molecular collisions (concerns the classification scheme for A+M data).
15	Wiese	Inquire into the feasibility of quoting compilations of energy levels and transition probabilities of interest to fusion in the Atomic Collision biblio- graphy to be published by the NDS.
16	Wiese	Send NBS publications to all centres and organizations represented at this meeting.
17	Delcroix	Send to NDS/A+M Unit a list of all the molecules included in the CAPHYOR system; this list could be used by the A+M Unit in preparation of a questionnaire to the fusion community concerning molecules of interest.
18	Delcroix	Send the geographical abbreviations as used in GAPHYOR to the NDS/A+M Unit.
19	NDS/A+M Unit	On the basis of the items agreed upon for in- clusion in a bibliographic index (Paper CM-13), develop the first draft of a format proposal by 1 October and send examples to the cooperating centers represented at this meeting: Orsay, ORNL, JILA, USSR (Kurchatov Institute), Japan (JAERI and Nagoya). Smith (Belfast), ZAED (Karlsruhe) and CCDN (Saclay) are to be included in the format discussions.
20	Barnett	Send to Dr. Martynenko the list of journals in- cluded in the ORNL bibliographic index.
21	Delcroix	Send to Dr. Martynenko data from GAPHYOR with which it will be possible to check for completeness the coverage of Russian language literature in- cluded in GAPHYOR.

22	Martynenko	Ascertain what gaps exist in the coverage of the Russian language journal literature between 1 Jan. 1970 and 1 Jan. 1977. Fill in the gaps for the years 1970 - 1976 and provide full coverage for 1977 by providing us by 1 April 1978 at the latest bibliographic information items as decided upon. As much as possible the information should be provided in English. A weaker part of this action is to try and send at least some of this information in computerized format.
23	Japanese Repre- sentatives	Send by 1 April 1978 at the latest a computerized version of the input for the references from the Japanese literature for calendar years 1976 and 1977.
24	Smith	Sena a tape to NDS/A+M Unit containing the biblio- graphic references and data such as they are now available at Belfast.
25	Barnett	Send as soon as possible a tape containing the most recent bibliographic library so that the NDS/A+M Unit can experiment with it.
2 6	JILA	Send as soon as possible a tape containing the most recent bibliographic library so that NDS/A+M Unit can experiment with it.
27	Delcroix	Send as soon as possible a tape containing the most recent bibliographic library so that NDS/A+M Unit can experiment with it.
28	Wiese	Send the description of the structure data bibliographies under preparation at NBS to all the cooperating centres.
29	Meeting Participants	Eliminate FRG/Garching from the list of Members of the A+M Data Centre network as contained in Appendix A of INDC(NDS)-82/GB.
30	Martynenko	Send completed works in structure data evaluations to Dr. Wiese, the NDS/A+M Unit, and all other participating centres. Even though the works may be written in Russian, the main contents in tabular form will still be very valuable to other users.
31	Martynenko, Suzuki and Wiese	Exchange letters that detail the scope of their work and their plans in structure data compilation over the next few years. Overlapping areas should then be eliminated; there is plenty of work for all.
32	Meeting Participants	Inform the A+M Unit about work in progress on A+M data reviews and assessments to assist in pre- paring a survey on this topic.

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33	Itikawa	Send to all participants and centres the Japanese language report IPPJ-DT-44 by K. Takayanagi in
		the Appendix of which is given a list of reviews and compilations. It is understood that the list is incomplete, but it does include works carried out all around the world.

- 34 Drawin, Fuketa, and Martynenko Bartynenko Drawin, Fuketa, and Martynenko Bartynenko Barty
- 35 Barnett Send to the NDS/A+M Unit the ERDA and National Academy of Science reports in which the fusion research data needs are outlined.
- 36 Barnett, NDS/A+M Unit Within the next couple of months as time allows, communicate with each other to develop a common understanding on the content of an evaluated A+M collision data library, and develop a proposal on format for use in intercenter exchange of such data. It is understood that there may be a difference between in-house storage formats and the format used for intercenter communication. Send the format proposal to the participants named in the next action.
- 37 Smith, Fuketa, Report back to NDS/A+M Unit with comments on the Martynenko, Suzuki, proposed format within four to six weeks of Barnett, Ebel receipt thereof.
- 38 NDS/A+M Unit Incorporate recommendations received from the various centers and send to Dr. Barnett a fully described format for use in transmitting evaluated A+M collision data.
- 39 Barnett Transmit his computerized data sets to NDS/A+M Unit in the agreed-upon format; NDS will be responsible for forwarding them to other interested data centres.
- 40 Fuketa Recognizing that A+M collision data do not now exist in computerized form at JAERI, send any available data to NDS/A+M Unit with which they can work in developing the proposed common format for data exchange.
- 41 Smith Send to the NDS/A+M Unit a tape containing the data stored in his computer files for use in developing the common format for data exchange.

42	Martynenko	If there are data available which could be compiled in computerized form, communicate them to NDS/A+M Unit in any form so that they may be used in developing the common format for data exchange.
43	Delcroix, Drawin	Put together some works on A+M collision data and communicate them to NDS/A+M Unit for use in developing the common format for data exchange.

First Meeting of the Atomic and Molecular Data Centre Network Vienna, 19-13 May 1977

Opening speech by Prof. A.V. Shalnov, Director Div. of Res. and Labs.

It gives me great pleasure to welcome you to this meeting on behalf of the Director General and wish you a successful and productive meeting.

As you know the Agency has been asked to initiate an international programme for the systematic collection, exchange and distribution of atomic and molecular data required for fusion research, which has become known as the Agency's A+M data programme.

This programme has two aspects. The first one has to do with "what" has to be done. To do that, we haw to identify the specific data required by the fusion community, and compare these requirements with the existing data. As this field of activity was new to the Agency, the first step we took in this direction was to hold a topical meeting on Atomic and Molecular data for Fusion in order to inform us of the current status in this field. This meeting was hold last November at the Culham Laboratory in the UK, and I believe some of you have attended it. This meeting was very important from our point of view, in that it focussed the current A+M data needs in three data fields important to fusion, namely atomic collisions, atomic structure and surface interaction. These recommendation should provide the initial guidance to the Agency's A+M programme.

The second aspect has to do with "how" to do the job. In order to help us define the priorities of this task, and identify an initial set of tasks which could be performed within a reasonable time, the Agency formed a "joint sub-committee on A+M data for fusion" composed of representatives of the fusion, nuclear and atomic data communities, under the general auspices of the International Fusion Research Council and the International Nuclear Data Committee. Both of these are permanent advisory bodies to the Agency's Director General. At the same time, the Agency created a new unit within the Nuclear Data Section and staffed it with experts who have already started to implement some of the recommendations of the joint A+M subcommittee.

As you may imagine, the needs for A+M data required for the development of fusion research and technology, and the effort to compile, evaluate and disseminate these data are very large. It is therefore almost impossible for any one country or organization to meet these needs alone. This fact was also realized by the participants of the Culham Meeting, who recommended that an international network of A+M data centres be formed to work with the Agency's A+M Data Unit in establishing a system of international cooperation.

Some definite tasks have been given to the A+M Data Unit to achieve within the initial two year period of this programme. I understand that some of the ground work has already been done, but a considerable amount of work remains to be done. I would therefore like to invite your cooperation and assistance by helping us to achieve these tasks.

April 1977

A Bibliographic Index for Surface Interaction Data

G. Ebel

Zentralstelle für Atomkernenergie-Dokumentation (ZAED) 7514 Eggenstein/Leopoldshafen 2

W. Heiland

Max-Planck-Institut für Plasmaphysik 8046 Garching

Since 1966 the Max-Planck-Institut für Plasmaphysik at Garching issues a monthly documentation entitled "Surface and Vacuum Physics Index". 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. In addition to these indices it contained up to 1976 a subject index in logical order that has now been discarded.

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.

This ensures the topicality of such information. It is thus possible to inform scientists engaged in the field of surface and vacuum physics within a short time about the latest publications and reports, arranged according to subject matter. 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 1976 about 3000 documents were covered.

The index is edited in cooperation with and supported by the International Union for Vacuum Science, Techniques and Applications (IUVSTA) and is published and distributed by the Zentralstelle fur Atomkernenergie-Dokumentation (ZAED). The ZAED handles also requests for the original literature and for literature searches.

At the IAEA Advisory Group Meeting on Atomic and Molecular Data for Fusion at Culham in November 1976 it was recommended to establish an index to surface interaction data. Therefore ZAED and IPP Garching have considered the possibility to extend the "Surface and Vacuum Physics Index" to a bibliographic index for surface interaction data. This can be done in the following way:

All papers containing numerical data will be given a special treatment in addition to the usual procedure for compiling the Surface and Vacuum Physics Index. They will be indexed with additional keywords on a formatted worksheet specifying the type of data contained in the papers. These keywords will 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 will be stored in a computer as it is already done with the present "Surface and Vacuum Physics Index". This will allow the generation of different types of indices, arranged e.g. by reactions, measured quantities or measuring methods. These indices could be added to the existing author and subject indices in the Surface and Vacuum Physics Index as well as cumulated and published in a separate form.

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Suggestions and comments from the participants of this meeting regarding the scope and the format of the planned Surface Interaction Data Index will be welcommed.

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JOINT INSTITUTE FOR LABORATORY ASTROPHYSICS



UNIVERSITY OF COLORADO

UNIVERSITY OF COLORADO BOULDER, COLORADO 80309

April 27, 1977



NATIONAL BUREAU OF STANDARDS

JILA Atomic Collision Information Center

The Joint Institute for Laboratory Astrophysics (JILA) is a research institute located at the University of Colorado and sponsored jointly by the University of Colorado and the National Bureau of Standards. The scientific scope of the institute is centered around the physics of relatively low temperature plasmas such as occur in astrophysics, gas discharges including lasers, the Earth's ionosphere and plasma power generators. Included in the JILA scientific program is an Atomic Collision Information Center where data on the collision processes involved in low temperature plasmas are compiled, evaluated, and distributed.

The principal objective of the Information Center is to assist scientists who are engaged in the mathematical modeling of low temperature plasmas. The Information Center regularly reviews the published literature to identify papers which report data in the areas of concern. In addition, for the critical areas of electron and photon impact, retrospective literature searches have been done. The result is an indexed bibliography which is maintained as computer files and which is printed and distributed as Information Center Reports. Copies of all the papers are obtained and are on file in the Information Center and are available for interested scientists to consult. Numerical data are extracted from the papers on an "as needed" basis. The numerical data are also maintained as computer files and selected portions are printed and distributed.

The full scope of collision data which is useful in these applications is very large and the Information Center has concentrated its efforts on those processes which are judged to be particularly important and for which the requisite technical expertise is available. The most important data concern electron collision processes and continuum photoabsorption by atoms and simple molecules. The range of molecules includes all diatomics and a selected list of more complicated molecules.

Because free electrons are effective at producing excitation, even low temperature plasmas have relatively high concentrations of excited states of atoms and molecules. Collisions between excited and ground state atoms or molecules can result in the transfer of the energy of excitation. The "energy transfer" collisions are particularly important in laser plasmas. The Information Center is beginning to compile and evaluate data on energy transfer collisions.

The evaluation of data is generally done on an extensive basis as developments in the field require. As the needs are recognized, experts from outside the normal staff of the Information Center are invited to use the Information Center files to critically review the data available on some selected topic. These cooperative critical reviews are normally published in the open, refereed literature.

- 33 -LAWRENCE LIVERMORE LABORATORY



Alex Lorenz Nuclear Data Section Division of Research & Laboratories IAEA Kaerntner Ring 11 P.O.Box 590 A-1011 Vienna, A U S T R I A

April 27, 1977

Dear Alex,

As communicated to you earlier, I regret that I will not be able to attend First Meeting of the Atomic and Molecular Data Centre Network because of pressing work commitments at LLL.

I would appreciate representing LLL and the USA in future meetings. The work which we are now doing for laser induced isotope separation, and atomic and molecular data in general, should be an asset to your future planning. Also, we will be involved in preparing data files, textual and numeric, for use on the MFE computer center.

With regard to your meeting, I would like to make the following comments:

1. Bibliographic A&M Data Base

The data base prepared by C.F. Barnett during the past decade should be of considerable interest to the A&M community. This at least was the concensus at the Culham meeting.

We are prepared to assist in the standardization of the data base, and reformatting where required, should the request for this undertaking, and our making the data base available over the MFE network, be approved by Jim Decker, with appropriate funding through the MFE programs at LLL.

I suspect this may require 0.5 FTE, when compared to a similar effort that we are doing for the LLL laser program, in cooperation with the University of Rochester, in the field of Multiphoton Reactions.

Several different bibliographic storage and retrieval programs could be used for this purpose on the MFE machine.

In addition, a cleaned-up copy of the data base could be made available to the ERDA/RECON interactive information network.

2. Numerical A&M Data Base

As you know, the Lawrence Livermore Laboratory hasvery extensive programs in laser induced and magnetic fusion energy programs. The computers and numerical data play an important role.

At the present time, LLL and other MFE research centers, are still using their own data files and data generation programs for calculations. This will change only slowly as researchers change their working locations yet retain familiarity with their preferred sets of constants. Here the situation is not unlike that in the nuclear fission field with neutron cross section data 1-2 decades ago. And yet one would hope that the proliferation of disparate numerical data could be avoided as the fusion program is gaining momentum.

At LLL, users of atomic and molecular data express needs for computerized data banks especially in two areas:

- radiation damage data for optimization of blankets and reactor designs;
- aggregation and standardization of the numerous publications of the National Bureau of Standards.

We are starting to pursue actively the identification of radiation damage data. The computerization of the NBS data, and their conversion to a uniform set of units, has been discussed repeatedly with David Lide, NBS/NSRDS. The NBS publications have - in some cases - magnetic tapes that were used to drive the linotype printing machines of the GPO. We have had some experience in converting these files into corresponding data bases. To do this would require at least one FTE for an extended period of time. It would also require some extension of our ongoing work toward the development of a portable *Scientific Data Base Management System (SDBMS)* so that the customary notations of the AGM field could be faithfully reproduced, i.e., upper and lower case, subscripts and superscripts, extended character sets, etc. At LLL, we have in operation the Hershey character sets and capabilities on the FR80s and CRT screens to store and reproduce these types of scientific notations.

Guidance and support for any of these activities must necessarily come from ERDA and the MFE and laser research community.

3. Data Exchange Formats

As indicated in our report to the Culham meeting, UCRL-79286, The Time for Atomic and Molecular Data Bases is Now!, the Interlaboratory Working Group for Data Exchange of ERDA has prepared an extension to the ANSI standard, X3.22-1967 and X3.27-1969 to include numerical data. I was favorably received, I am told, and should become the next ANSI standard for exchange of data by magnetic tape. One of the latest drafts is contained in the appendix of LBL-5329. Copies of the proposed standard were also sent to you earlier this year and should be considered by the working group.

Alternately, the EXFOR system should be used.

With best regards and good wishes for your timely work,

Viktor E. Hampel, Leader DATA MANAGEMENT RESEARCH PROJECT

enclosures

cc: James F. Decker, ERDA J. V. Martinez, ERDA J. S. Kane, ERDA/DPR M. Harrison, LLL/MFE C. Taylor, LLL J. D. Lee, MFE Dieter Fuss, MFE Computer Center J. Ranelletti, LLL/USD W. L. Wiese, NBS/NSRDS C. F. Barnett, ORNL Basis for a General Classification Scheme for A+M Data for Fusion

by K. Katsonis and A. Lorenz

The A+M data needs for fusion depend on the type and technology of the fusion device. The most common among such devices are closed or open magnetic lines confinement devices and compression laser systems. Although the physical principles are various, only some A+M data types are common to the first two of them (i.e. Tokamak and Theta-pinch).

Actually, closed magnetic line devices like Tokamaks, are currently the most investigated. The A+M data needs for the conceptual reactors of this category are of primary interest, and during the initial stages of the Agency's A+M unit programme, the effort will be restricted to them (Ref. 1).

The scope of interest involves particle processes and collective phenomena pertinent to the following aspects of controlled fusion devices (Ref. 2):

- 1. Nuclear Reactions
- 2. Energy and particle losses
- 3. Impurities
- 4. Injection heating
- 5. Refuelling
- 6. Diagnostic (spectroscopic and by probes)

The theoretical aspects of A+M data used in fusion research are summarized in ERDA-76/106 (Ref. 3).

With regard to the nuclear reactions, it is expected that initially the fuels will be restricted to deuterium and tritium in the following reaction:

$$D + T \longrightarrow {}^{4}He + n$$

Also the initiation of the nuclear reactions in the plasma will demand a preionization of the D - T mixture. The tritium fuel is planned to be bred in a lithium blanket by interaction of the fast neutrons generated in the plasma:

6
Li + n \longrightarrow 4 He + T

In closed magnetic-line systems the energy losses come mainly from the radial diffusion of e and ions, from radiative losses (bremsstrahlung in the mass of the plasma, and line radiation by atoms or non-stripped ions) and charge exchange collisions. As the plasma in fusion devices is optically thin, the radiative energy losses are substantial.

The appearance of impurities which results from a series of atomic processes presents another energy loss mechanism with a resultant decrease of the plasma temperature. For instance, in the present-day conceptual Tokamaks the hydrogen molecules are ionized and further dissociated by e impact giving rise to fast hydrogen atoms; also higher energy hydrogen atoms are created through charge exchange, finally leading to impurities by interactions (sputtering, release of impurity gases, etc.) with the wall material.

Injection of neutral beams (or α -particles) is foreseen as one possible method to raise the plasma temperature in the fusion device. This involves charge exchange and proton impact ionization interactions for which data must be available. Refuelling is also expected to be done by the injection of strong neutral beams or frozen D - T high velocity pellets.

Finally the diagnostic methods applied in the experimental fusion devices require extensive data pertinent to the atomic spectroscopy field.

The specific A+M data which are currently needed by the fusion community, can be (refined synthese) summarized from the six areas of emphasis mentioned above. A proposed list of these data, structured into a general A+M data classification scheme, is given in the <u>Appendix</u>. The main section of this scheme has been used in the presentation of the information in the Quarterly International Bulletin on Atomic and Molecular Data for Fusion, issued by the A+M Data Unit at the NDS. This classification scheme is also expected to serve as the basis for the storage of bibliographic and numerical A+M data in computerized files.

The data in the first Part of the list, on A+, structure and spectroscopy, are indispensable for plasma diagnostic, for the calculation of radiative processes, and collisions between $e^{-}(e^{+})$, atoms and ions, for the evaluation of experimental results, and for plasma modelling. In addition, data in this category are especially needed to determine wavelengths of resonance and other strong lines, mostly of heavy, high ionized ions related to the significant loss of energy in Tokamaks, and for the evaluation of the concentration of impurities. The electronic and vibrational structure of H₂, H₂⁺, H₂⁻, D₂, etc., should be useful in understanding the basic processes of ion sources.

Most of the radiative reactions, given in Part 2 of the list, relate to plasma cooling and the presence of impurities. A detailed review of the corresponding processes is given by Drawin (Ref. 4).

The largest and most important part of the data has to do with collisions of e⁻(or e⁺) with atoms, ions and molecules, given in Part 3 of the list, as well as collisions between atoms, ions and molecules given in Part 4. A comprehensive list of these processes is given by the Atomic Data Study Group, Nagoya University, Japan, which was taken into consideration in the scheme mentioned above.

The list of processes which relate to plasma surface interactions given in Part 5 of the list are based on the recommendations of the Working Group on Surface Interactions (Ref. 5). For an extended review of this topic, see Review Paper A2 by H. Vernickel (Ref. 6).

Part 6 consists of macroscopic and chemical data, as well as bulk data used for diagnostic purposes. The different coefficients describe, on a macroscopic scale, the results of microscopic processes given in parts 2, 3 and 4. Finally, data related to the overall description of the fusion devices are also included.

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List of A+M Data needed in Fusion

1. ATOMIC AND MOLECULAR STRUCTURE, SPECTROSCOPY

- 1.1 Energy levels and constants, wavelengths, vibrational and rotational levels; line identification
- 1.2 Wavefunctions (orbitals; SCF, LCAØ, variational ...); electronic structure, electron correlation (configuration interaction)
- 1.3 Oscillator strengths, lifetimes, transition probabilities
- 1.4 Electric and magnetic moments; polarisability
- 1.5 Bords, interatomic potentials, force constants
- 1.6 Level crossing, optical pumping

2. RADIATIVE PROCESSES AND INTERACTION (Interaction with photon)

- 2.1 Total scattering
- 2.2 Elastic scattering (Thomson, Rayleigh ...)
- 2.3 Not specified non-elastic (inelastic-superelastic) processes
- 2.4 Free-frec transitions (direct and inverse Bremsstrahlung)
- 2.5 Photoexcitation-deexcitation
- 2.6 Photoionization-radiative recombination
- 2.7 Radiative attachment-photodetachment (from negative simple or compound ions)
- 2.8 Multiphoton processes
- 2.9 Photodissociation

3. COLLISIONS OF e or e WITH ATOMS, IONS, MOLECULES

- 3.1 Total scattering
- 3.2 Elastic scattering
- 3.3 Not specified non-elastic (inelastic-superelastic) processes

- 3.4 Homentum or spin transfer
- 3.5 Excitation-de excitation (electronic, vibrational, rotational, relaxation)
- 3.6 Ionization-recombination (three body, dissociative)
- 3.7 Attachment (three-body, dissociative) detachment concerning simple or compund ions
- 3.8 Dissociation
- 3.9 Binary e-e
- 3.10 Radationless transitions, autoionization, dielectonic recombination

4. COLLISIONS BETWEEN ATOMS, IONS (INCLUDING PROTON), MOLECULES

- 4.1 Total scattering
- 4.2 Elastic scattering
- 4.3 Not specified non-elastic (inelastic-superelastic)
- 4.4 Momentum or spin transfer
- 4.5 Charge transfer
- 4.6 Excitation-deexcitation (electronic, vibrational, rotational)
- 4.7 Ionization-recombination
- 4.8 Detachment (concerning simple or compound ions)
- 4.9 Association-dissociation

5. SURFACE INTERACTIONS

- 5.1 Combined effects
- 5.2 Sputtering (physical: liberation of materials due to beams; chemical: without moment transfer)
- 5.3 Absorption
- 5.4 Desorption (release of gas by ions, e, ph, thermal effects)
- 5.5 Blistering (by hydrogen isotopes, α radiation ...)

- 5.6 Backscattering
- 5.7 Ionization-neutralization and deexcitation
- 5.8 Pellet refuelling
- 5.9 Impurity control (gettering, baking, discharge cleaning)
- 5.10 Chemical reactions or surfaces

6. MACROSCOPIC AND CHEMICAL PLASMA DATA; DIAGNOSTIC

- 6.1 Chemical reaction patterns
- 6.2 Transport coefficients
- 6.3 Radiative coefficients (of photoexcitation, deexcitation, radiative recombination ...)
- 6.4 Collision and radiationless transition coefficients (of exciation, deexciation, ionization, autoionization, three body and dielectronic recombination ...)
- 6.5 Line shape, broadening and shift
- 6.6 Diffusion
- 6.7 Distribution functions
- 6.8 Fundamental quantities (pressure, temperature, density, conductivity ...). Plasma modelling

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Activities of the ZAED in the field of data information and documentation G. Ebel Zentralstelle für Atomkernenergie-Dokumentation (ZAED) 7514 Eggenstein-Leopoldshafen, Germany

1. General outline

In 1974 the government of the Federal Republic of Germany passed a program for the promotion of information and documentation which intends the establishment of 16 Specialized Information Systems. The Zentralstelle für Atomkernenergie-Dokumentation (ZAED) will be combined with some other documentation centers for aerospace science, physics and mathematics to form the center of the Specialized Information System for Energy, Physics and Mathematics. It will be formally founded within the next months and will be located at the Karlsruhe Nuclear Research Center.

The main purpose of these Specialised Information Centers will be the information on relevant documents and data in their respective subject fields. As a consequence, the ZAED has been commissioned by the Federal Ministry of Research and Technology to substantially improve the situation in the field of physics data by establishing a data information system. For this purpose, data compilations are regularly to be published in a rumber of physics subfields and to be kept up to data. Moreover, as complete as possible, a list of world wide existing data compilations is to be organized in order to inform about existing data compilations and to facilitate the search for data. Another task of the information center will be the collection and distribution of existing data compilations for the Federal Republic of Germany. This applies in particular to data compilations on magnetic tape, for which ZAED will act as a distribution center. In order to avoid duplication of work in compiling physics data, ZAED will also have the task of coordinating activities in this field to a certain degree. At the same time, close international cooperation in this field is envisaged.

2. Publication of new data compilations

One of the main tasks of the data information system is the publication of new data compilations in active fields of physical research. The data are compiled and evaluated by groups of scientists who are working at research instituions and are actively engaged in the field in which tney compile data. The ZAED functions as a central office for the coordination of the work and provides technical and financial assistance to the groups. This includes searches for the relevant literature from which the data are extracted, computer processing of the data, publication and distribution of the data compilations.

Up to now data compilations have been completed in the fields of elementary particle physics, nuclear physics, ion interactions in matter and thermodynamics and wore published as separate booklets in the series "Physikdaten/Physics Data". Further compilations for other fields are in preparation as well as updates of already published compilations.

3. Bibliography of existing data compilations

In addition to the establishment of new data compilations a bibliography of worldwide existing tables and other data sources has been compiled and published in the series "Physikdaten/Physics Data". This bibliography contains up to now about 2000 data sources and most of them are present in a reference library at the ZAED. The bibliography is also available on magnetic tape and allows the retrieval of compilations for specific data.

4. Classification scheme for physics data

Attempts are being made to establish a classification scheme for physics datar One of the most comprehensive physics data compilations are the tables by Landolt and Börnstein, "Zahlenwerte und Funktionen aus Naturwissenschaft und Technik" in its two latest editions (6th edition and New Series). The data contained in it are therefore

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used to draw up a subject index for the "Landolt-Börnstein" which will then be extended into a modern subject classification for data. This classification system will, of course, be suitable for manual as well as for computerized searches. It will also serve as a basis for a physics data bank planned for the future.

5. Computerized data services

A further task of an information center is to make available to users data files on magnetic tapes. In this respect we have started with the distribution of the Cambridge Crystallographic Data Files that contain the crystal structures of about 13000 organic and organometallic compounds. The idea is to serve as an affiliation center to provide users either with the data or with the copies of the whole files. At the moment we are implementing the Evaluated Nuclear Structure Data File from the Nuclear Data Group at the Oak Ridge National Laboratory. It is hoped to make available the content of the most important physical data files to users within the Federal Republic of Germany in the future.

6. International cooperation

Great emphasis will be put on an international cooperation, as in the long run a field of this magnitude can only be managed in this way. ZAED has made a start in this direction by joining into a project within the field of the nuclear structure data as partner in an international collaboration for the compilation and evaluation of nuclear structure data organized 1976 by the IAEA. In the past the whole effort of compilation and evaluation has been done by the Nuclear Data Project of the United States.

7. <u>Contribution to the international cooperation on atomic and</u> molecular data for fusion

The ZAED is willing to cooperate in the field of atomic and molecular data in a similar way as is already done in the field of nuclear data. It will coordinate the data activities within the Federal Republic of Germany and will act **as** the German partner in the envisaged international data center network. A first step in this direction will be the establishment of a bibliographic index on surface interaction data on the basis of the existing Surface and Vacuum Physics Index.

Appendix 11

Memorandum

A REPORT ON ACTIVITIES OF THE ATOMIC DATA STUDY GROUP, IPP/NAGOYA

Prepared by Hirosi SUZUKI Sophia University, Chiyoda-ku, Tokyo, 102 Japan Chairman of the Atomic Data Study Group, IPP/Nagoya

This is a short report on the current and projected work of the Atomic Data Study Group, Institute of Plasma Physics/ Nagoya University (SG) in compilation and dissemination of atomic and molecular data for fusion research. New programs which will be started in the near future in the SG will be also described briefly. An establishment of the newly authorized scientific information center, which is tentatively named the Fusion Research Center for Data Analyses and System Studies, in the IPP/ Nagoya University will be informed. Finally some proposals for the possible collaborations to the data center network from the SG and the new Center, IPP/Nagoya will be offered.

1. SURVEY OF THE WORK OF THE SG, IPP/NAGOYA

In response to urgent and expanding demands on atomic and molecular data for fusion research, the SG was organized by K.Takayanagi in 1973, and continues a series of systematic efforts in compilation and dissemination of numerical data of interest in fusion, under the leadership of H.Suzuki. The working group of the SG consists of about twenty physicists in the fields of atomic collision and atomic and molecular spectroscopy, who participate in the cooperative research project from different universities and institutes all over Japan. A list of the members in the main group of the SG is presented in Appendix 1.

After an extensive survey on request of data for atomic processes within the fusion research community in Japan, a report was published in 1974 [1], which includes a comprehensive list of cross section data for atomic processes in the urgent needs. This report also contains a list of bibliographical references relevant to data and informations for atomic processes.

The first volume of numerical data compilation " Cross Sections for Atomic Processes Vol.1 " was published in May 1975 as the First Edition . The revised and enlarged edition of Vol.1 was issued in November 1976 [2]. This volume contains the cross section data for all types of processes involving hydrogen isotopes and their ions, electron and photons. Both experimental and theoretical values of data are plotted mainly in figures. Preparation for publication of the English Edition of Vol.1 is in advance.

First edition of " Cross Sections for Atomic Processes Vol.2 " [3], which contain systematic compilation of data on all types of atomic processes involving helium, hydrogen atoms and molecules, their ions, electrons and photons, is in print and expected to be issued in May 1977.

Efforts to compile and evaluate atomic data relating to impurity problems in fusion plasmas, neutral injection heating, and plasma diagnostics are organized in various styles of work shops. Several parts of the compilation tasks will be published in preprints from the IPP shortly as follows:

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

KATO, T., "Excitation and Ionization of Ions by Electron Impact - a Review of the Calculation by Means of Semi-Empirical Formulae" IPPJ-AM-2.

MORI, K. et al., "Energy Levels and Grotrian Charts of Highly Ionized Ions of Iron (Feⁿ⁺) n=8-26" IPPJ-AM-3.

OKUNO, K., "Bibliography of Charge Transfer Collisions of Highly Ionized Ions with Atoms".

IWAI, T., "Experimental Cross Sections for Ionization and Excitation of Ions by Electron Collisions". etc. Besides to these activities, a sub-group was organized in the SG to compile and evaluate fundamental data concerning with the plasma-wall interactions, in 1976 under the leadership of J. Okano. Members of this group consist of about 10 specialists in the research fields of surface physics and vacuum technology. A list of members of the sub-group is given in Appendix 2. This group is preparing for publication of a review involving compilation of bibliographic references on varieties of particle-wall interactions. Expected contents of this review are shown in Appendix 3.

REFERENCES

- TAKAYANAGI, K., editor, "Report of Research Group in the IPP on a Planning of Atomic and Molecular Data Compilation" IPPJ-DT-44 (1974).
- [2] TAKAYANAGI, K., SUZUKI, H., ed., " Cross Sections for Atomic Processes" Vol.1, Processes Involving Hydrogen Isotopes, Their Ions, Electrons and Photons, IPPJ-DT-48 (1976).
- [3] TAKAYANAGI, K., SUZUKI, H., OHTANI, S., ed., "Cross Sections for Atomic Processes" Vol.2, Processes Involving Helium, Hydrogen Atoms and Molecules, Their Ions, Electrons and Photons, IPPJ-DT-50 (1977).

2. PLANS OF THE SG IN THE 1977 FISCAL YEAR

Biobliographic Compilation

The SG has depended mainly on bibliographies and reference indexes of K. Takayanagi or reference library of W. Shearer-Izumi and T. Watanabe for its reference sources which are necessary to its compilation tasks of numerical data. The SG considers to support of updating of those reference libraries from this fiscal year and has no plan to begin its own compilation of references except for the case of plasma-wall interactions.

Compilation of Numerical Data

In addition to the effort to complete the enlarged part of "Cross Section for Atomic Processes" Vol. 2, a series of compilations of cross sections or rate constants for the processes involving impurity ions in high temperature plasmas has shared by about ten members. It will be a main work for this fiscal year. Several parts of this compilation will be published as soon as they are finished.

Workshops for Solving Urgent Problems

The SG is preparing to organize several workshop meetings which convene the investigators who have special subjects in the high temperature plasmas, and specialists in atomic-and astro physics, in order to ask them to solve their common problems. During these meetings informations or data will be compiled if they are available. Estimations of data by calculations using semi-empirical methods will be also useful to respond the urgent needs, if they are not available in the published literatures. The reports on results of discussions and created informations in these meetings will be published for each occasion. One of possible subjects is considered to be diagnostics in the JIPP-T2 device concerning to the cold particles in the plasma-gas interface.

3. ESTABLISHMENT OF THE FUSION RESEARCH CENTER FOR DATA ANALYSES AND SYSTEM STUDIES (tentative name) IPP/NAGOYA UNIVERSITY

This Center is officially established in the 1977 fiscal year. Its organization is in progress. According to the schedule by the arrangement committee, it will be composed of three sections on a three year program. One of these sections will have the function of an information center for atomic and molecular and other relevant data for fusion research and related fields. In near future, several scientists will be engaged in the businesses for atomic data center as a full-time staff. Activities of the present SG will be succeeded by the center and will be developed further on the official basis.

4. PROPOSALS FOR POSSIBLE COLLABORATIONS TO THE DATA CENTER NETWORK FROM THE SG AND THE NEW CENTER IPP/NAGOYA

The SG and the Center IPP/Nagoya will be able to propose the following possible contributions to the data center network at this stage of the program for the international cooperation.

- Publication of English Edition of "Cross Sections of Atomic Processes" Vol.1 and Vol.2.
- (2) Future Publications of Compilations of Numerical Data in English.
- (3) <u>Management for Promotion of Contributions of Prepublished Data and</u> <u>New Requests of Data to the IAEA/NDS Bulletin from Research Groups</u> <u>in Japan.</u>

In order to promote contributions of prepublished data to the IAEA/NDS bulletin from the active research groups in Japan, it should be most effective that the SG or the Center will take services for management of sending the request letters and collecting the contributions in adequate formats, for the NDS itself. It will be also effective that the SG serves to propagate the informations on the Bulletin to encourage the contributions from active investigators. As an example of these actions, the chairman and the secretary of the SG recently presented invited talks at the Annual Meeting of the physical Society of Japan, where they requested the cooperation to the international Bulletin to Atomic and Molecular Physicists. *

Main investigators and their institutes who are expected to be contributors of their fresh data to the Bulletin are listed in Appendixes 4,5, 6, and 7. Names of several institues which are expected to be responsible to the new requests of data are listed in Appendix 8.

(4) Collaboration in the Creation of the Format of the Bibliographic Index and the Imput to the Index.

The SG or the Center IPP/Nagoya will share the work for the creation of the international format of the bibliographic index for collision data and the future imput of references into the index. The Center will consider the transformation of reference libraries of Prof. Takayanagi or Dr. Shearer-Izumi to the international format, if it is desired.

(5) Collaborations in the Future Plans for Compilation of Numerical

Data

The Center IPP/Nagoya is considering to take part of the international collaboration for compilation and evaluation of numerical data and their exchange, which will be coordinated by the IAEA/NDS in the future.

* OHTANI, S., "Atomic Processes which are essential in Thermonuclear Fusion Research."

SUZUKI, H., "International Cooperation in the Data Bank Activities for Atomic and Molecular Data."

Invited Talks in the Spring Meeting of the Physical Society of Japan, (4-7 April 1977 , Yamaguchi University).

Members of the Atomic Data Study Group

Institute of Plasma Physics, Nagoya University, Japan

May, 1977

Main Group

Hiroshi Suzuki	(Sophia University, Chairman of the SG, atomic collisions, experimental)	
Hajime Narumi	(Hiroshima University, elementary processes in plasmas, atomic collisions, theoretical)	
Kazuo Takayanagi	(Institute of Space and Aeronautical Science, University of Tokyo, atomic collisions, theoretical)	
Yukikazu Itikawa	(Institute of Space and Aeronautical Science,University of Tokyo, atomic collisions, theoretical)	
Yozaburo Kaneko	(Tokyo Metropolitan University, atomic collisions, mass spectroscopy, experimental)	
Tsuruji Iwai	(Osaka University, atomic collisions, molecular spectroscopy, experimental)	
Kazuo Mori	(Institute of Physical and Chemical Research, plasma spectroscopy, experimental)	
Tsutomu Watanabe	(University of Tokyo, atomic/molecular structure and collisions, theoretical)	
Michio Matsuzawa	(University of Electro-Communications, atomic/molecular structure and collisions, theoretical)	
Hiroki Nakamura	(University of Tokyo, atomic/molecular structure and collisions, theoretical)	
Tatsuo Arikawa	(Tokyo University of Agriculture and Technology, atomic collisions, experimental)	
Hiroyuki Tawara	(Kyushu University, atomic collisions, experimental)	
Kazuhiko Okuno	(Tokyo Metropolitan University, atomic collisions, mass spectroscopy, experimental)	
Walter C. Shearer-Iz	umi (University of Tsukuba, applied atomic physics, experimental)	
Toshinobu Takayanagi	(Sophia University, atomic collisions, experimental)	
Takako Kato	(Nagoya University, astrophysics, theoretical)	
Takasi Fujimotc	(Kyoto University, plasma spectroscopy)	
Masamoto Otsuka	(IPP, plasma spectroscopy, experimental)	
Junji Fujita	(IPP, plasma diagnostics, experimental)	
Yoshinosuke Terashima (IPP, plasma physics, theoretical)		
Takaichi Kawamura	(IPP, plasma physics, theoretical)	
Shunsuke Ohtani	(IPP, acting as Secretary of the SG, atomic collisions and plasma diagnostics, experimental)	

Subgroup for Data Compilation on Plasma-Wall Interactions

Jun Okano	(Osaka University, Leader of the Subgroup, surface physics, mass spectroscopy, experimental)
Gen'ichi Horikoshi	(National Laboratory for High Energy Physics, vacuum physics, accelerator technology, experimental)
Hideo Akimune	(Kyoto University, CTR technology, experimmntal)
Yasuo Fujii	(Osaka City University, surface science, experimental)
Hazime Shimizu	(Electrotechnical Laboratory, surface technology, experimental)
Yukio Ishibe	(Institute of Physical and Chemical Research, vacuum technology, experimental)
Akira Miyahara	(IPP, CTR technology, experimental)
Yoshi-hiko Ichikawa	(IPP, plasma physics, theoretical)
Kenya Akaishi	(IPP, acting as Secretary of the Subgroup, vacuum technology, surface physics, experimental)

Bibliography on Plasma-Wall Interactions in preparation by the SG, IPP/Nagoya Editors: J.Okano, A.Miyahara and K.Akaishi Preface Chapter 1. Sputtering by Neutral Particle- and Ion-Impact and Its Relation to Plasma-Wall Interactions. Cooperative Effects in Sputtering (Akaishi and Miyahara) Chapter 2. Chemical Sputtering (Shimizu) Chapter 3. Blistering (Akimune) Chapter 4. Desorption of Gases by Electron- and Ion-Impact (Ishibe) Chapter 5. Desorption of Gases by Photon Impact and Thermal Desorption (Horikoshi) Chapter 6. Secondary Electron Emission by Electron-, Ion- and Photon-Impact. Getter Materials. (Fujii) CHapter 7. Surface Phenomena -Reflection, Diffusion, Absorption, Surface Migration, etc. Chapter 8. Surface Diagnostics: SIMS, QWAAS, etc. (Okano) Chapter 9. Surface Influx (Ichikawa) Chapter 10. Related Problems: Ion Source Design, etc.

A list of research groups on Atomic Collision Data with key personnel

S. Ohtani, T. Iwai, K. Okuno [Institute of Plasma Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya-shi, 464] Measurements of excitation, ionization and charge transfer cross sections of highly ionized ions in collision with electrons or neutral atoms are being prepared. J. Fujita, K. Kadota [Institute of Plasma Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya-shi, 464] Diagnostics of JIPP-T2 by means of fast neutral analysis. Excitation cross section measurement for neutral-neutral collision, to utilize it for the active plasma diagnostics with the use of neutral beam. S. Ohtani, H. Suzuki, H. Nishimura [Institute of Plasma Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagova-shi 4641 Differential cross sections for ionization and excitation of hydrogen atoms by low energy electron impact are being measured. Auger electrons ejected from an atom by electron impact near threshold are also being observed. H. Suzuki, Y. Wakiya, T. Takayanagi [Faculty of Science and Technology, Sophia University, Kioicho 7, Chiyoda-ku, Tokyo 102] Differential cross sections for excitations of some atoms and molecules by electron impact are being measured with electron spectrometry. Autoionizations and Auger effects are being investigated in detail. T. Iwai, S. Tsurubuchi, M. Kimura [Faculty of Science, Osaka University, Machikaneyama-machi 1-1, Toyonakashi, Osaka-fu 560] Inelastic collision processes of water molecule by electron and ion impact are being investigated. Spectroscopical methods are used in a variety of collision experiments. K. Kuchitsu, T. Kondow, T. Hirooka [Department of Chemistry, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113] Ionizing collisions of long-lived highly-excited atoms. Visible emission spectroscopy of dissociation fragments. Y. Hatano [Department of Chemistry, Tokyo Institute of Technology, Ookayama 2-12-1, Meguro-ku, Tokyo, 152] Doppler profile measurements of Balmer α radiation by electron impact on H_2 . Y. Kaneko, K. Okuno, N. Kobayashi [Faculty of Science, Tokyo Metropolitan University, Fukazawa 2-1-1, Setagaya-ku, Tokyo 158] Ion neutral reactions are being studied using an ion-drift tube and double mass spectrometer. Measurements of vibrational excitation cross sections for ionmolecule collisions by means of ion energy-loss spectra are in progress.

N. Oda, F. Nishimura

[Research Laboratory of Nuclear Reactor, Tokyo Institute of Technology, Ookayama 2-12-1, Meguro-ku, Tokyo 152] Atomic processes as the fundamental processes of radiation effects on the materials are being studied. Differential cross sections for ionizing collisions of electrons with atoms and molecules have been measured. Experiments on ion-e, ion-hv collisions are in preparation.

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H. Inoue, Y. Sato

[Research Institute for Scientific Measurements, Tohoku University, Sanjo-machi 19-1, Sendai-shi 980] Integrated and differential cross sections for elastic and inelastic collisions of alkali ions with rare gas atoms and some diatomic molecules are being measured.

T. Makita

[Department of Chemistry, Kyoto University, Kitashirakawa-oiwake-cho, Sakyo-ku, Kyoto-shi, 606] Differential cross sections for charge-changing processes are being measured.

M. Inoue

[The University of Electro-communications, Chofu-gaoka 1-5-1, Chofu-shi, Tokyo 182] Ion-neutral reactions are being studied using an ion cyclotron resonance

mass spectrometer.

T. Arikawa

[Faculty of Technology, Tokyo University of Agriculture and Technology, Naka-machi 2-24-16, Koganei-shi, Tokyo 184] Low energy ion-neutral collision processes are being studied by crossedbeam method.

N. Hishinuma

[College of General Education, University of Tokyo, Komaba 3-8-1, Meguro-ku, Tokyo 153] Scattering of thermal-energy H-atom beams by atoms and molecules are studied experimentally.

S. Morita, K. Ishii, H. Tawara*

[Faculty of Science, Tohoku University, Aoba, Aramaki, Sendai-shi 980] [*Faculty of Engineering, Kyushu University] Measurements of inner shell ionization cross section of various elements by heavy-charged-particle impact, using a 4 MeV van de Graaff accelerator. The similar measurements in electron impacts, using 300 MeV Lineac.

M. Sakisaka, F. Fukuzawa

[Faculty of Engineering, Kyoto University, Yoshida-Honmachi, Sakyo-ku, Kyoto-shi, 606] Innershell ionization of atoms by ion impact, beam-gas spectroscopy, using

4 MeV van de Graaff accelerator.

[The Institute of Physical and Chemical Research, Hirosawa 2-1, Saitamaken 351]

Measurements of inner shell ionization and excitation cross sections for the x-ray production, by high energy and highly ionized ions, using 160-cm cyclotron.

K. Ozawa

[Division of Physics, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken, 319-11]

Measurements of the K X-ray emission cross section from various solid targets in collision with high energy ions, using 2 MeV van de Graaff accelerator.

Y. Nakai, H. Ryufuku

[Division of Physics, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken, 319-11] Planning of measurement of cross sections for charge-changing processes of highly ionized ions, by the use of van de Graaff accelerator.

I. Koyano

[Institute for Molecular Science, Myodaiji-machi, Okazaki-shi, Aichi-ken 444] Measurement of state-selected ion-molecule reactions by a coincidence method.

T. Mochizuki

Institute of Laser Engineering, Osaka University, Suita-shi, Osaka 565]

K. Takayanagi, Y. Itikawa, I. Shimamura

[Institute of Space and Aeronautical Science, University of Tokyo, Komaba 4-6-1, Meguro-ku, Tokyo 153] Electronic atomic and molecular collision processes are being studied theoretically. Among others, electron transfer processes from highlyionized atoms to protons and inelastic collisions between highlyexcited hydrogen atoms and charged particles have been studied recently, and collision processes in a magnetic field are being investigated.

S. Nakazaki

[Faculty of Engineering, Miyazaki University, Nishi-maruyama-machi 118, Miyazaki-shi 880] Excitation cross sections are being calculated in the Coulomb-Born approximation for some electron-positive ion collisions.

H. Narumi, A. Tsuji

[Faculty of Science, Hiroshima University, Higashisenda-machi 1-1-89, Hiroshima-shi 730] Calculations of ionization and excitation cross sections by Glauber approximation. Atomic structure of exotic atoms. [The University of Electro-communications, Chofugaoka 1-5-1, Chofu-shi Tokyo 182]

Reactions of highly excited Rydberg atoms with other atoms and molecules are investigated theoretically.

T. Watanabe, H. Nakamura

[Faculty of Engineering, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113]

Theoretical studies of electronic and atomic collisions in a variety of collisional systems. Structure studies on atoms in excited states, including super-excited states. Various kinds of resonances are also interested in.

J. Hata

[Faculty of Science, Osaka City University, Sumiyoshi-ku, Osaka 558] Calculation of resonance scattering of electrons with atoms.

F. Koike

[Department of Medicine, Kitasato University, Asamizo-dai 1, Sagamiharashi, Kanagawa-ken, 228] Theoretical study on various processes in electron-atom and -molecule collisions.

S. Hara, T. Ishihara, W. Shearer-Izumi

[University of Tsukuba, Sakura-mura, Niihari-gun, Ibaraki-ken 300-31] Atomic collision theory. - 57 -

A list of research groups on Atomic Structure Data with key personnel

K. Mori, K. Ando

[The Institute of Physical and Chemical Research, Hirosawa 2-1, Wako-shi Saitama-ken, 351]

Plasma Spectroscopy, particularly in extreme ultra-violet and soft x-ray regions.

K. Fukuda, K. Ishii, H. Suemitsu, R. Okasaka, T. Fujimoto

[Faculty of Engineering, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto-shi, 606] Plasma spectroscopy in extreme ultraviolet region.

Beam-foil spectroscopy.

Determination of population density of atoms and ions in plasmas, using Hook method.

Other studies on elementary processes including excited atoms.

M. Nakamura

University of Tsukuba, Sakura-mura, Niihari-gun, Ibaraki-ken, 300-31] Atomic and molecular spectroscopy, and photoelectron spectrometry of rare gases and small molecules in vacuum ultraviolet region.

H. Takeyama, T. Oda, R. Ikee, M. Yamagishi*

[Faculty of Science, Hiroshima University, Higashi-Sendamachi 1-1-89 Hiroshima-shi 730] [*Faculty of Education, Tottori University] Plasma spectroscopy.

M. Otsuka, K. Sato

[Institute of Plasma Physics, Nagoya University, Furoo-cho, Chikusa-ku, Nagoya-shi 464] Plasma spectroscopy, spectroscopic studies of plasmas in contact with some neutral gases.

A. Funahashi

[Division of Thermonuclear Fusion Research, Japan Atomic Energy Research Institute, Tokai-mura, Naka-gun, Ibaraki-ken 319-11] Plasma spectroscopy, particularly in extreme ultraviolet region, JAERI JFT-2 and JFT-2a.

I. Hirota, Y. Maejima

[Tanashi Branch, Electrotechnical Laboratory, Mukodai-machi 5-4-1, Tanashi-shi, Tokyo, 188] Plasma spectroscopy.

T. Sasaki, S.Yamaguchi*, M. Nakamura**, T. Sagawa***

[College of General Education, University of Tokyo, Komaba 3-8-1, Meguroku, Tokyo 153] [*Faculty of Science, Tokyo Metropolitan University] [**University of Tsukuba] [***Faculty of Science, Tohoku University] Atomic, molecular and solid state spectroscopy, in extreme ultraviolet region, using a 300 MeV storage ring for synchrotron orbital radiation (SOR-RING).

M. Seya, T. Namioka

[Institute for Optical Research, Tokyo University of Education, Hyakunin-cho, Shinjuku-ku, Tokyo 160] Instrumentations in vacuum ultraviolet spectroscopy. High resolution spectroscopy of simple molecules.

T. Ishimura

[Faculty of Engineering, Osaka University, Suita-shi, Osaka 565] Plasma spectroscopy in extreme ultraviolet region.

T. Kagawa, T. Murai

[Department of Physics, Nara Women's University, Nishi-machi, Kita-Uoya, Nara-shi, 630] Relativistic multi-configuration self-consistent field calculation of atomic energy levels. Exact-electronic energies and wave functions of simple molecules by B-0 approximation.

K. Ohno, F. Sasaki, K. Tanaka

[Faculty of Science, Hokkaido University, Nishi 8, Kita-10jyo, Sapporoshi, 060]

Quantum mechanical calculations of atomic and molecular structures. Atomic level and oscillator strength by CI and SCF calculation. ab initio LCAO SCF MO calculation of polyatomic molecules.

H. Tatewaki

[Research Institute for Catalysis, Hokkaido University, Nishi 9, Kita-11 jyo, Sapporo-shi 060] Atomic SCF calculations using Slater-type bases.

S. Iwata

[The Institute of Physical and Chemical Reserach, Hirosawa 2-1, Wakoshi, Saitama-ken, 351] CI calculation with perturbation of molecular states.

O. Matsuoka, H. Taketa*

[The University of Electro-Communication, Chofugaoka 1-5-1, Chofu-shi, Tokyo 182] [*General Education Department, Kyushu University]

SCF calculation of diatomic molecules, using Gaussian type orbitals.

E. Ishiguro, H. Sato

[Department of Physics, Ochanomizu University, Otsuka 2-1-1, Bunkyo-ku, Tokyo, 112]

SCF calculation of molecules, using Slater-type orbitals.

K. Oohata, R. Akamatsu

[Faculty of Science, Kyushu University, Hakozaki 6-10-1, Higashi…ku, Fukuoka-shi 812] Calculation of electronic states and reaction process in molecules using BO approximation. List of research groups on data of surface interactions for fusion technology

J.Ckano College of General Education, Osaka University, Machikaneyamamachi, Toyonakashi, Osakafu 560] Secondary ion mass spectrometry by various ion impact from solid targets H.Akimune Research Center for Heliotron Device, Kyoto University, Gokasho, Ujishi, Kyotofu 611] Blistering on solid surfaces by proton impact K.Okamoto, Y.Ishibe [Laboratory of Nuclear Fusion Research, The Institute of Physical and Chemical Research, Hirosawa, Wakoshi, Saitamaken 351] Measurement of outgassing rate from solid surfaces by electron impact A.Miyahara, K.Akaishi Institute of Plasma Physics, Nagoya University, Furoocho, Chikusaku, Nagoya 464] Studies of plasma-wall interaction by means of the ion back-scattering technique and measurements of sputtering yields using a microbalance K.Sone, Y.Murakami Division Thermonuclear Fusion Research, Japan Atomic Energy Research Institute, Tokaimura, Nakagun, Ibarakiken 319-11] Measurement of sputtering yields of molybdenum and graphite by low energy (0.1-6 keV) proton impact. Sputtering and blistering experiment by high energy (30-400 keV) ion impact is in preparation. K.Kamada [Division of Physics, Japan Atomic Energy Research Institute, Tokaimura, Nakagun, Ibarakiken 319-11] Blistering on solid surfaces G.Horikoshi National Laboratory for High Energy Physics, Ohomachi, Tsukubagun, Ibarakiken 300-32] Desorption of gases by photon impact N.Itoh Faculty of Engineering, Nagoya University, Furoocho, Chikusaku, Nagoya 464] Channeling, color-center formation, irradiation defects in solids by ion impact R.Watanabe, H.Shiraishi

[National Research Institute for Metals, Nakameguro, Meguroku, Tokyo 153] Metallurgical properties of reactor materials

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List of research groups on astrophysics of interst to atomic data

S.Hayakawa, T.Kato X ray and IR astronomy K.Kawabata radio astronomy [Department of Physics, Nagoya University, Furoo-cho, Chikusaku, Nagoya 464] physics of sun Z.Suemoto (Director) J.Hirayama spectral analysis Nariai modeling of stars, theoretical [Tokyo Astronomical Observatory, Oosawa, Mitakashi, Tokyo 181] K.Nariai K.Kodaira astronomical spectroscopy T.Tssuji atmosphere of stars [Department of Astronomy, University of Tokyo, Hongo, Bunkyoku, Tokyo 113] physics of upper atmosphere T.Tohmatsu [Geophysical Research Laboratory, University of Tokyo, Hongo, Bunkyoku, Tokyo 113] M.Shimizu atmosphere of planets [Institute of Space and Aeronautical Science, University of Tokyo, Komaba, Meguroku, Tokyo 153] Y.Fujita atmosphere of low-temperature stars [Faculty of Engineering, Tokai University, Tomigaya, Shibuyaku, Tokyo 151]

List of fusion research groups expected to be contributors and proposers to the Bulletin

K.Takayama director head of the research group for JIPP-T2 K.Matsuura Institute of Plasma Physics, Nagoya University, Furoocho, Chikusaku, Nagoya 464] S.Mori head of the division of TFR M.Yoshikawa, K.Sako, T.Tajima design of JT-60 [Division of Thermonuclear Fusion Research, Japan Atomic Energy Research Institute, Tokaimura, Ibarakiken 319-11] K.Uo director Fusion Research Center for Heliotron Device, Kyoto University, Gokasho, Ujishi, Kyotofu 611] H.Itō director [Plasma Physics Laboratory, Faculty of Engineering, Osaka University, Yamadaue, Suitashi, Osakafu 565] C.Yamanaka director Research Center for Laser Fusion, Osaka University, Yamadaue, Suitashi, Osakafu 565] T.Sekiguchi T.Uchida N.Inoue [Faculty of Engineering, University of Tokyo, Hongo, Bunkyoku, Tokyo 113] S.Nagao [Faculty of Engineering, Tohoku University, Aoba, Aramaki, Sendai 980] I.Katsumata [Research Institute for Atomic Energy, Osaka City University, Sugimotocho, Sumiyoshiku, Osaka 558] S.Yano Kobe University of Marcantile Marine, Fukaeminamicho, Higashinadaku, Kobe 658] T.Kawabe, S.Miyoshi [University of Tsukuba, Sakuramura, Niiharigun, Ibarakiken 300-31] K.Okamoto fusion research T.Dote plasma physics Institute of Physical and Chemical Research, Hirosawa, Wakoshi, Saitamaken 351] T.Tamaru chief of plasma laboratory Tanashi Branch, Electrotechnical Laboratory, Mukaidai, Tanashishi, Tokyo 188]

Appendix 12

4 May 1977

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

compiled by Toyojiro FUKETA Nuclear Data Center, JAERI Tokai-mura, Ibaraki-ken, Japan

Activities on atomic and molecular data for fusion in Japan Atomic Energy Research Institute (JAERI) are carried out in co-operation with many Divisions and groups in JAERI especially with the Divisions of Thermonuclear Fusion Research, of Large Tokamak Development and of Physics. We also ask co-operation with the specialists other from JAERI's through many channels especially through the Research Committee on A + M Data of JAERI which will include non-JAERI members and be inaugurated about the middle of this year taking over the present Committee on A + M Data which is formed by JAERI's staffs only. A section for the A + M data in the Nuclear Data Center, JAERI (JAERI/NDC) is going to act as center and secretariat for the above activities. The section is led by Dr. Yohta Nakai with two concurrent staffs and two students specially received from the postgraduate doctoral courses of universities, and we are requesting to increase the staff of this section. We intend to characterize our data center activities in close connection with the development of actual fusion devices, especially of JT-60, a large tokamak with plasma volume of 60 m^3 .

A brief description of the related program and activities in JAERI is given in the following. ["Review of the Recent Activities on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute" compiled by Y. Obata, Y. Nakai, T. Shirai and M. Kase (4 May 1977), and a report by Y. Nakai at the Culham Meeting, November 1976 are also referred to.]

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1. Data Evaluation and Compilation

We are planning to make the A + M data evaluation and compilation on the specific items requested from the fusion programs in turn, and the following items are planned in this fiscal year, April 1977 to March 1978:

- (1) Cross sections of ionization and charge transfer for multicharged heavy ions in gases. Evaluation and compilation on this item are closely connected with the experimental and theoretical research programs mentioned later.
- (2) Electron-Atoms and -Molecules (especially hydrogen and its isotope atom and molecules) collision data.
 Electron energy range: thermal to 50 keV.

We are willing to contribute to the possible inter-centre exchange of numerical A + M data at least in Japanese literatures in cooperation and coordination with the JAP/Nagoya.

Common computer exchange formats for A + M collision data will be agreed relatively easily compared with the other A + M data. Among the difficult ones, sputtering data may be easier than blistering data to deal with. Convenient descriptive symbols should be devised to classify the surface condition of the samples in the compilation of sputtering or blistering data for example. However, descriptive comments on the experimental conditions, method of analysis, errors and so forth are more or less necessary in any computerized compilation of the numerical data. And at the present stage, we might propose to submit ideas on the common exchange formats for all type of A + M data of fusion interest in the next several months well before the next A + M data centres' meeting so as to discuss them practically at the next meeting.

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2. Bibliographic Indexing

We are willing to contribute to the international network by making the bibliographic indexing of the Japanese literatures on all type of A + M data of fusion interest in cooperation and coordination with JAP/Nagoya. The INIS may be utilized at least supplementally. Our investigation on the Japanese entry to INIS in 1976 shows that all Japanese literatures relevant to the A + M data for fusion research seem to be entered into INIS. These literatures in Nuclear Science Information of Japan, Vol. 7, Nos. 1 - 6 (1976) amount to 60.

3. Some Recent Topics of the Other Research Activities in JAERI

3.1. Cross sections of ionization and charge transfer

- (1) Measurements of ionization and charge transfer cross section for Ne⁺ and Ne²⁺ in H_2 , He and Ar
 - by Y. Nakai, K. Ozawa, T. Shibata, T. Takagaki, C. Kobayashi, and T. Shirai
 - To be published.

Energy Range: Ne⁺: 0.3 - 0.85 MeV

Measured Cross-sections:

 $\sigma_{ion}, \sigma_{10}, \sigma_{12}, \sigma_{21}, \sigma_{20}, \sigma_{23}$

for the following reactions:

Ne⁺ + A
$$\rightarrow$$
 Ne⁺ + A⁺ + e (σ_{ion})
 \rightarrow Ne⁰ + A⁺ (σ_{10})
 \rightarrow Ne⁺⁺ + A + e (σ_{12})

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$$Ne^{++} + A \longrightarrow Ne^{++} + A^{+} + e \qquad (\sigma_{ion})$$

$$\longrightarrow Ne^{+} + A^{+} \qquad (\sigma_{21})$$

$$\longrightarrow Ne^{0} + A^{++} \qquad (\sigma_{20})$$

$$\longrightarrow Ne^{+++} + A + e \qquad (\sigma_{23})$$

where A's are H2, He and Ar.

(2) Theoretical Studies

(i) Charge transfer processes of highly stripped ions

by H. Ryufuku and T. Watanabe* (*Univ. of Tokyo) Submitted to 10th Int. Conf. of Physics of Electronic and Atomic Collisions.

In the study of the atomic processes in the controlled fusion reactor, the charge transfer processes by impurity gas atoms and ions are very important. The electron capture from H atom by an impurity ion is considered as one of the rate-determining processes in plasma heating by neutral hydrogen beam injection.

In this paper symmetric charge transfer processes:

 $X^{Z+} + X^{(Z-1)+}(1s) \longrightarrow X^{(Z-1)+}(1s) + X^{Z+}$

and also one of asymmetric charge transfer processes of highly stripped ions: $H + 0^{8^+} \longrightarrow H^+ + 0^{7^+}(n, 1, m)$

are investigated theoretically in the high energy region with use of the semiclassical impact parameter method. In this work the two-level formula taken into account the trajectory deflection of incident particle due to Coulomb force is employed.

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(ii) Ionization collisions between two excited hydrogen atoms

by H. Nakamura*, T. Shirai, K. Iguchi** and Y. Nakai
 (*Univ. of Tokyo, **Waseda Univ.)

Submitted to 10th Int. Conf. of Physics of Electronic and Atomic Collisions.

Atomic collision processes involving excited species have been the subject of considerable recent interest from not only a practical but also a theoretical point of view. These processes have usually large cross sections and are important in many fields of applications such as a nuclear fusion plasma and so forth.

In this paper the type of process between two excited hydrogen atoms: $H^*(n_A, l_A) + H^*(n_B, l_B) \longrightarrow H^+ + e + H(n_B^+, l_B^+)$ is investigated theoretically in the high energy region with use of the semiquantal theory. The main purpose of the work is to know the dependence of the ionization cross section on the combination of the states (n, l) in the initial and final channels, where n and l are the principal and azimuthal angular quantum number respectively.

- 3.2. Multiple ionization of inner shell by heavy ion bombardment by K. Kawatsura, K. Ozawa, F. Fujimoto* and M. Terasawa** (*Univ. of Tokyo, **Tokyo Shibaura Electric Co.,Ltd.)
- Chemical effects on beryllium K X-ray spectra produced by heavy ion bombardment

Published in Phys. Lett. <u> 60Λ </u> (1977) 327 - 329 with the following abstract:

Beryllium X-ray spectra from Be and BeO targets by proton, helium, nitrogen and argon ion bombardment have been measured. In the oxide, chemical shifts of K_{α} and K^2_{α} X-ray lines are similar magnitude and the intense satellite KL and hypersatellite K²L lines are observed by heavy ion bombardment.

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(2) Double K-shell ionization of light elements by hydrogen and helium ion impact

Submitted to 10th Int. Conf. of Physics of Electronic and Atomic Collisions.

The X-ray production cross sections for the double K-shell ionization of Be and B atoms have been measured using H⁺ and He⁺ ion bombardment (0.25 - 2 MeV). The result shows the cross section for double K-shell ionization obeys the scaling relation of Z_1^{-4} law:

$$\sigma/Z_1^4 = f(E/\lambda U).$$

3.3. Ion bombardment on graphite and molybdenum

(1) Graphite surface erosions by 100 keV helium and hydrogen bombardment by K. Sone, T. Abe, K. Obara, R. Yamada and H. Ohtsuka Submitted to J. Nucl. Material.

Surface erosions in pyrolytic graphite by 100 keV ⁴He⁺ and 200 keV H_2^+ ion bombardment have been observed by scanning electron microscope. The particle fluence ranged from 1×10^{17} to 5×10^{18} particles/cm². Although the surface is eroded at 1×10^{17} particles/cm² in helium bombardment, it is not eroded so heavily even at 5×10^{17} particles/cm² in hydrogen bombardment. In helium bombardment flaking is significantly observed at 1×10^{18} particles/cm², and a cone structure appears at 5×10^{18} particles/cm², which is produced after the first cover all flakes off. In hydrogen bombardment at 1×10^{18} particles/cm², many circular blisters are formed, which are sputtered off at 5×10^{18} particles/cm².
- (2) Sputtering yields for 0.1 ~ 6 keV protons incident onto molybdenum and graphite targets
 - by K. Sone, H. Ohtsuka, T. Abe, R. Yamada, K. Obara, O. Tsukakoshi* T. Narusawa*, T. Satake*, M. Mizuno*, and S. Komiya* (*ULVAC Corporation)

In molybdenum, the sputtering yield at ambient temperature was obtained by in situ measurement of Auger electron signals from sputtered molybdenum atoms deposited onto substrate. An electro-micro-balance was used to calibrate the Auger signals. The present experimental sputtering yeild for molybdenum in the proton energy above 1 keV is about three times as large as the experimental one obtained by Finfgeld. Below 1 keV it rapidly decreases with decreasing energy, and reaches the small value of 1.9 X 10⁻⁴ atoms/ion at 0.15 keV. In pyrolytic graphite, physical sputtering yield at 500°C was measured by the same way as for The absolute value of the yield in pyrolytic graphite is molybdenum. about an order of magnitude as large as that in molybdenum, whereas the energy dependence is very similar to the molybdenum case, In addition, chemical sputtering (methane production) yield for pyrolytic graphite was measured at 1 keV, whose temperature dependence shows the maximum value of about 0.1 CH4 molecules/ion near 800°K.

(3) Very interesting phenomenon of "grain ejection" was observed in hydrogen ion bomberdment on molybdenum.

> by Y. Nakamura, T. Shibata, and M. Tanaka Submitted to J. Nucl. Material. The typical results are shown in photographs of Fig. 1.

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3.4. Dielectronic recombination of carbon, oxygen and iron in low-density and high-temperature plasmas

> by Y. Nakamura*, S. Kasai, and T. Tazima (*On leave from Sumitomo Heavy Industries, Ltd.)

JAERI-M 7019 (March 1977)

The coefficient of dielectronic recombination, which is one of the important atomic processes in tokamak plasmas, is evaluated by a semiclassical method neglecting the effects of the density and the radiation fields. Those of carbon, oxygen and iron, which play important roles in such as plasma resistivity and energy losses, are calculated numerically in the range of the electron temperature of 10 eV - 10 keV. Compared with the results obtained from Burgess equation, which is most useful for the ions with effective nuclear charge $z \leq 20$, our results show that Burgess formula is applicable for ions with $z \leq 25$ without much inclease in error. Our formula obtained in the present report may be more useful for the estimation of the dielectronic recombination coefficients of ions with z > 25 such as molybdenum.

3.5. Surface damage studies by ion bombardment

by K. Kamada, Y. Kazumata, H. Naramoto, and Y. Higashida

Blistering of Mo single crystal on high energy Ar^+ ion bombardment and flaking of pyrolytic graphite on bombardment with Ar^+ , N^+ and He⁺ ions have be**om** investigated.

Theoretical works based on the elasticity theory to clarify the mechanisms for the blistering and the flaking are also progressing, and satisfactorily quantitative explanations for the flaking in the pyrolytic graphite are given.





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200 pm 100 pm $M_{o} \leftarrow H^{+}$ Fig. 1

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4 May 1977

Reviews of the Recent Activities on Atomic and Molecular Data for Fusion in Japan Atomic Energy Research Institute (JAERI)

compiled by

Y. Obata, Y. Nakai, T. Shirai and M. Kase

Nuclear fusion plasma is composed of various elementary atomic and molecular processes which have complicated correlations with each other. The processes involving impurity atoms and ions, especially, have been the subjects of considerable recent problems related to not only plasma diagnostics but also radiative plasma coolings. Impurity atoms are mainly released from the first walls, i.e., limiter and liner in the fusion device of tokamak, due to atomic and ionic bombardments of the plasma such as sputtering and blistering, and also local evaporation and desorption of adsorbed and occluded gases. Since these adultarations of plasma are inevitable in feasibility experiment device (JT-60) and future thermonuclear fusion reactors, atomic and molecular data for fusion become important in order to analyse the problems of the interactions of plasma particles with impurity atoms and ions.

The studies in the past two years related to atomic and melecular processes in Japan Atomic Energy Research Institute (JAERI) are summarized in the gross form of classifications as follows:

1. Plasma Diagnostics; spectroscopic measurements of electron and ion temperatures, plasma density and confinement time and spacial distributions of impurity ions,

2. Surface Phenomena

2.1 Surface Damages; experimental stuies on damages (blistering and boyd) of the first wall materials by bombardments of ions and electrons.

2.2 Impurity Particles Released Form Surface; experimental studies of the quantities of impurity atoms and ions sputtered by neutral and ion beams to plunge into plasma,

3. Transport Phenomena Of Impurity Atoms And Ions; theoretical studies of the spacial distributions of impurity ions transported in various plasmas characterized by their densities, temperatures and confinement times,

4. Plasma Coolings by Impurity Atoms And Ions; theoretical and experimental studies of radiative energy losses upon recombinations, bremsstrahlungs, excitations and ionizations of impurity atoms and ions,

5. Plasma Heating By Neutral Beam Injection; experimental study of plasma heating by atomic hydrogen beam injection,

6. Theoretical And Experimental Studies Of Elementary Atomic And Molecular <u>Processes</u>; calculations and measurements of cross sections of elementary atomic and molecular collision processes, and also atomic and molecular structures such as energy level, transition probability and/or oscillator strength to identify ionic and atomic impurity species. The bibliography of the recent studies is given in the form of the above mentioned category.

1. Plasma Diagnostics

A. Funahashi, S. Kasai, T. Matoba and N. Fujisawa, <u>Measurement of Impurity=</u> <u>Ion Lines and Particle Confinement Time in Tokamak-Plasmas JFT-2</u>; JAERI-M <u>5961</u>, <u>30 (1975)</u>

H. Takeuchi, K. Takahashi, H. Shirakata and A. Funahashi, <u>Multi-Channel Neutral</u> Particle Energy Analyser for Measuring Ion Temperatures in Tokamak Plasmas, JAERI-M <u>6048</u>, 18 (1975)

A. Funahashi, K. Takahashi, Y. Shimomura, A. Kitsunezaki, T. Nagashima and K. Kumagai, <u>Fringe-Shift Interferrometric Apparatus for Tokamak-Plasma Diagnostics</u>; JAERI-M 6166, 53 (1975)

H. Takeuchi, A. Funahashi, K. Takahashi, H. Shirakata and S. Yano, <u>10-Cannel</u> <u>Neutral Particle Energy Analyser Apparatus and its Application to Tokamak Plasmas</u>; JAERI-M 6605, 50 (1976)

S. Kasai, A. Funahashi and T. Sugie, <u>Measurements of balmer H_{d} -line emitted</u> from tokamak plasmas in JFT-2a device; JAERI-M 6662, 23 (1976)

T. Matoba, A. Funahashi, T. Itagaki, K. Takahashi, K. Kumagai and T. Yamauchi, <u>Comparison in Electron Density Distribution of Tokamak Plasma Between Ruby-Laser</u> <u>Scattering and Milli-Meter Wave Interferometric Measurements</u>; JAERI-M <u>6685</u>, 21 (1976)

T. Matoba and A. Funahashi, Experimental Evaluation of Electron Heat Conductivity in High-Temperature Tokamak Plasmas; JAERI-M 6720, 22 (1976)

S. Kasai, A. Funahashi, T. Tazima and Y. Nakamura, <u>Spectroscopic Investigations</u> of the Vacuum Ultra-violet Emission in a Normal-incidence Region from JFT-2 Tokamak Discharge; JAERI-M 6761, 38 (1976)

H. Takeuchi, A. Funahashi, K. Takahashi H. Shirakata and S. Yano, <u>A 10-Channel</u> Neutral Particle Energy Analyser for Measurements of Ion Temperatures on Tokamak Plasmas; Jap. J. Appl. Phys., <u>16</u> 139 (1977)

2. Surface Phenomena

2.1 Surface Damages

K. Kubo, Interferometric Investigation of Ion-Bombarded Surfaces; JAERI-M 5977, 25 (1975)

K. Sone, and K. Shiraishi, <u>Calculations on Displacement Damage and Its Related</u> Parameters for Heavy Ion Bombardment in Reactor Materials; JAERI-M 6094, 39 (1975)

M. Tanaka, K. Fukai and K. Shiraishi, <u>Observation of Blisters formed on the</u> surface of Molybdenum irradiated with Ar⁺ ions at Ambient Temperature; JAERI-M 6585, 25 (1976) K. Kamada, <u>Surface Damage after Ion Bombardment; Mainly on Blistering;</u>
J. Atomic Energy Soc. of Japan,<u>17</u>, 517 (1975)

A. Hishinuma, Y. Katano, K. Fukaya and K. Shiraishi, <u>Radiation Damage in</u> <u>Stainless Steel Electron Irradiated in a High Voltage Electron Microscope</u>; J. Nucl. Sci. Technol. (Tokyo), 13, 656 (1976)

2.2 Impurity Particles Released From Surface

K. Sone, <u>Review of the works on Plasma-Wall Interactions in Fusion Reactors;</u> JAERI-M 6243, 29 (1975)

Y. Gomay and T. Tazima, <u>Recycling Process of Impurities in Tokamak Discharges;</u> JAERI-M 6297, 14 (1975)

Y. Gomay, S. Nomura, K. Fukuda, S. Muraoka and H. Nakamura, <u>An Estimate of Low-Z Materials for the First Wall of JT-60; JAERI-M 6432, 100 (1976)</u>

Y. Gomay, T. Tazima, N. Fujisawa, N. Suzuki and S. Konoshima, <u>The Study of</u> <u>Discharge Cleaning in the JFT-2 Tokamak with Surface Observation by AES</u>; JAERI-M 6647, 16 (1976)

3. Transport Phenomena Of Impurity Atoms And Ions

T. Tuda, Effect of a Radial Electric Field on the Impurity Transport; JAERI-M 6096, 11 (1975)

T. Amano and M. Okamoto, <u>Numerical Study of the Time Behavior Impurity</u> Concentration in a Tokamak; JAERI-M 6143, 15 (1975)

T. Tuda and M. Tanaka, <u>Impurity Drift Instability of Dissipative Type</u>; JAERI-M 6167, 6 (1975)

M. Okamoto and T. Amano, <u>Impurity-Evolution Code IMPHPCG and Analysis of the</u> <u>Impurity Measurements for JFT-2 Tokamak</u>; JAERI-M 6343, 44 (1975)

T. Amano and M. Okamoto, <u>A method of Solving the Rate Equations</u>; JAERI-M <u>6401</u>, 31 (1976)

T Tuda and M. Tanaka, <u>Pfirsch-Schluter Diffusion of a Plasma with Multiple Ion</u> Species; J.Phys. Soc. of Japan,<u>38</u>, 1228 (1975)

T. Tuda and M. Tanaka, <u>Impurity Drift Instability Due to Trapped Ions</u>; J. Phys. Soc. of Japan, <u>38</u>, 1792 (1975)

T. Amano and M Okamoto, <u>Numerical Investigation of the Time Evolution of Impurity</u> Concentration in a Tokamak; J. Phys. Soc. of Japan, 42, No. 3 (1977)

4. Plasma Coolings By Impurity Atoms And Ions

T. Sato, T. Hirayama, M. Maeno and N. Fujisawa, <u>Measurements of Plasma Energy</u> Losses to the Wall in JFT-2; JAERI-M 6577,16 (1976)

T. Tazima, K. Inoue and Y. Nakamura, <u>Density Distributions of Impurities and</u> Related Energy Losses in Tokamak Plasmas; JAERI-M 6606, 38 (1976) Y. Nakamura, S. Kasai and T. Tazima, <u>Dielectronic Recombination of Carbon</u>, <u>Oxgen and Iron in low-density and high-temperature plasmas</u>; JAERI-M 7019, 45 (1977)

5. Plasma Heating By Neutral Beam Injection

Y. Ohara, S. Matsuda, H. Shirakata and S. Tanaka, <u>Beam Focusing in the</u> Multiaperture Ion Sources; JAERI-M 6438, 20 (1976)

S. Matsuda and H. Yamato, <u>Conceptual Design of the Neutral Beam Injection</u> System for the 2000MWt Tokamak Reactor; JAERI-M 6222, 25 (1975)

6. Theoretical And Experimental Studies Of Elementaly Atomic And Molecular Processes

T. Iwata, K. Komaki, H. Tomimitsu, K Kawatsura, K. Ozawa and K. Doi, <u>Channelling</u> of H⁺ and He⁺ Ions in Pyrolytic Graphite; Radiat. Eff., 24, 63 (1975)

K. Okazaki, S. Sato and S. Ohno, <u>The Contribution of the Double Collision</u> Occurring in an Atom to the Yield of the Ionization and excitations of Noble Gases Irradiated by 100keV Electrons; Bull. Chem. Soc. Jap., 48,1411 (1975)

S. Ohno, <u>Calculation of the Ionization Yield in He by Incident Ar⁺ and H⁺ Ions</u> with the Initial Energies of 1 and 0.1 MeV; Bull. Chem. Soc. Jap., <u>48</u>, 2229 (1975)

K. Ozawa, K. Kawatsura, F. Fujimoto and M. Terasawa, <u>X-Ray Emission from Boron</u> and Boron Nitride by Bombardment with Nitrogen and Argon Ions; Nucl. Instrum. Methods, 132, 517 (1976)

F Fujimoto, K. Kawatsura, K.Ozawa and M. Terasawa, <u>Beryllium Double K X-ray</u> Emission by Proton and Helium Ion Bombardment; Phys. Lett., A, 57 263 (1976)

H. Ryufuku, <u>Calculation of Charge Transfer Cross Sections in Atomic Collision</u> by Impact Parameter Representation; JAERI-M 6274, 50 (1975)

H. Ryufuku and T. Watanabe, <u>Semi-Classical Treatment of Symmtric Resonant</u> <u>Charge Transfer between Coulomb Interacting Ions;</u> J. Phys. Soc. of Japan <u>41</u> 991 (1976)

Proposed Framework for a Bibliographic Index for A+M Collision

Data for Fusion

A. Lorenz

A bibliographic data index is a reference listing of existing numerical data sets in a given data field, which is designed to provide information about the existence and whereabout of the data. To be useful, a bibliographic data index should be as complete and up-to-date as possible, and present the information in a condensed, ordered and easy-to-scan manner.

If one defines a "data set" as one or more numerical values which resulted from the measurement, calculation or evaluation of a certain physical process involving one or more reactants in a given energy range, which was performed by one or more investigator at a given time and place, then it is possible to identify every existing data set uniquely by a limited number of identification descriptors. In the case of reaction and collision data, these basic descriptors are 1) incident particle(s), 2) target(s), 3) reaction process, 4) name of investigator(s) and 5) date. In a computerized index system, these basic identification descriptors should be coded, according to accepted conventions in order to allow easy computer sorting to produce desired output, and to perform selective retrievals on the data base.

In addition to the basic identification descriptors required to define a data set, it is desirable to include supplementary (non-structured) information providing the user with additional criteria in the performance of his search. In the case of reaction or collision data, these could be: 1) the state and nature of the reaction product(s), 2) the energy or energy range of the incident particle, 3) whether the work was experimental or theoretical, 4) which experimental or theoretical method was used, 5) nature of the reference, 6) place of origin of work, 7) a comment, and 8) title of reference.

The reference - that is where and when the investigator(s) publicized the work - is not needed to define the data set, but to inform the user where to find the description of the work performed, and perhaps where to find the data. Nowadays, however, in the neutron data field, it is not unusual not to find the numerical data in publications: they are often presented in graphical form, and therefore unreliable, or if produce in large quantities, they are not accepted by the publishers and are instead sent directly to the data centres, or included in separately published compilations.

Having ascertained the existence of a given data set, a bibliographic data index user must be given one additional item of information to enable him to obtain the numerical data. This information can be included in the index in the form of a referral pointer, indicating the inclusion of the desired numerical data in a published compilation or in the files of a data centre.

The items of information which have been proposed to form the bibliographic index for A+M collision data (e.g. identification descriptors, supplementary information, and referral pointer) are summarized in the Appendix. For convenience, they have been regrouped under three general titles: Physics Information, Bibliographic Information, and Reference to Data. All identification descriptors and the referral pointer are indicated as being <u>obligatory</u>, that is they have to be included in the index; the supplementary information items are indicated as being <u>optional</u>.

List of Information Items Proposed to be Included in Bibliographic Index

for A+M Collision Data

1. Physics Information

1. Incident particle(s):	identification of the most light-weight of process interactants. For more than one incident particle, list both. Sorted as a function of mass. States of ionization and/or excitation are given by conventional notation (Obligatory).
2. Target (particle):	identification of target particle, atom, ion or molecule. Same convention as for incident particle. In case of undefined target, specific convention can be adopted for individual cases (e.g. for nitrogen plasma, etc.) (Obligatory).
3. Reaction process:	defined by adopted classification scheme (see pro- posal in Appendix of Working Paper CM-7) (Obligatory).
4. Final product:	descriptive information on state and nature of reaction products, if needed (Optional).
5. Dhergy range:	energy or energy range of the incident particle. Given as E, E_{\min} and/or E_{\max} , or "larger than" or "smaller than" indicated energy. Also should have option to give temperature instead of energy, and the use of conventional terms, i.e. thermal, max- wellian, etc. (Optional).
6. Type of work:	indication whether referenced data is the result of experiment, theory, calculation, evaluation, or deduced from other data (Optional).
7. Nethod:	type of experimental or theoretical method used to obtain the referenced data (Optional).
8. Comment:	Abbreviated commentary relating to the experiment or the results (see CINDA) (Optional).

Bibliographic Information

1. Reference date: or "date of work", indicated by year and month of first publication; this information should be given independently of the manner in which the Reference is treated as a whole (Obligatory).

2. Reference type:	indication whether reference is a journal article, a lab report, a book, a conference proceedings, a thesis or a private communication (Optional).
3. Origin of work:	laboratory/institute or country where work was performed (Optional).
4. Reference:	principal part of the bibliographic citation (e.g. name of journal, vol., page, year of publication): can be given in the index proper (as in CINDA), or included in a separate bibliographic citation listing as Annex to index, with reference number given in index, or both (Obligatory).
5. Author(s):	part of bibliographic citation, can be given in full (i.e. all authors) as part of the full bibliographic citation in the Annex, or partially (first author as in CINDA) in the index proper, or both <u>(Obligatory).</u>
6. Title:	part of bibliographic citation which can be given in the index proper or in the bibliographic citation listing in Annex (Optional).
Reference to Data	
1. Data:	reference to the existence of the pertinent numerical

C.

reference to the existence of the pertinent numerical data in a published compilation or in the files of a data centre.

Appendix 15

TENTATIVE OPTIMIZATION OF THE FUTURE BIBLIOGRAPHIC INDEX

FOR A+M COLLISION DATA

J.L. DELCROIX

Rapport L.P. n° 164 Mai 1977.

TENTATIVE OPTIMIZATION OF THE FUTURE BIBLIOGRAPHIC INDEX FOR A+M COLLISION DATA

J.L. DELCROIX Université Paris-Sud - 91405 ORSAY - France

1 - INTRODUCTION

Following the recent meeting of an Advisory group on Atomic and Molecular (A+M) Data for Fusion in Culham (1-5 november 1976), a series of recommendations were prepared by the group and edited by the Nuclear Data Section of the International Atomic Energy Agency (IAEA/NDS) in a Summary Report hereafter mentioned as CSR (Culham Summary Report).

One of the first short-range tasks assigned by CSR to the IAEA/NDS is the creation of an international bibliographic index for atomic collision data. The description of the proposed bibliographic index is given in Appendix B of CSR from which we extract the two following pieces :

Limits of coverage

The index should cover the properties of collisions between electrons, photons, atoms and molecules (including ions) in chemical systems composed of either pure hydrogen (including D and T), or of hydrogen (and/or D, T) plus one or two other elements, such as H+Mo or H+CO...

Formats

... The experience and the methods developed at the IAEA in the development of the CINDA index on neutron reaction data should also be used, recognising, however, the greater complexity of the problem in A+M data. A semi-quantitative description of the collision process according to its initial and final states, energy range, etc. is desirable. If possible, the indexing of any one collision should fit on one line of an appropriate computer print-out format to be sorted according to a number of desirable criteria. The limits of coverage is of course a very important question and an optimization of these limits must be chosen in such a way as to satisfy the fusion community as well as possible, without accumulating and publishing a too large amount of information which would be costly and troublesome. The experience gained during the last six years of operation of our GAPHYOR system [1] may help to solve this problem by consideration of some simple statistics. The present note is an attempt to use these statistics to propose an optimization of the future International Bibliographic Index for A+M Collision Data. For shorter and by similarity with CINDA we shall call this new index CIAMDA (Computer Index of Atomic and Molecular Data).

2 - THEORETICAL "VOLUME" OF CIAMDA

Let us start from the methods used in our GAPHYOR system [1] : the information is classified by using firstly the following descriptors :

```
a) Process categories K
```

K = 1 properties of atoms and molecules ("Structure")

- K = 2 photon collisions
- K = 3 electron collisions
- K = 4 heavy particle collisions
- K = 5 macroscopic properties

The proposal made in CSR is to limit the scope of CIAMDA to K = 2, 3 or 4.

b) <u>Mendeleev families</u> A, B, C of the elements composing the chemical system under study. The proposal made in CSR is to limit the scope of CIAMDA to systems where

- B (and/or) C is blank

- A, B, C are not blank but one of them is hydrogen.

c) Structures of molecules P, Q, R/S, T, U taking part into a collisions.

In the most general case the chemical formulae of each P, Q ... molecule is written as

A₀ B_m C_n

(1)

No recommendation was made in CSR as to the complexity of molecules one wishes to cover. In GAPHYOR it was decided to limit this complexity by the relation :

$$l + m + n \leq M = 8 \tag{2}$$

Since in hot plasmas, large molecules are not expected to exist one could in CIAMDA propose to use the same condition with some smaller value of M. As a guide for this decision one may show $\begin{bmatrix} 1 \end{bmatrix}$ that the numbers P(M) of different molecules of type (1) limited by the relation (2) are those shown in the following table :

M	1	2	3	4	5	6	7	8
P (M)	4	10	20	35	56	84	120	165

d) Other descriptors and theoretical volume of CIAMDA

The theoretical volume V_0 of CIAMDA is defined as the number of different cases in the file. It can be estimated using the same methods as for GAPHYOR in reference [1] but taking into account the limitations proposed above in a) b) c). One finds the results shown below

М	1	2	3	4	5	6	7	8
vo	2,0 10 ¹⁵	2,0 10 ¹⁷	6,3 10 ¹⁸	1,0 10 ²⁰	1,1 10 ²¹	8,2 10 ²¹	4,9 10 ²²	2,4 10 ²³

Let us recall that these very large figures are some what academic. The available information is indeed much smaller as we shall see in the next section.

3 - EXPERIMENTAL "VOLUME" OF CIAMDA

The theoretical "volume" V_0 estimated in the above section is not realistic because most of the cases are empty by lack of available information. A more realistic approach consist in starting from the statistical properties of GAPHYOR. The experimental "volume" V of such a file will be defined as the number of computer lines per year (1 computer line = 1 bibliographic reference). In GAPHYOR and for the year 1975 this volume was :

V = 11420 (3)

Assuming that this material would be published with the same format as CINDA (66 lines per page) the resulting yearly book would extend over 173 pages or something like 200 pages taking into account the appendixes. This is reasonably small, but it is expected that the international cooperation would semewhat increase the volume of information extracted from the litterature (possibly by a factor 1,5).

Let us now discuss the simplifications brought by the limits of coverage proposed in CSR and by a possible value of M smaller than eight :

a) Categories of processes

The statistics in GAPHYOR are as follows

К	1	2	3	4	5
72	46,3	7,6	10,5	27,5	8,1

If one decides the limitation K = 2, 3, 4 for CIAMDA, then the experimental volume should be multiplied by

$$\alpha_{\rm K} = 0,46 \tag{4}$$

b) Mendeleev families

The difference of volumes of GAPHYOR and CIAMDA due to the limits on Mendeleev families given in 2.b above would be the following.

ĸ	2	3	4
GAPHYOR	100	100	100
CIAMDA	98,4	99,9	97,4

It is clear that these differences are not significant (in spite of a predictible visual simplification of the listings and of the book).

c) Complexities of molecules

The "volume" occupied in GAPHYOR by collisions with different values of M has been analysed statistically for a period of three monthes in 1975. The results are shown in the following table.

K	1	2	3	4	5	6	7	8
2	121	187	289	300	310	312	314	322
3	146	227	322	327	331	335	336	344
4	131	370	517	544	569	578	583	591
Σ	398	784	1128	1171	1210	1225	1233	1257

These statistics in spite of their inaccuracy show that to obtain a significant reduction in volume it would be necessary to decrease drastically M to the value 2 (which means including only diatomic molecules). If this decision would be taken the "volume" would be multiplied by a factor

α_M(2) ∿ 0,62

d) Nature of the analysed documents

In CSR the proposal was the following :

The index should include references to publications in regular journals, books, review reports (like NBS reports), proceedings of major conferences in the A+M data field (i.e. ICPEAC[#] and ICAP^{##}), and to theses if these are readily available, but not to internal reports ...

The present statistics in GAPHYOR is as follows

^{*} International Conference on the Physics of Electronic and Atomic Collisions.

^{**} International Conference on Atomic Physics.

JOURNALS and Review Reports	86 %
Books	3 %
Conferences	8 %
Theses	2 %
Internal reports	1 %

If one follows the above proposal the "volume" would be multiplied by a factor

e) Expected volume of CLAMDA

Collecting the preceding factors and introducing an amplification factor β due to international cooperation one would expect that the actual volume of CIAMDA would be of the order

$$V' = V \alpha_K \alpha_M \alpha_P \beta$$

With $\beta = 1,5$ (a reasonable value⁽¹⁾) one is left with two possibilities :

- Describe rather complex molecules up to M = 8 this means α_M = 1 and would give

V'∿ 7640

⁽¹⁾One specific problem is the inclusion of electron-ion recombination coefficients. In GAPHYOR they are partly described in K = 3 (electron collisions) and partly in K = 5 (macroscopic phenomena). Considering their importance in fusion research they should be included in CIAMDA and this would produce an increase factor $\beta \sim 1$, 015.

- Limit CIAMDA to mistomic molecules (M = 2) which would make α_M^{-1} 0,62 and consequently

V'∿ 4740

The first solution is obviously simpler for us in Orsay, because it produces a minimum of perturbation in our system. But the report gives the elements to decide whether the second solution could be considered as more efficient.

Reference

[1] J.L. DELCROIX. J. de Phys., à paraître (1977).

Appendix 16

CONTROLLED FUSION ATOMIC DATA CENTER

OAK RIDGE NATIONAL LABORATORY

Physics Division

FUNDING AGENCY

DIVISION OF MAGNETIC FUSION ENERGY ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

ESTABLISHED: 1962

STAFF

- C. BARNETT, DIRECTOR
- I. WILKER COMPUTER IMPUT
- S. HAWTHORNE EDITORIAL DUTIES

PART-TIME STAFF (20%)

- G. McNeilly Computer System
- M. WRIGHT PROGRAMMER
- D. CRANDALL PHYSICIST
- J. RAY ENGINEER
- R. PHANEUF PHYSICIST
- H. KIM PHYSICIST
- F. MEYER PHYSICIST

UNIVERSITY PERSONNEL (LITERATURE SEARCH, DATA COMPILATION AND EVALUATION)

- E. McDaniel Georgia Institute of Technology
- E. THOMAS GEORGIA INSTITUTE OF TECHNOLOGY
- H. GILBODY QUEEN'S UNIVERSITY, BELFAST
- T. MORGAN WESLEYAN UNIVERSITY
- R. MCKNIGHT UNIVERSITY OF VIRGINIA

A. HEAVY PARTICLE-HEAVY PARTICLE INTERACTIONS

- 1. GENERAL
- 2. ELASTIC SCATTERING COLLISIONS
- 3. EXCITATION
- 4. DISSOCIATION
- 5. INELASTIC ENERGY LOSSES (NO DETAILED PROCESSES)
- 6. Electron Transfer (between bound states)
- 7. IONIZATION AND STRIPPING
- 8. RECOMBINATION (ION-ION)
- 9. COLLISIONAL DEEXCITATION, BROADENING AND RELAXATION
- 10. HEAVY PARTICLE INTERCHANGE, REARRANGEMENT AND RECOMBINATION REACTIONS (ONE OR MORE IONIC REACTANTS)
- 11. HEAVY PARTICLE INTERCHANGE, REARRANGEMENT AND RECOMBINATION REACTIONS (ONLY NEUTRAL REACTANTS)
- 12. Spin Exchange
- 13. ELECTRON DETACHMENT (FROM NEGATIVE IONS INTO CONTINUUM)
- 14. INTERACTION POTENTIALS
- 15. TOTAL SCATTERING (ELASTIC AND INELASTIC)

- 1. EXCITATION
- 2. DISSOCIATION
- 3. IONIZATION
- 4. DETACHMENT
- 5. QUENCHING
- 6. GENERAL

- C. PARTICLE PENETRATION IN MACROSCOPIC MATTER (IONS, NEUTRALS AND ELECTRONS)
 - 1. GENERAL
 - 2. Energy Losses
 - 3. Energy to Create an Ion Pair
 - 4. PARTICLE RANGE
 - 5. MULTIPLE SCATTERING
 - 6. CHARGE STATE POPULATIONS
 - 7. Excited State Populations

D. PARTICLE INTERACTIONS WITH SOLIDS

- 1. GENERAL
- 2. SPUTTERING (ELECTRON AND HEAVY PARTICLE)
- 3. Secondary Electron Ejection by Electron Impact
- 4. Secondary Electron Ejection by Heavy Particle Impact
- 5. PHOTOELECTRIC EJECTION OF ELECTRONS
- 6. Reflection of Electrons from Surfaces (backscattering)
- 7. REFLECTION OF HEAVY PARTICLES FROM SURFACES
- 8. PRODUCTION OF ELECTROMAGNETIC RADIATION BY ELECTRON IMPACT
- 9. PRODUCTION OF ELECTROMAGNETIC RADIATION BY HEAVY PARTICLE IMPACT
- 10. SURFACE IONIZATION
- 11. DEEXCITATION AND NEUTRALIZATION AT SURFACES
- 12. GAS DESORPTION BY ELECTRONS, IONS AND PHOTONS
- 13. BLISTERING AND VOIDS IN METALS
- 14. RADIATION DAMAGE IN METALS
- 15. ION IMPLANTATION IN METALS

E. ELECTRON-PARTICLE INTERACTIONS

- 1. GENERAL
- 2. ELASTIC COLLISIONS
- 3. EXCITATION
- 4. DISSOCIATION
- 5. IONIZATION (CROSS SECTIONS)
- 6. RECOMBINATION (ELECTRON-ION)
- 7. Collisional Deescitation, Broadening and Relaxation
- 8. NEGATIVE ION FORMATION (CROSS SECTIONS)
- 9. Spin Exchange
- 10. FREE-FREE TRANSITIONS
- 11. TOTAL SCATTERING (ELASTIC AND INELASTIC)
- 12. POSITRONS WITH HEAVY PARTICLES
- 13. ELECTRON DETACHMENT FROM NEGATIVE IONS
- 14. BINARY ELECTRON-ELECTRON COLLISIONS

- G. TRANSPORT PHENOMENA AND AVERAGE PROPERTIES IN GASES
 - 1. GENERAL
 - 2. DIFFUSION OF NEUTRALS
 - 3. DIFFUSION OF ELECTRONS
 - 4. DIFFUSION OF IONS
 - 5. DRIFT VELOCITIES OF ELECTRONS
 - 6. DRIFT VELOCITIES OF IONS
 - 7. Scattering and Energy Loss Parameters of Neutrals in Gases
 - 8. Scattering and Energy Loss Parameters of Electrons in Gases
 - 9. Scattering and Energy Loss Parameters of Ions in Gases
 - 10. ELECTRONIC ENERGY DISTRIBUTION (VELOCITY AND ENERGY DISTRIBUTION OF ELECTRONS IN GASES WITH APPLIED ELECTRIC AND MAGNETIC FIELDS)
 - 11. MOMENTUM TRANSFER
 - 12. FIRST AND SECOND TOWNSEND IONIZATION COEFFICIENTS
 - 13. ELECTRON ATTACHMENT COEFFICIENTS
 - 14. PHOTON TRANSPORT

- H. PHOTON COLLISIONS WITH HEAVY PARTICLES, ELECTRONS AND PHOTONS
 - 1. GENERAL
 - 2. TOTAL ABSORPTION (GAS TARGETS)
 - 3. ELASTIC SCATTERING
 - 4. EXCITATION
 - 5. DISSOCIATION
 - 6. IONIZATION
 - 7. ELECTRON DETACHMENT FROM NEGATIVE IONS
 - 8. LUMINESCENCE IN GASES BY PHOTON ABSORPTION
 - 9. MULTIPLE PHOTON ABSORPTION
 - 10. PHOTOCHEMISTRY OF GASES
 - 11. FREE-FREE ABSORPTION ON INVERSE BREMSSTRAHLUNG
 - 12. PHOTON-ELECTRON SCATTERING
 - 13. PHOTON-PHOTON COLLISIONS
 - 14. COHERENT PHOTON EFFECTS

- I. GENERAL THEORY
- K. DATA COMPILATIONS

۰.

- L. POSITRONIUM AND MUONIUM
- M. REVIEWS AND BOOKS IN FIELD OF ATOMIC AND MOLECULAR COLLISIONS

N. BIBLIOGRAPHIES ON ATOMIC COLLISIONS

SECOND PRINT OUT



Aut	ΤНΟ	R]	ND	ΕX

BAYFIELD, J	. E.	24,	155
KHAYRALLAH,	G. A.	24,	155

FIRST PRINT OUT

- 98 -

CURRENT WORK

- 1. Newsletter
 - A. SUPPLEMENTS
- 2. COMPILATIONS
 - A. ATOMIC DATA FOR CONTROLLED FUSION RESEARCH ORNL-5206, ORNL-5207, February 1977
 - B. MULTICHARGED ION CROSS SECTIONS
 - 1. CHARGE EXCHANGE
 - 2. ELECTRON IONIZATION
 - 3. ELECTRON EXCITATION
- 3. BIBLIOGRAPHIES 1950-1975
 - A. CHARGE EXCHANGE
 - B. HEAVY PARTICLE EXCITATION
 - C. HEAVY PARTICLE IONIZATION
 - D. HEAVY PARTICLE DISSOCIATION
- 4. CONVERSION OF CROSS SECTIONS TO REACTION RATES; FIT REACTION RATES TO POLYNOMINAL; STORE CROSS SECTIONS, REACTION RATES AND POLYNOMINAL COEFFICIENTS IN CTR COMPUTER AT LIVERMORE FOR ON-LINE RETRIEVAL.

FUTURE PLANS

- 1. Update ORNL-5206 and 5207
 - 1. EQUILIBRIUM FRACTIONS
 - 2. Sputtering
 - 3. PARTICLE REFLECTION
- 2. EVALUATION OF THEORETICAL LITERATURE
- 3. Restructure A09, E-07
- 4. Replace Present Card Input System with Remote Terminal Input

Experiences from an international cooperation in data exchange

Draft H.D. Lemmel, 6 May 1977

A. Introduction

The neutron data centers (at Brookhaven, Saclay, Vienna, Obninsk) have now more than 12 years experience in the compilation of numerical data, in the production of related data indexes and bibliographies, and particularly in such systems usable for multilateral input and international exchange. I would like to report on some of the experiences which these centers have gained, mainly in the field of neutron data, but also in the field of more complex nuclear reaction data induced by charged particles and photons. There is no important difference between nuclear reaction data and reaction data for atoms, ions and molecules, except that for the latter ones one must invent some additional coding rules for molecules, ionization, and excited states. Thus I believe that the experiences gained by the neutron data centers can well be applied for all reaction data.

Until 1964, there was practically only one neutron data center, the Sigma Center in Brookhaven, which covered neutron reaction data from all the world. At that time it became obvious, that the importance and growing volume of the data required some kind of international cooperation, quite similar as is today the case for atomic and molecular data. For neutron data, additional regional or national data centers were then created. There was nowever little experience in the practices of international data exchange, and it took about five years until the neutron data centers had agreed on a common exchange format for their data exchange. This is now in successful operation since 1969. It seems therefore advisable, when starting an international cooperation for another data category, to study the experiences gained from the neutron data exchange. I should like to report on some of the principles of this cooperation.

B. Basic consideration

1. The main goal is the <u>compilation of numerical data sets</u>. For this purpose one has first of all to find a mechanism by which the data centers obtain awareness of new and old data sets and of experiments being in progress. This means essentially a bibliography, oriented to numerical data sets, or briefly a "bibliographic data index". There is quite some difference between a normal bibliography and a "bibliographic data index" required as a basis for numerical-data compilation. I shall explain this difference later.

2. Basic requirements for a useful mamerical data compilation are <u>sneed</u>, <u>completeness and reliability</u>. For this reason, the <u>limited manpower</u> available must be concentrated on the really important items, and all items not really needed must be omitted from the compilation. One must consider carefully, what items are really needed.

Speed, completeness and reliability of a simple-structured "bibliographic data index" can relatively easily be achieved for the full scope considered by a systematic scanning of literature in <u>regional data centers</u> and by continuing contacts of these centers with the authors.

For the numerical data compilation, completeness for the full data scope can be achieved only in a rather long-term project, and one will have to start with a limited data scope or from a certain date onwards.

Thus, one must envisage the <u>dual system</u> of a "bibliographic data index" which should be complete, disregarding whether the numerical data have been compiled or not, and a numerical data file which will be complete at first for a limited data scope only and later fo a gradually growing scope. 3. A basic requirement for a <u>system usable for an international coopera-</u> <u>tion</u> is simplicity, both for the "bibliographic data index" and for the numerical data file. If a system shall be operated in <u>only one center</u>, one can make use of all facilities of the computer available. But a system usable <u>for international cooperation</u> must be restricted to the least common denominator of the computers of the cooperating centers, present and future ones, and the potential customers of these centers. Therefore, any such system myst be restricted to the basic character set of capital letters, digits, and the 10 special signs generally available. The system must probably have a fixed record-length, possibly a record length of 80 characters.

4. In all such considerations one must clearly distinguish between the <u>center-to-centerexchange format and other special formats</u>. Simplicity is required for the center-to-center exchange format. But each cooperating center may develop different special formats for input, strorage and output. These special formats may be more refined and optimized for the computer available, with the only restriction that thay must be compatible with the simple center-to-center exchange format. In fact it is only about the exchange format that one has to reach agreement between the cooperating centers.

5. If the one or other of the cooperating centers has already a <u>computer-ized file in operation</u>, one can try to design an exchange format which is compatible to the systems in operation. However, if this is not possible, the systems in operation will have to be changed.

6. A <u>typical example</u> on the one side is the dual system of <u>CINDA</u> and <u>EXFOR</u>, <u>CINDA</u> being the "bibliographic data index" for neutron nuclear data, and EXFOR being the exchange format for numerical nuclear reaction data. Both systems fulfill the requirement of simplicity as needed for the international cooperation. Yet fancy output is still possible from both systems. Both systems in their exchange formats, are restricted to the set of capital characters, digits and 10 special signs. Yet the output, e.g. the CINDA book, contains lower case characters, Greek characters, "larger than" symbols, fat print, etc. If it were required for the scope of CINDA, the CINDA book could quite well also include superscripts, subscripts and all the facilities available on a photo-typesetting machine, but still maintain the requirement of the simple basic character set in its exchange format.

7. A typical example on the other side is the system of "<u>Recent Refer</u>ences" which was developed for operation at one center only, with quite some refinement, but which is usable for international exchange only with difficulties.

C. The "bibliographic data index"

1. A "bibliographic data index" must first of all have a <u>data classifica-</u> <u>tion scheme</u> which is detailed enough but not too detailed within the scope required by the data centers and their users. This is the main reason why each data compilation effort, be it in neutron nuclear data or in atomic collision data, must maintain its own "bibliographic data index".

2. The <u>depth of data classification</u> must be carefully considered according to the existing retrieval needs. Here we can learn from a recent experience: The system of "Recent References", although it covers chargedparticle nuclear reactions, could not be adopted as a basis for the recently started international effort of charged-particle nuclear data compilation, because the retrieval parameter "integral cross-sections" versus "differential data", which turned out to be important, did not exist in "Recent References". For this reason (and also because of the complexity of the "Recent References" system), a new "bibliographic data index" had to be created, along the principles of CINDA, for the purpose of charged-particle nuclear data compilation.

The unit of information for a conventional bibliography is "a reference". For a "bibliographic data index" the unit of information should not be "a reference" but rather "a data set". A data set can be defined as the measurement of a certain reaction-parameter on a certain target in a certain energy range of incident particles performed at a certain institute. There is not a one-to-one correspondence between a data set and a published reference, but rather a many-to-many correspondence. Each published reference may contain several data sets, and each data set may be published more than once or even not at all. CINDA therefore has the following structure: it lists the existing data sets sorted first by target material, then by reaction or reaction parameter, and then it lists in chronological order all existing data sets defined by energy range and laboratory. Then, for each data set all pertinent bibliographic references are listed. This typical data-set structure of CINDA shows the main difference of a "bibliographic data index" as compared to a conventional bibliography. This structure is important for the data compilation, because it helps avoiding duplicate compilation when a data set is published twice or more often, and it helps keeping track of data sets that have been published but become superseded by a revised data set issued later by the same author(s).

4. For reasons of <u>economy</u> and <u>handingss</u> the SINDA book had to be kept very compact, even at the cost of legibility. If the economic boundary conditions were less stringent, one could as well produce an easier readable book by replacing a code like "PR/C" by "Phys. lev.C", and by replacing "HAR" by "Harwell". This, in fact, is done in individual computer retrievals from the CINDA file. If one can afford a more volumbous and more costly publication, such cosmetic improvements are possible, of course. For the <u>convenience</u> of the users it turned out to be more practical to code a reference in the form PR/C 8 711 5/73 which is easily understood, rather than to code it in the form AB73 or similar with an inverted reference index.

5. CINDA is in so far a closed system, as in neutron physics only a
limited number of reactions and reaction parameters, are of interest. These are grouped in 49 so-called "quantities". For charged particle muclear data a <u>revision to CINDA</u> had to be made by introducing an openended data classification scheme. This more generalized CINDA is now in operation at the US National Nuclear Data Center at Brookhaven [T.W. Burrows and J.S. Burt: The bibliography of integral charged particle muclear data. ENL-NCS-50640, March 1977, covering the literature from 1 January 1976 to 31 January 1977]. This system can rather easily be adapted for atomic and molecular reaction data, by introducing conventions for the coding of molecules and ionizations. It gives in an self-explanatory string of coded information the target material, the incident particles, the process and/or the reaction products and, where needed, their state. Then follows the parameter measured such as crosssection or yield.

D. The numerical data file

1. With respect to numerical data files I would first like to explain the <u>different types of numerical data files</u>.

There are files for <u>evaluated data</u> optimized for data processing, for scientific computatitions or other applications. These require data in well defined and rigid formats. There are general-purpose evaluated data files and others specialized for specific purposes. Contents and format of such files is determined by the application envisaged. I will not discuss such files in further details; I only want to mention that also for evaluated data files one must distinguish between the exchange format, which must be easily acceptable by all types of computers, and center-internal formats, often packed binary, optimized for use on a given computer.

2. On the other hand, <u>experimental data</u> require a more flexible format. Experimental data exist in a large variety of different representations. There may be Legendre-coefficients of which a dozen of different representations exist. There may be upper limits of data, unsymmetric errors, various different error contributions, normalization values, flags, different units and other odd things. There may be linear tables with a single variable, or multidimensional tables with double or tripel differential data and with several variables.

If one wants to compile experimental data, all such information must be stored without a loss of information. For experimental data one needs a flexible system which can hardly be optimized for data processing, which must however be sufficiently defined that compiter processing of the data is nevertheless possible.

3. <u>Earlier systems</u> for storing experimental data had been designed in too rigid formats. Consequently, certain data types could be entered only after transformation into another representation, and such transformation decreased speed and reliability of compilation. Other data types could not be entered without loss of information, in particular loss of information about errors or error analysis. Consequently, experimental data compiled in too rigid systems were often not regarded as sufficiently reliable. The users did not trust the data, and the authors hesitated to submit their data to the centers.

4. Based on such experiences, the EXFOR system has been designed in 1969

for the international exchange of experimental nuclear reaction data. It fulfills all essential requirements:

- simplicity in structure and permitted character set, as required for the international exchange;
- flexibility as required to include all types of experimental data without loss of information;
- precise definitions, such that all essential information can be identified by computer programs and extracted for computer processing and information transformation into more rigid systems for specific purposes.

5. A brief <u>description of EXFOR</u> is available in a separate paper. I should restrict myself to explaining the most essential features.

Each EXFOR <u>entry</u> may consist of several subentries. Thus, different data sets resulting from the same experiment are entered in different subentries of the same entry.

A subentry consists of three sections:

- the numerical <u>data</u> table itself;
- a section for numerical parameters which are <u>common</u> to all lines of the data table;
- and the so-called <u>BIB</u>-section which contains text information giving a minimum of physics background needed for the understanding and correct interpretation of the data table.

The <u>data table</u> may contain an unrestricted number of columns with a field width of eleven digits. The meaning of the contents of each column is identified by certain column heading keywords. Examples are

> EN for the energy of the incident particles, EN-RSL for the energy resolution. ANG for the angle of an outgoing particle, etc.

The column heading keywords are mostly self explanatory and the list of permitted keywords is open-ended. The experimental results are entered under the column heading DATA, and the meaning of the data given is explained in the BIB-section under a keyword previous y called "ISO-QUANT", now called "REACTION". Under this keyword a coded information string is given which includes

- the target isotope and its state, or the :arget material,
- the incident particles,
- the process (such as inelastic scattering) and/or all reaction products and, where needed, their state.

These items of information define the reaction considered. The coded information string continues by describing, in coded form, the parameter

measured, such as

cross-section, yield, angular distribution, energy spectra, and others,

and continues, where necessary, to describe in coded form the representation in which data are given, such as

point data, Legendre coefficients, absolute or relative data, and so on.

This string of coded information, which accurately defines the experimental data given, is certainly a very important part of the system. We believe that we have found a convenient and precise formalism for describing all kinds of reaction data. For atomic and molecular data obviously a few more codes have to be defined to describe molecules, ionizations and excited states. This would certainly be possible by a rather trivial extension of the existing system.

The other items in the <u>BIB-section</u> concentrate on a minimum of text information needed to identify the origin of the data and to judge upon their quality. These items are grouped under certain keywords such as:

AUTHOR	(all authors)
INSTITUTE	(country and institute in coded form)
REFERENCE	(all pertinent bibliographic references)
STATUS	(including the source of the numerical data, a note whether the author has seen and approved the compiled data, etc.)
HISTORY	(who did the compilation and when, when was it revised and for what reason)
REACTION	(defining the data as described above)
FACILITY	
METHOD	
DETECTOR	
etc	
ERR-ANALYS	(defining the type of errors given; statistical, systematic, etc.)
CORRECTION	(explaining briefly which correction for experimental uncertainties have been considered)

Any mumerical data compiled are not meaningful without a minimum of such accompanying information which is needed to unlerstand meaning and reliability of the data. Since the compilation of this important explanatory information is already quite time consuming, one must carefully avoid the compilation of all less important items.

6. The most important source of data are the authors. The most important publications to scan by the data compilation centers are new progressreports. When a work of interest shows up in a progress-report, then it is the time to contact the author for obtaining the numerical results.

Published data tables, even in so-called archival journals, are not reliable. It is essential that a data set compiled from a printed source is sent back to the author for obtaining his approval for the data compiled. A surprisingly large fraction of published data is subsequently revised by the author. On the average each data set compiled will have to be revised at least once. This is a fact which one has to take into account, and for this reason the regional data centers are well advised to stay in permanent close contacts with the authors. There are many examples that the data centers found by means of their data checking programs errors in published data which had escaped the attention of the authors. Also, the authors are usually grateful when being asked by the data centers about items of error-analysis or normalization, which they had forgotten to mention in their publication.

E. Conclusion

The purpose of this paper was to demonstrate that whenever new cooperation schemes for data compilation and exchange are to be started, the experiences gained in the long-lasting international cooperation of the neutron data centers should be carefully studied and in particular the systems EXFOR and CINDA which are the results of a long learning process.

Admittedly, if one would have to re-design EXFOR and CINDA from scratch, certain details would perhaps find a somewhat different solution, but the principles would certainly remain the same.

I therefore recommend to consider carcfully whether not systems close to EXFOR and CINDA should be recommended also for atomic and molecular data, for which only small modifications to existing computer programs would be required.

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Appendix 1

A sample page from CINDA

						49 Indium	1	
Quantity	Energy Min	(ev) Max	Lab	т	ype	Documentation Ref Vol Page	Author, Comments Date	Data
Evaluation	-2	+3	WIN	Eval	Prog	UKNDC(75)P71	Jul75 Pope+ THERMAL+RESON PARAMETERS	
Diff Elastic	1.1+7		ОНО	Expt	Prog	ERDA-NDC-2 156	May75 Ferrer + NDG.TOF.	
Diff Elastic	8.0+6		OHO	Theo	Jour	NP/A 249 29	Sep75 Carlson + OPTMOD PARAM FROM PN REACT	
Emission	1.5+7			Expl	Rept	7.FK - 277	Jul74 Hermsdorf + DIFFSIG AT SANGS.TBL + GRPH	
	1 5+7				Data	EXEOR30275	ADT74DOUBLDIF(SANG467PTS) + PARTIAL ANGDIS	+
Emission	1.4.17		EC1	E	lour	VE 20 852	Nav74 Sal'Nikov+ TOFTRI DOURIDIFF+INTEGRI	•
a Emision	1.4 1/		FEI	CAPI	four		May76 ENGLISH OF YE 20 852	
	5011	80.4	E.F.I	Feet	Dept	VK- 10 57	75 Shorin + SIC(NEUT - E) TRI CRARH	
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	60.1				Date	EVEOD (0122 001	M-71 SIGMA FOR 22 EN RANGES GUN	L.
<i>L</i> .	5.0+5	8.4+4		F	Card	EAFOR+0222.003	Marra JUMA FOR 32 EN-RANGES OVN	т
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(a,p)	1.4+7		KYU	ExTh	Jour	NP/A 245 509	Jul75 Niidome+ SIG VS EP.ANG DISTR	
						49 Indium	n 113	
Quantity	Energy	(cv)	Lab	т	ype	Documentation	Author, Comments	Data
	Min	Max				Ref Vol Page	Date	
Reson Params	4.7+0	2.0+3	COL	Expi	Jour	PR/C 10 1910	Nov74 Rahn+49 RES.WG=0.075 EV	
Reson Params	None		COL	Revw	Conf	75Wash, 779	Mar75 Hacken+ TBL AVG WG.STF,NUMBER GWN,WG	
Tot Inelaste	3.9+5	1.0+7	ANL	Expl	Abst	BAP 20 562	Apt75Smith+ ACT TECHNIQUES USED CFD EXPT	
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					Prop	INR-1197 18	May70 - + SIGMA AT 10 ES GRAPH+TABLE	- +
	1.5+7				lour	APP 33 409	Mar68 Kozlowski+ SIGMA TO ISOMER=1 & HR	
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Quanny	Min	Max	Lao	1	ype	Ref Vol Page	Autor, Comments Date	Dat
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The Bibleogniphy of Integral Charged Particle Nuclear Data

T. IV. Burrow and J.S. Burb

	EXPERIMENTAL REFERENCES(cor	nt)	
No. Lab Reference	tmin Emax Author, Cor (MeV) (MeV)	mments Branch, Particle and Modifier	
Tilp, absorption) e(E	<u>}</u>		Reaction and quantity measured
89 mañ ñ feith 21 789	76 2.0+1 5.0+1 NASR+ NUG.		
Ti(p,x) ⁴⁸ Y (E) 90 RIC J JGR 01 5509 J JGR 79 314 J JGR 78 6920	76 1.7+1 4.3+1 MOLTON+ TBL. 5 74 1.7+1 4.3+1 + PART, SUPER, 73 1.7+1 4.1+1 PART, SUPER,	TAINLESS STOLL TYPE 302. CORR. TO JCR 78.6420(73) BY JCR 79.314(74)	Energy range of incident particle (in laboratory system unless otherwise noted in comments, 1,7 + 1 = 17.)
31V(p,n)31Cr (E) 91 K17(n 1m/15 3/ 234/1	N/6 4.0+0 4.4+0 SEKHARAN. NDG.	Emn/Par G	Branch, particle and modifler (see Appendix B for definitions)
02 RIC / JGR 01 5000 Cr(p.x) ³² Mn (E)	76 1.9+1 4.4+1 Unt TUN+ TUL. U	COUCCO FROM 55-302 NEALUR	Laburatory code (see Appendix D for expansions)
93 KIC J IGK 81 5689 **Er(p+n)***Mn *(E) 94 F50 J 1477 8 711	76 1.9+1 UALTON+ (45+-10 23 8.5+0 8.6+0 HCKENNA+ CURV.	0)HB FRUM 55-302 MENSURE. 	Reference code (see Appendix C for explonation of notation and for expansions)
\$0Cr(p,n)\$0050 (E) 95 FSU 3 PR/C 8 /11	73 8.6+0 9.0+0 #CKENNA+ FURY.	172=0.7905. <u>199650-(6.</u> 837+0.01 0.02) PAR	Entry number of reference Llock (see Section V)
4 124 0880010.003 32Cr(p.n)528n (E) 96 81 0 J 8120 224 53	76 8.8.0 9.0.0 . 11 ENTRIES. U D/G 6.3.0 7.3.0 INTLOR. IVI. EC	5732-1.279 REL TO .168 PAR C	Data index line data avoltable from cooperating centers (see table 2)
334n(p.4n)34Fe (E) 97 Hite U.B.NIE(/G)-180 558n(o.m)35Fe (E)	276 IR 1.5.2 STHE. CURV. P.	28	
98 KUU L CIP 53 2601 99 100 0 1000(SEC)-50	75 2.8+0 3.6+0 PMB: Atson+ Ciks 176 1.4+0 5.4+0 KHII NJ+ NUG. 41	v. 92-1409 KEV GANNAS, PORZENT 6	(see Appendix E for axpansion s of commonly used obbreviations)
F#(p+x)**Cr = 4(E) 100 R1C J 166 - 81 - 5689 - 1 158 - 75 - 114 - J 158 - 76 - 5528	26 1.9+1 4.4+1 UNLION+ TBL. 51 24 1.9+1 4.4+1 . PART. SUPEN. 23 1.951 4.9+1 . PORT. SUPER.	TAINLESS STIEL TYPE 302. FURR. TO JAR 28.6928(23) BY JAR 29.314(24)	

FIGURE 1. DESCRIPTION OF MAIN SUBSECTION

:

- 109 -Appendix

N

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

SHORT GUIDE TO EXFOR

EXFOR - a computerized EXchange FORmat - presents in a convenient compact form experimental numerical data as well as physical information necessary to understand the experiment and interpret the data. <u>Keywords</u> and <u>codes</u> make the information computer intelligible. The structure of EXFOR is briefly described in the following.

Each EXFOR "entry" consists of two or more "subentries". The first subentry of an entry contains information which is common to all the following subentries of that entry. Each subentry may include two types of information: Descriptive text information and numerical data. Each item of descriptive text information is identified by keywords such as TITLE, STANDARD, ISO-QUANT, which may exhibit a code within parenthesis, such as (GELI), (SCIN) for the keyword DETECTOR or (TOF), (COINC) for the keyword METHOD. The meaning of most keywords is self-explanatory. The meaning of most codes is given in the free text following the code. Of particular importance is the keyword <u>"ISO-QUANT"</u>. Under this keyword are coded the "isotope and quantity" or, in other words, the reaction and parameter measured.

EXFOR information is available in two formats:

- the "standard format" primarily designed for the international exchange of data in computer processable form, and
- the "edited format" in which coded information and data tables are edited in an easily legible form.

The EXFOR structure, the standard and edited formats are illustrated in example 1.

There are several categories of numerical data:

- In the DATA TABLE the numerical data of the quantity defined above under ISO-QUANT are given under DATA (or RATIO) together with the columns of independent variables, errors, etc.
- Constant numerical values which are common to the entire data table of a given subentry, are given in the CONSTANT PARA-METERS (also called COMMON in the standard format) section.
- Constant numerical values which are common to all subentries of a given entry, are given in the CONSTANT PARAMETERS (resp. COMMON) section of the first subentry of that entry.

All numerical data are defined by <u>Data-heading</u> keywords (e.g. DATA, EN = incident neutron energy, STAND = standard) and by <u>Data-unit</u> keywords (e.g. EV, MB). The list of Data-heading keywords presently used is given on page 6.

Some data tables may have a more complex structure, for example there may be several ISO-QUANT per subentry; in this case each ISO-QUANT is connected to its pertinent column in the DATA TABLE by means of a <u>"pointer"</u>, as illustrated in example 2. More generally a pointer can be used to connect related pieces of information (see example 3).

WUCLEAR C	DETA SECTICA, INTERNATIONAL ATOMIC ENERGY AGENCY, VIENNA, ACCESSION NUMBER	<u>2.208_352824</u>	EXFO	<u>R ENIRY</u>	30284	<u>(.</u>	
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EXAMPLE 1



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PRESENTED IN THE "EDITED" LISTING

IN THIS EXAMPLE, A POINTER LINKS AN ANGLE AND THE CORRESPONDING DIFFERENTIAL CROSS - SECTION ALSO NOTE THAT TABLES WITH MORE THAN 6 COLUMNS WHICH ARE TEDIOUS TO DECIPHER IN "STANDARD" FORMAT, ARE CLEARLY

919 - PROINTER . WHICH LINKS RELATED FIECES OF MUMERICAL AND/OR TEXT INFORMATION

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EXAMPLE 3

OF DATA - HEADING KEYWORDS LIST

KEYWORD EXPLANATION

EXPLANATION (cont'd)

HIGH LIMIT CF COSINF-HANGE OF ANGLE. LAR-SYSTEM
HIGH LIMIT CF COSINF-HANGE OF ANGLE. C-M-SYSTEM
COSIMO OF ANGLE.LIMITOR
HIGH LIMIT CF COSINF-HANGE OF ANGLE. C-M-SYSTEM
COSIMO OF ANGLE.LIMITOR
HEADING FCW COLUMN GIVING THF QUANTITY SPECIFIED
UNDER 'ISC-OMMAT'.
DATA GIVYS IN THE CITTER OF MASS SYSTEM
APPROXIMATE VALUT CF DATUM
HIGH LIMIT CF BATUM
HIGH LIMIT CF BATUM
HIGH CIMITOR 'EART-ANALYS'.
SECHH DATA-FARDON, IF MCGF THAN UND FRIEND-COL IS GIVEN.
EXPLANATICN UNDFR 'EART-ANALYS'.
COMMAT'. NOFF 'ISC-OMMAL'.
UNSYMPETRIC DATA-FARDON, FXULANATIN UNDER 'EART-ANALYS'.
COMMAT'. NO TH HOGE THAN ONS CHAID-CAL IS GIVEN.
'UNSYMPETRIC DATA-FARDON, FXULANATIN UNDER 'EART-ANALYS'.
UNSYMPETRIC DATA-FARDON, FXULANATIN UNDER 'EART-ANALYS'.
'UNSYMPETRIC CALUMN GIVING THE ANALYS'.
'UNSYMPETRIC SATID-FARDAG. FXULANATIN UNDER 'EART-ANALYS'.
'UNSYMPETRIC CALUMN GIVING THE AND NO FARTID-FARDON IS GIVEN. EARLANTISN UNDER 'EART-ANALYS'.
'UNSYMPETRIC CALUMN GIVING THE AND NO FARTID-FARDON IS GIVEN. EARLANTISN UNDER 'EART-ANALYS'.
'UNSYMPETRIC CALUMN GIVING THE NOTE AND NUBER 'EART-ANALYS'.
'UNSYMPETRIC GALUMN GREETER 'ANALYS'.
'UNSYMPETRIC GALUMN GREETER 'EART-ANALYS'.
'UNSYMPETRIC GALUD-FARDON FARDON GENER'.
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KEYWORD

EXPLANATION (cont'd)

A+M surface interaction data currently required for fusion which need to be evaluated

W. Heiland

This issue has been summarized at the meeting at Culham (IAEA Advisory Group Meeting on A + M Data for Fusion, Nov.1976). Since then the tasks in fusion research have not changed. Therefore only the main items are listed below in the order of the report from the last meeting:

A: PARTICLE SURFACE INTERACTIONS

- 1) Reflectior of hydrogen and helium
- 2) Accommodation of hydrogen atoms
- 3) Trapping of hydrogen and helium
- 4) Detrapping processes for hydrogen and helium
- 5) Sputtering by hydrogen, helium and "impurities" (C,O,..)
- 6) Blistering by hydrogen, helium
- 7) Desorption by ions (hydrogen, helium, impurities)
- 8) Desorption by electrons
- 9) Desorption by photons
- 10) Chemical reactions of hydrogen with surfaces
- 11) Secondary electron emission due to ions and electrons
- 12) Arcing
- 13) Energy loss

B: SURFACE MATERIALS OF INTEREST

- 1) Stainless steels and Inconels
- 2) Refractory metals: Mo, Nb, V, W...
- 3) Low Z materials: C,SiC, B4C,...
- 4) Trapping materials: Ti, Zr,...
- 5) Coatings

C: CHARACTERIZATION OF SURFACES

- 1) The source of materials
- 2) Surface preparation
- 3) Measurement of composition and structure

77-4168 Translated from Russian

> WORK AT THE KURCHATOV INSTITUTE ON ATOMIC AND MOLECULAR DATA

Yu.V. Martynenko Kurchatov Institute of Atomic Energy

The current tendency towards the construction of large thermonuclear fusion devices is giving rise to a real need for the detailed information which is essential to an understanding of the physical processes that occur in thermonuclear facilities and indispensable if future thermonuclear reactors are to have the soundest possible design. Physicists and engineers need atomic and molecular (A+M) data.

The leading fusion research organization in the USSR is the I.V. Kurchatov Institute of Atomic Energy (IAEh). Work has already started at the IAEh on compiling A+M data for thermonuclear fusion, although the A+M data centre has not yet been officially established and the A+M data compilation service is still in its formative period.

The present staff consists of one full-time specialist and three part-time specialists. The technical work is performed by the centralized services of IAEh. The staff is to be expanded in the future.

The compilation of bibliographical and numerical A+M data has already been started.

The bibliographical data are being compiled from Soviet literature from 1976 onwards, including preprints and proceedings of conferences, on the following topics:

A.1. Energy levels, wavelengths and line identification

- A.2. Transition probabilities
- A.3. Atomic collisions
 - (1) Collisions of electrons with atoms
 - (2) Collisions of heavy particles
 - (3) Photo-excitation and photo-ionization

A.4. Surface phenomena

- (1) Sputtering
- (2) Ion backscattering

- (3) Discomposition, free paths, changes in composition and structure of surface
- (4) Blistering
- (5) Chemical reactions on the surface
- (6) Inelastic processes
- (7) Desorption and gassing
- (8) General questions concerning surface phenomena

A.5. Plasma diagnostics

- (1) Optical methods
- (2) X-ray methods
- (3) Corpuscular methods
- (4) Laser methods
- (5) Calculation of ionic equilibrium and level population

A.6. Reviews, general papers.

The format of entries in the bibliography is about the same as that of the bibliographic compilation "Atomic data for fusion", edited by Barnett and Wiese.

We think it would be useful to collect bibliographic data from Soviet work and exchange all the information so collected. It is important that many national or regional centres should participate in this.

Initially the bibliographic data will be published in the form of preprints. Computer entry and processing of these data will begin after a unified international bibliographic index has been developed.

We have also started compiling numerical A+M data for thermonuclear fusion. The first such work, "Veroyatnosti radiatsionnykh perekhodov ionov C I-C V" (Probabilities of radiative transition of the ions C I-C V), was produced by V.A. Abramov and T.I. Zhukova. There are carbon impurities in the plasma owing to oil pumping or carbon contained in the wall material. The authors also performed experiments on tokamaks with limiters made of carbon or a material containing carbon. Therefore, carbon ion transition probabilities are necessary for optical methods of plasma diagnosis and for accurate calculation of energy losses through radiation. The authors also give, for each transition, wavelength, initial and final term characteristics and lifetime or oscillator power, and they refer to the sources from which their data are taken. If different sources present different data, they give all the data. No data evaluation was performed.

In the future we are going to compile the transition probabilities for oxygen and a selection of other elements, data on surface phenomena, excitation and ionization cross-sections for collisions of electrons with atoms and ions and charge exchange cross-sections. The schedule of work at the initial stage is determined by the needs of the plasma physicists and physicists dealing with the engineering problems of fusion at the IAEH, and is also based on the recommendations of the Advisory Group on Atomic and Molecular Data for Fusion, Culham, 1976.

Later on, A+M data requirements will also reflect inquiries and recommendations from competent scientific centres in the USSR.

Currently contacts are being established with other scientific centres in the USSR (such as the Leningrad Physico-Technical Institute, the Uzhgorod State Institute, the Khar'kov Physico-Technical Institute, etc.) for the following activities:

- (1) Exchange of information on A+M data (e.g. exchange of preprints);
- Use of libraries of bibliographic and numerical data available at these institutions;
- (3) Data of some types will be compiled in the laboratories of other institutions. This work will be co-ordinated by the A+M data centre of the IAEh;
- (4) The collected data will be evaluated in specialized laboratories and also by IAEh experts. Besides, contacts are being established with other A+M data centres in the USSR: e.g. the Centre for Atomic Spectra of Highly Excited Atoms, Spectroscopy Institute, USSR Academy of Sciences, and the Centre for Spectral Lines for Plasma- and Laser-Physicists, IAEh. Co-operation with these centres will be in the following fields:
 - (1) Co-ordination of work on data selection,
 - (2) Information exchange,
 - (3) Data evaluation,
 - (4) Replies to inquiries received from other institutions
 (e.g. we ask another centre to answer an inquiry on which we have no information).

The A+M data centre will distribute the collected information as well as information received from other Soviet institutions and the IAEA to the interested institutions and laboratories. Once a sufficient data bank has accumulated the Centre will answer inquiries.

We think it would be useful to compile the data by subject in the Soviet A+M data centres and to exchange all the information.

We intend to use material presented at conferences. Some all-union conferences are held in the USSR at which the A+M data required for thermonuclear fusion are presented: they include the all-union conferences on interactions between atomic particles and solids. The last such conference took place in Khar'kov in 1976 and the next is planned for 1978 in Vilna. There are also all-union conferences on the physics of electronic and atomic collisions. The last was held in Tiflis in 1975 and the next will be in Petrozavodsk in 1978. An international conference on atomic collisions in solids, at which data of value to fusion research may also be presented, is to be held in Moscow from 19 to 23 September 1977.

We highly value international collaboration in collecting A+M data and welcome the successful initial moves in this direction. For instance, we find the publication "Atomic data for fusion" which Dr. Barnett kindly sends us most useful, and the same applies to information provided by other colleagues.

As time goes on we propose to intensify the exchange of both bibliographic and numerical information relating to A+M data. Other forms of co-operation should also become possible, e.g. in the field of data evaluation.

In connection with all these prospects, we highly appreciate the IAEA's nuclear data activities.

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