International Atomic Energy Agency

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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

SIXTH MEETING OF THE

ATOMIC AND MOLECULAR DATA CENTRE NETWORK

IAEA Headquarters, Vienna, Austria
10-12 September 1986

SUMMARY REPORT

Prepared by A. Lorenz

November 1986

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

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Abstract

Summary report of the Sixth A+M Data Centre Network Meeting convened by the IAEA Headquarters, Vienna, Austria, on 10-12 September 1986. The meeting was attended by ten representatives of centres from four Member States concerned with the coordination of the international management of atomic and molecular data pertinent to controlled fusion research technology.

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A. Meeting Summary

1. Introduction

The sixth A+M Data Centre Network (DCN) meeting was convened by the IAEA Nuclear Data Section at IAEA Headquarters in Vienna, from 10-12 September 1986. The meeting was attended by ten representatives of data centres from four Member States, concerned with the coordinated international management of atomic and molecular data pertinent to controlled fusion research and technology. The meeting was chaired by D.H. Crandall.

The participants in this meeting are listed in Appendix 1, the Adopted Agenda is given in Appendix 2, and the List of Actions which resulted from this meeting, is given in Appendix 3.

2. Meeting Conclusions

The meeting

- recommended that the final report of the IAEA Advisory Group Meeting be published as a special supplement to the Nuclear Fusion journal, and that the iron data recommended by that meeting be incorporated in the internationally recommended A+M collision data file;

- decided to initiate a co-operative inter-centre project on atomic data characterizing the collision of H, D, He molecules and their ions and electrons of importance to plasma edge effects, and to have IAEA convene a meeting on this topic in 1987;

- reviewed the final version of the CIAMDA-86 index on atomic collision data, and made a number of suggestions with regard to its publication;

- decided to change the publication frequency of the International Bulletin on A+M Data for Fusion from quarterly to semi-annually;

- agreed that the A+M Data Centre Network be the body responsible to recommend A+M data for inclusion in international A+M Collision Data file, and made specific recommendation on the initial content of this file.

3. Next A+M Data Centre Meeting

The next meeting of the A+M Data Centre Network was proposed to be held at the Oak Ridge National Laboratory in November 1987.

B. Meeting Proceedings

1. Opening Statement by the Meeting Chairman, Dave Crandall

The A+M Data Network can be the primary instrument for attaining the common goals of the IAEA and the National Data Centres in their efforts to develop and distribute atomic data for fusion. The objective is to define "recommended" atomic data and compile these data in forms readily applied to magnetic fusion problems. A centrally agreed upon set of atomic data is likely to be widely used to minimize atomic physics as a source of uncertainty in fusion development.

To accomplish this, the A+M Data Network needs to move beyond individual data center efforts. There should be stronger data centre involvement in the collaborative IAEA efforts; data centres should avoid duplication as much as possible. The Network should be the body which is to recommend those A+M data for fusion that are to be included in the IAEA data base. There should be agreement among the data centers to divide the work and how to present the data to the users. A+M Data Centre Network meetings should become more data-specific, involving workshop-type activities. The Network should respond to the data requirements by choosing a problem, defining specific species and reactions, and, after sharing the work among themselves, transfer the data to the IAEA to be included in the data base of recommended data. The IAEA and the Network should interact more with INTOR and other fusion organizations that define atomic physics needs of fusion and use these data.

Together, the data centres have the manpower and skills required to assess and compile atomic data for fusion in a compelling manner that will result in recognition of the effort and use of the best data.

2. Progress Reports

2.1. The JAERI Activities on A+M Data for Fusion. Status Report, September 1986 (presented by H. Tawara). Appendix 4.

2.2. Progress Report from RIC/IPP/Nagoya. H. Tawara. Appendix 5.

2.3. Data Centres on Atomic Spectroscopy at the National Bureau of Standards (presented by W.L. Wiese). Appendix 6.
I. Atomic Energy Levels Data Center
II. Data Center on Atomic Transition Probabilities

2.4. Controlled Fusion Atomic Data Center. Oak Ridge National Laboratory. 5 September 1986 (presented by H. Hunter). Appendix 7.

2.5. Recent Numerical Data Activities at the Atomic Data Centre GAPHYOR. K. Katsonis. 5 September 1986 (presented by J.-L. Delcroix). Appendix 8.

2.6. GAPHYOR Status Report. J.-L. Delcroix. Appendix 9.

2.7. Progress Report of the A+M Data Unit. A. Lorenz. September 1986. Appendix 10.

3. Status of Report on the AGM on Iron

The report consists of four chapters

- Charge exchange (chapter by R.A. Phaneuf has been received).

- Ionization (chapter by M. Pindzola with input from Belfast was presented to this meeting in draft form).

- Excitation (chapter by A.E. Kingston with input from J.G. Hughes and T. Kato will be ready in a month or two).

- Dielectronic recombination (the chapter by H.P. Summers has not yet been submitted. W. Wiese will suggest to Rozman (USA) that he send the iron-like dielectronic recombination data to H.P. Summers).

It is estimated that the report will have approximately 250 pages. J.G. Hughes will write the introduction to the report. The deadline to have the report ready for publication was set to 31 December 1986.

This report will be submitted for publication to the IAEA Nuclear Fusion journal, and has been suggested to be published as a special supplement to this journal. This report will not be distributed free of charge to the subscribers of Nuclear Fusion; the cost per issue is estimated to be approximately US-$ 30.-, and will be available at half the cost when ordered through official government channels. The data centres were asked to investigate the possibility to have their respective governments order this report in bulk, and to inform the IAEA of such a possibility before the end of the year.

Action 1

There was an action on all authors of the report to send the recommended numerical data on tape to the IAEA.

Action 2

The follow-up action is to have the IAEA combine these data, and send them to all data centers on tape, and include them in the database of recommended data.

Action 3

It was questioned whether fits of the data should be included in the final report. It was suggested that only the data for the main transitions in excitation should be included in the report; also the report should include references to the spectroscopic data reports published by NBS, and to the proton-iron collision data by T. Kato at Nagoya.

It was agreed that the resulting iron data should be tested by modellers at JET and INTOR. M.F.A. Harrison agreed to ask INTOR officially on behalf of the Subcommittee and the A+M Data Centre Network their opinion on the use and testing of the iron data. M.F.A. Harrison shall transmit INTOR's reply to the network by letter through the IAEA.

Action 4

M.F.A. Harrison also agreed to ask the JET modellers to test the iron data in their modelling studies.

4. Co-operative Network Project

Three specific data topics which the network could work on co-operatively were discussed:

- Collision of H, D, He molecules and their ions and electrons at low energies (these data are of importance to plasma edge effects divertors and ion sources).

- Charge exchange cross sections for C and O, and spectra

- Complete data on Ni (similar to the Fe project).

The first of these three topics was chosen by the Network. For this purpose IAEA shall organize a specialists meeting (convened at no cost to the IAEA) convening plasma modellers and data centre representatives. Although the venue of such a meeting, suggested at the time of the data centre meeting, was the 2nd week of April 1987 at either Garching, Jülich,

Princeton or General Atomics, it was decided subsequently for logistical reasons to have the meeting in Vienna on 18-21 May, to take advantage of the presence of potential participants who would be attending the INTOR meeting on 4-15 May 1987 in Vienna.

Action 5

It was concluded that the participants of the meeting should consist of eight plasma phycicists and eight atomic physicists. It was suggested that Drs. M.F.A. Harrison, D.H. Crandall, H.W. Drawin, A. Miyahara and A. Shurygin be asked to nominate two plasma physicists, plus one alternate, each, to represent INTOR, the USA, Europe, Japan, and the USSR, respectively. The following groups were suggested to be drawn from: Princeton, GA, MIT, Garching, Nagoya, Jülich.

The title of the meeting was decided to be: "A+M Physics for Plasma Edge Studies". The objective of the meeting was concluded to be: "Identification of the fundamental processes in the plasma edge with special emphasis on H, He, and their molecules and ions". The meeting is to bring together plasma physicists and atomic physicists to address primarily data needs for the modelling of the plasma edge". The energy range of interest for this study is a few hundred ev and below.

In preparation for the meeting, the data centres agreed to bring the following data to the meeting:

- Belfast: electron impact ionization data,
- Nagoya: all other electron collision data,
- Oak Ridge: heavy particle collision data,
- NBS: spectroscopic data for the relevant molecules.

The Gaphyor and the IAEA centres volunteered to distribute a bibliography from their bibliographic databases for the pertinent processes and species.

Actions 6 and 7

The results of this meeting and of subsequent similar studies are planned to be published in the form of IAEA reports, and are intended to provide input to the IAEA recommended numerical A+M collision database.

5. Publication of the CIAMDA Index

The following recommendations and suggestions were made with regard to the content and appearance of CIAMDA-86.

- Remove Sections 5 and 6 of the non-indexed part of the publication.

- Give Section 4 of the same part a more descriptive title.

- Introduce a new Section in the beginning of the publication which lists the most important, and most used, (including spectroscopic) references. In this context, all participants were asked to send to the IAEA as soon as possible a list of the most useful references for inclusion in CIAMDA.

Action 8

- Consideration was given to the suggestion to include in CIAMDA-86 all the references included in CIAMDA-80. As such an alteration to the planned content would delay the preparation of the publication beyond the

absolute deadline, and would also result in a voluminous and more costly publication, it was decided by the majority of the participants to restrict the scope of CIAMDA-86 to the material added to the database since the publication of CIAMDA-80.

- The title on the cover of the publication should clearly indicate that CIAMDA-86 is a Supplement to CIAMDA-80. It was also suggested that the appearance of CIAMDA-86 be similar to CIAMDA-80.

The following recommendations and suggestions were made with regard to the sales and advertisement of CIAMDA-86:

- The Network was requested to inquire with their national authorities about the possibility of ordering CIAMDA in large quantities. The IAEA shall announce the publication of CIAMDA to the Member States and send copies of the letter to the A+M Data Centers.

Action 9 and 10

- It was suggested that CIAMDA be advertised at international and national physics and fusion meetings, such as the next ICPEAC, and the American Physical Society, and European Physical Society meetings. The network was asked to advertise CIAMDA wherever possible.

Action 11

- It was suggested that free copies of CIAMDA be sent by IAEA to physics and fusion journals for review.

Action 12

6. Publication of the Bulletin

- In order to give more time for the IAEA A+M Data Unit to devote to the compilation of recommended A+M collision data and to the development of the IAEA database of numerical data, it was decided by the Network to change the publication frequency of the IAEA Bulletin from quarterly to semi-annually. The last issue of the Quarterly Bulletin will be published in October 1986; the publication of the Semi-annual Bulletin will start in April 1987.

- The Oak Ridge A+M Data Center will continue to supply the periodic update to the bibliographic A+M database. The IAEA was asked not to devote extra time to add information to improve the quality of the updates.

- In an effort to guarantee the completeness of the bibliographic input of the Oak Ridge and Gaphyor centres, the two centres were encouraged to arrange a method to compare their literature coverage, and to report at the next meeting of the Network on the results of this comparison.

Action 13

7. IAEA Recommended Numerical Database

It was agreed by the Netwrok that the database of the internationally recommended numerical A+M collision data shall be compiled by the IAEA from data sets contributed by the A+M data centre network. The sets of A+M collision data to be included in the IAEA database shall be approved by the Network at their annual meetings. Data proposed to be recommended by the Network must be distributed to all data centres at least one month before a data centre meeting.

Action 14

The IAEA shall develop a publication format for the dissemination of the recommended data to the fusion community in accordance with the needs and requirements of the data users.

Action 15

It was agreed that the recommended A+M collision data shall be published in a new report series of the IAEA Nuclear Fusion journal. The outward appearance of these reports should be readily associated by the user community with the Nuclear Fusion journal. The IAEA was asked to devise a cover for this report series.

Section 16

It was proposed that the IAEA A+M data reports shall be distributed as a cost-free supplement to the subscribers of Nuclear Fusion. The cost of publication of these reports shall be covered by the budget of the Nuclear Data Section. At the present time, Nuclear Fusion has a distribution of 800 paid and 200 cost-free issues.

The initial composition of the IAEA A+M collision database shall include the following recommended data sets:

- the Belfast electron impact ionization datafor ions up to oxygen;
- the Belfast electron impact ionziation datafor ions up to nickel;
- the Nagoya excitation data on carbon and oxygen ions (IJJP-AM-27);
- the internationally recommended data on iron which resulted from the September 1985 IAEA meeting (see Section 2 above);
- the recommended atomic collision data which resulted from the March 1985 Daresbury workshop on A+M Data for Fusion.

The recommended data to be compiled by the IAEA shall be on isolated atoms, excluding density effects. In conjunction with the above list of recommended data, Belfast and Nagoya were asked to send their coefficient data with the computer programs to generate the curves to the IAEA on tape.

Actions 17 and 18

Also IAEA is to request the Daresbury data from Belfast for incorporation into the database.

Action 19

In order to incorporate fitting coefficients into the database, IAEA is to devise a format for parametric representation of the data in EXFOR.

Action 20

8. Publication of IAEA 1982-1984 CRP Report

It was announced that the summary report of the three-year IAEA Co-ordinated Research Programme on Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas (1982-1984), written by K. Katsonis and R. Janev, will be submitted for publication in the IAEA Nuclear Fusion journal before the end of 1986. IAEA was asked to ask Dr. Katsonis to include a list of authors and CRP participants in the report, and to add a Table of Contents.

Action 21

9. Review of Process Classification

In response to an action from the 1985 Data Center Network meeting, J.-L. Delcroix produced a report on a proposed classification scheme for atomic collision processes, and their definitions. The report (DG 24) was distributed at the meeting, and the participants were asked to communicate their comments to J.-L. Delcroix and to the other members of the Network.

Action 22

10. Miscellaneous

- Distribution Lists. It was requested that each A+M Data Centre send a copy of their distribution lists (including full names and mailing addresses), one for atomic physicists and one for fusion physicists who are users of atomic collision data, to the IAEA. The IAEA will combine the lists and send them out to the A+M Data Centres.

Action 23

- Telephone numbers of participants. As requested by the Network, the telephone numbers of all Network members and meeting participants are included in the List of Participants attached to this report.

- Dates of future meetings. A number of meetings related to the activities of the Network were mentioned in the course of our meeting; their dates and locations, where known, are listed here for general information:

- Next INTOR meeting, IAEA 1 December 1986
- IPAT 87 Int. Conference on Ion and Plasma assisted Techniques, Brighton, UK, 27-29 May 1987
- Next ICPEAC meeting, Brighton, UK, 22-28 July 1987
- ICPEAC satellite meeting organized by H.P. Summers, 6-8 August
- European Physical Society Meeting, Madrid, end of June 1987
- 1989 ICPEAC Meeting, Australia
- APS Division of A+M Optical Physics, end of May 1987

11. Next A+M Data Centre Network Meeting

The next meeting of the A+M Data Centre Network was proposed provisionally to be held at the Oak Ridge National Laboratory, in the USA, in November 1987. The following topics, mentioned during this meeting, should be on the agenda of the next meeting:

- Proposals of recommended data sets,
- On-line access to data
- Discussion of large Advisory Group Meeting Data Review meeting in 1989,
- Review of plasma edge meeting results,
- Production of a single bibliographic data base
- Discussion proposed process classification report by J.-L. Delcroix.

Appendix 1

Sixth Meeting of the A+M Data Centre Network

10 - 12 September 1986
IAEA Headquarters, Vienna, Austria

List of Participants

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Appendix 2

Sixth Meeting of the A+M Data Centre Network

10 - 12 September 1986
IAEA Headquarters, Vienna, Austria

Adopted Agenda

- Introductory and preliminary items
- Adoption of Agenda
- Review of Actions from 1985 meeting

1. Report from A+M Data Centre and Groups

2. Report from the IAEA A+M Data Unit

3. Numerical Data (Atomic Collision Data)

* - Status of A+M data base
* - Numerical data index
* - Data compilation (priorities, inter-centre exchange)
* - Procedures for the recommendation of data (see 1984 IFRC Subcommittee meeting recommendations)
* - Compendium of numerical data and data distribution to users (see 1984 IFRC Subcommittee meeting recommendations, November 1984 Report, page 3, item 5)
- Review of A+M EXFOR dictionaries
- Graphic and parametric representation of data
- On-line access of data
- Terminology and definition of processes

4. Bibliographic Data

* - Status of the A+M bibliographic data base
* - Exchange of bibliographic data
- Production of the A+M Data Bulletin
- Publication and sale of CIAMDA

5. A+M Data Meetings and Publications

- Status of final report of AGM on Atomic Data for Plasma Modelling and its publication
- Publication of final report of Collision Data for Diagnostics CRP conclusions and recommendations
- Next A+M Data Centre Meeting

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* To be discussed on Wednesday with the participation of IFRC Subcommittee

Actions

1.	Network	Investigate with authorities the possibility to order copies of the iron meeting report from the IAEA in large quantities, for distribution in own country.
2.	Authors of iron report	Send recommended iron data on tape to the IAEA.
3.	IAEA	Combine the recommended data on tape and send tape to the Network.
4.	Harrison	Ask INTOR to test the iron data, and inform the Network through the IAEA of their reply.
5.	IAEA	Organize the meeting on the plasma edge data.
6.	Gaphyor	Distribute bibliography of pertinent processes and species to the Network in preparation for the plasma edge meeting.
7.	IAEA	Same as Action 6.
8.	Network	Send in to the IAEA as soon as possible a list of most used data references for inclusion in CIAMDA-86.
9.	Network	Inquire with their authorities about ordering large quantities of CIAMDA-86 for distribution in own country.
10.	IAEA	Announce the publication of CIAMDA-86 to Member States, and send copy of the announcement to the data centres.
11.	Network	Advertise the publication of CIAMDA-86 to physics and fusion journals for review.
13.	Oak Ridge, Gaphyor	Arrange to compare coverage of their bibliographic databases, and present the results of comparison at the next meeting.
14.	Network	Distribute to all data centers data proposed to be recommended at least one month before the next DC meeting.
15.	IAEA	Develop a publications format for the dissemination of internationally recommended data.
16.	IAEA	Devise a cover for the atomic data series reports to be published by the IAEA.
17.	Belfast	Send to the IAEA on tape, the coefficients and the computer programs to generate the curves of the data which have been recommended.

Appendix 4

The JAERI Activities on A+M Data for Fusion
Status Report, September 1986

Y. Nakai, T. Shirai and K. Ozawa
JAERI, Tokai-mura, Japan

Construction of large tokamak device, JT-60 has been completed and its operation was started in April 1985 and the first plasma was achieved. In parallel to the investigation of JT-60, activities on A+M Data for fusion at JAERI has been carried out by A&M Data Section of Nuclear Data Center, in cooperation with Research Committee on A&M Data consisting of the members both in and outside of JAERI. The works in data compilation and evaluation are continued on the following 3 fields: atomic collision data, particle-material interaction data and atomic structure data, and Japanese Evaluated A&M Data Library, 1st Volume (JEAMDL-1) and 2nd Volume (JEAMDL-2) programs are in progress. These are the systematic sets of compilations of evaluated A&M data on specific items of above 3 fields relevant to fusion research. The data base compiled up to now have been stored in the Atomic and Molecular Data Storage and Retrieval System (AMSTOR).

I. Activities on Data Compilation for Ion-Atom Collisions.

Data on total cross-sections for charge transfer in collisions between ions, atoms and molecules have been compiled. Data compilation for partial cross-sections for the same processes is in progress. The data on the total cross-sections have been fitted with analytic formulas for the convenience of interpolation and extrapolation.

Part of the results of data compilation has been published in JAERI-M Report series: JAERI-M 8849 (1980), JAERI-M 83-013, 83-143 (1983) and JAERI-M 84-069, 84-169 (1984). The data are stored in the AMSTOR at JAERI. The results of fitting analytic formulas to data are summarized below. Fitting to the partial cross-sections is under consideration.

I-1 Charge Transfer of Hydrogen with Gaseous Atoms and Molecules (1)

The total cross sections σ for charge transfer in collisions of hydrogen atoms and ions with gaseous atoms and molecules have been fitted with an analytic formula. The cross sections considered are σ_{10}, σ_{0-1}, σ_{1-1}, σ_{01}, σ_{-10} and σ_{-11}. The functional form of the formula is a modification of the Green-McNeal formula. Parameters in the formula are given in tables.

I-2 Charge Transfer of Hydrogen with Metal Vapors (2)

The same cross-sections as described above for the targets of metal vapors have been fitted with an analytic formula. The functional form used is also the same as above.

I-3 Charge Transfer of Helium with Gaseous Atoms and Molecules (3)

The total cross sections for charge transfer in collisions of helium atoms and ions with gaseous atoms and molecules have been fitted with an analytic formula in a manner similar to the case of hydrogen. The cross sections considered are σ_{-10}, σ_{-11}, σ_{0-1}, σ_{01}, σ_{02}, σ_{1-1}, σ_{10}, σ_{12}, σ_{20} and σ_{21}.

I-4 Single-Electron-Capture of Multiply-Charged Ions (4)

A universal semiempirical formula has been obtained for the total cross-sections $\sigma_{q,q-1}^{B}$ of the processes: $A^{q+}+B \rightarrow A^{(q-1)+}+B^{+}$, where A stands for the projectile of almost all atoms, and B the target of H, H_2 or He.

References

(1) Y. Nakai, T. Shirai, T. Tabata and R. Ito, At. Data & Nucl. Data Tables (to be published). A preliminary account is given in: T. Tabata et al., Radiat. Center Osaka Prefect. Tech. Rep. (RCOP-TR) No.5 (1986).

(2) T. Tabata, R. Ito, Y. Nakai, T. Shirai, M. Sataka and T. Sugiura, RCOP-TR (to be published).

(3) T. Tabata, R. Ito, Y. Nakai and T. Shirai, Ann. Rep. Radiat. Center Osaka Prefect. 26, 57 (1985); a more detailed report in a preliminary form will be published as an issue of RCOP-TR; a final report will be published elsewhere.

(4) Y. Nakai, T. Tabata, R. Ito, A. Kikuchi and T. Shirai, Ann. Rep. Radiat. Center Osaka Prefect. 25, 19 (1984); a more detailed paper is in preparation.

II. Activities on Data Compilation for Particle-Material Interaction.

These are composed of the following two items. (1) Data on elementary processes for hydrogen isotope recycling in fusion devices, such as (a) trapping and detrapping processes, (b) diffusion and (c) particle impact desorption. (2) Radiation effects through the atomic collision cascade in fusion materials by ion beams and fast neutron bombardments.

II-1 Compilation of Bibliographic Data on PWI Published in Japan

The bibliographic data sheets(121) with respect to the surface processes of PWI which appeared in domestic references published in Japan during 1983-1985 were compiled and sent to the IAEA Nuclear Data Section. We have surveyed mainly the fields directly relating to the PWI processes, but some important surface data in fusion technology, for example discharge cleaning of wall, were also collected. The abbreviations of codes are due to the IAEA report.

II-2 Hydrogen Re-emission Data Analysis in Austenitic Stainless Steel (1)

Diffusion constants of hydrogen in various austenitic stainless steels were computed from the analysis of hydrogen re-emission data, using the diffusion analysis code HRF-1. The computed re-emission rate was fitted to the experimental data and the effective diffusion constants were obtained neglecting the trapping and recombination process. The recombination constant in high temperature was also computed as a function of the material temperature.

II-3 Data Compilation for Trapping and Re-emission of Energetic Hydrogen Isotopes and Helium in Materials

During the last 3 years, the new data relevant to the trapping and re-emission of H and He in materials were compiled and stored in the AMSTOR system. It contains 36 data up to the end of 1985, dividing it into following 5 sections: 1) Re-emission(14), 2) Retention(9), 3) Thermal Release(9), 4) Damage Effects(1) and 5) Surface Recombination(3). The manuscript is being prepared for publication as the 2nd supplement of JAERI-M 82-118 and 84-093. The references for each experimental data are shown in the figures, and all the literatures concerning trapping and re-emission of hydrogen isotopes and helium are listed chronologically and alphabetically in each year at the end of the report.

II-4 Data Compilation for Particle Impact Desorption (2,3)

Data compilation for particle impact desorption has been continued as our multi-year effort. Previous results have been published on electron stimulated desorption and on ion impact and photon stimulated desorption in JAERI-M Reports. Our primary concern is the mechanism of ion impact desorption and we have approached to it by evaluating the dependence of the desorption cross section (σ) on the primary ion energy (E) up to 10 keV. We have found that σ for all adsorbate/substrate combination with a few exceptions can roughly be expressed by E^p where p is from -1 to 0 for light ions and from 0 to +2 for heavy ions. Theoretical calculations of σ by using the Winters-Sigmund model carried out for various systems on which experimental data are available in the literature, on the other hand, indicate that the model predicts well the data by light ion impact in addition to those for three systems by heavy ions, $Ne^+ \rightarrow O/Mo(110)$, $Ne^+ \rightarrow CO/Mo(110)$ and $Xe^+ \rightarrow N/Mo(100)$ where excellent agreement between theoretical and experimental cross sections has been obtained; this work will be published before the end of this year.

II-5 Data Compilation for Radiation Effects on Ceramic Insulators (4)

Data of radiation effects on ceramic insulators were compiled from the literatures up to the end of 1984 and summarized from the viewpoint of fast neutron irradiation effects. The data were classified according to the fellowing 5 properties and ceramics. The properties are i) dimensional stability (swelling), ii) mechanical property, iii) thermal property and iv) electrical and v) dielectric properties. The 56 data sheets for each table or graph in the literatures were made. The characteristic feature of the data base was also briefly described.

II-6 Evaluation of Interatomic Potentials and Molecular Dynamical Simulation of Detects in B.C.C. Metals (5,6)

Interatomic potentials used in the literatures have been surveyed, and the Johnson's method for constructing potentials was found to be the most practical and reliable at present. On the basis of the Johnson and Wilson potentials, systematic computer simulation for obtaining the anisotropic threshold energies of atomic displacements have been performed for b.c.c. Mo and Ta. The computer program used is a GRAPE which was developed in BNL.

The most characteristic point in the present calculations is that the interstitial configuration in tantalum crystal is found to be crowdion type along [100] and [111] directions. This situation differs fundamentally from the tendencies found in Fe and Mo, in which the [110] split dumb-bell type is the dominant configuration for an interstitial and no other type is observed. The vacancy configuration of Ta is found to be more shrunk comparing with that in Fe and Mo. These computational results reflect well some experimental results.

Based on the calculations of collision process, the contours of anisotropic displacement threshold energies are obtained. In the case of tantalum, it is compared with the results of experiment done by Julich group; the overall tendency coincides with each other except for a discrepancy of threshold energy along [110] direction.

The results obtained in the present calculations should be published in JAERI-M Report and elsewhere.

References

(1) K. Fukushima, K. Ozawa, K. Ebisawa and M. Terasawa, Hydrogen Re-emission Data Analysis in Austenitic Stainless Steel, JAERI-M 85-099 (1985).

(2) T. Oshiyama, S. Nagai, K. Ozawa and F. Takeuchi, Data Compilation on Electron Stimulated Desorption, JAERI-M 84-094 (1984).

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(4) K. Fukuya, K. Ozawa, M. Terasawa and S. Nakahigashi, Data Compilation for Radiation Effects on Ceramic Insulators, JAERI-M 86-127 (1986).

(5) M. Fuse and T. Iwata: Review on the Calculations of Atomic Collisions in Solids (in Japanese), JAERI-M 85-118 (1985).

(6) M. Yokota, Y. Taji and T. Iwata: Anisotropy of Displacement Threshold Energies Calculated by the Molecular Dynamical Method (in Japanese), JAERI-M 83-226 (1984).

III. Activities on Data Compilation and Evaluation for Atomic Structure of Highly Ionized Ions (Energy Levels, Transition Probabilities and Grotrian Diagrams).

Atomic energy level and transition probability data are necessary in the field of impurity diagnostics. Species of impurity are Ti, Cr, Fe, Ni and Mo constituting the first wall materials. We go on the compilation and evaluation for the data on the multiply charged ions of above atoms to put emphasis on the wavelengths, energy levels, oscillator strengths, transition probabilities and Grotrian diagrams by the AMSTOR system. Since 1984, the cooperation program "Compilation and Evaluation of Atomic and Molecular Data for Fusion" has been continued among NBS, ORNL and JAERI data centers as a part of the US-Japan fusion cooperation programs.

III-1 Data Compilation and Evaluation for Highly Ionized Ti Ions (1)

For the titanium ions Ti V to Ti XXII, wavelengths, energy levels, level configuration, oscillator strengths and radiative transition probabilities were critically reviewed and tabulated. Grotrian diagrams were also presented to provide a graphical overview. The report has been published in Atom. Data and Nucl. Data Tables.

III-2 Data Compilation and Evaluation for Highly Ionized Mo Ions (2,3,4)

Starting from the extensive survey of literatures, we have critically evaluated and tabulated the data for the atomic spectra of Mo VI - Mo XLII, with their wavelengths, intensities and classifications but except for Grotrian diagrams. A short review of the work on each stage of ionization is included. It was further revised and submitted for publication to JPCRD.

III-3 Data Compilation and Evaluation for Highly Ionized Ni Ions (5)

New compilation critically evaluated on the atomic spectra of Ni IX - Ni XXVII with their energy-level classifications and the Grotrian diagrams have recently completed. The report was submitted for publication to AD & ND Tables.

III-4 Data Compilation and Evaluation for Highly Ionized Fe and Cr Ions

The first report of the spectroscopic data and Grotrian diagrams for Fe VIII - Fe XXVI have been published by Mori et al. in AD & ND

Tables 23, 195 (1979); however, many revisions became necessary. The evaluation of a data base on the atomic spectra of Fe with their energy-level classifications and the Grotrian diagrams now is in progress and will be completed by March of 1979. The new data have been collected from Kelly's and Sugar & Corliss reports and other sources up to the end of 1985. We also start to begin compilation and evaluation of the data on the spectra of Cr-energy levels and wavelengths.

References

(1) K. Mori, W.L. Wiese, T. Shirai, Y. Nakai, K. Ozawa and T. Kato, Spectral Data and Grotrian Diagrams for Highly Ionized Titanium, Ti V - Ti XXII, Atom. Data and Nucl. Data Tables 34, 79 (1986).

(2) K. Ishii, K. Ozawa, Y. Nakai and T. Shirai, Bibliography on Spectra of Multiply Charged Molybdenum Ions. (Including Niobium, Zirconium and Yttrium), JAERI-memo 60-225 (1985).

(3) T. Shirai, K. Ishii, K. Mori, Y. Nakai and K. Ozawa, Spectral Data for Highly Ionized Molybdenum, Mo VI - Mo XLII, JAERI-M 85-173 (1985).

(4) T. Shirai, K. Ishii, J. Sugar, K. Mori, Y. Nakai and K. Ozawa, Spectral Data for Molybdenum Ions, Mo VI - Mo XLII, submitted to J. Phys. Chem. Ref. Data.

(5) T. Shirai, K. Mori, J. Sugar, W.L. Wiese, Y. Nakai and K. Ozawa, Spectral Data and Grotrian Diagram for Highly Ionized Nickel, Ni IX - Ni XXVII, submitted to Atom. Data and Nucl. Data Tables.

Progress Report at RIC/ IPP/ Nagoya

H. Tawara

1. AM working group

1.1 The up-dating of the previously compiled cross sections for ionization of atoms and ions by electron impact has been finished and is going to be published in Atomic Data and Nuclear Data Tables vol.36 (with data for 325 processes[1]).

1.2 A critical evaluation of the excitation of helium-like ions, in particular, the for n=1 → n=2 excitation by electron impact is under way. We are trying to find some empirical scaling law of the Z-dependence of ions for such excitation processes.

1.3 A compilation is completed on data of atomic and molecular hydrogens in collisions with electrons, photons and ions which are relevant to studies of edge plasmas[2].

1.4 Following our compilation of total cross sections of electron transfer of multiply charged ions with atomic and molecular hydrogens[3], we are now compiling the partial cross sections, that is, (n,ℓ) distribution in such multiply charged ions + H_1, H_2 collisions. A bibliography is completed on the (n,ℓ) distribution in the charge transfer[4]. It has been found that systematic experimental work on the (n,ℓ) distribution, in particular, for multiply charged ions is very scarce, though some theoretical calculations are available, with significant disagreement from each other sometimes.

1.5 Following a review on the energy loss of hevy ions in hot/dense plasmas[5], we are reviewing theoretical models of atomic structures such as the energy level and oscillator strength in hot/dense plasmas and some calculations are under way. This review will be published soon.

1.6 Our compiled data on the charge distribution of heavy ions after passage through foils have been published.[6)]

1.7 Atomic data in tokamak plasma modelling, in particular on Fe atoms and ions, have been discussed and summarized.[7)]

2. PSI working group

2.1 Some universal formulas for backscattering of ions from solid surfaces under normal and oblique incidence have been found and published.[8,9)]

2.2 A review is being continued on the plasma-surface interactions involving the edge plasmas with the emphasis on the following topics:

a) sputtering near thresholds

b) backscattering at very low energies (< 10 eV)

c) sputtering of compounds

d) synergistic effects in plasma-hydrogen recycling

Also some calculations of backscattering of hydrogen ions at the energies below 10 eV are under way, based on the Embedded Atom Model (EAM).

References

1) H. Tawara and T. Kato, ADNDT 36 (to be published)

2) H. Tawara and Y. Itikawa, Y. Itoh, T. Kato, H. Nishimura, S. Ohtani, H. Ohtani, H. Takagi, K. Takayanagi and M. Yoshino, IPPJ-AM-46(1986)

3) H. Tawara, T. Kato and Y. Nakai, ADNDT 32 (1985) 235

4) H. Tawara, N. Shimakura, N. Toshima and T. Watanabe, IPPJ-AM-45 (1986)

5) S. Karashima. T. Watanabe, T. Kato and H. Tawara, IPPJ-AM-42 (1985)

6) K. Shima, T. Mikumo and H. Tawara, ADNDT 34 (1986) 357

7) T. Kawamura (ed.), IPPJ-AM-44 (1986)

8) T. Tabata, R. Ito, K. Morita and H. Tawara, Radiation Effects 85 (1985) 45

9) T. Tabata, R. Ito, K. Morita and H. Tawara, Nucl. Instr. Meth. B 9 (1985) 113

Joint Workshop of U.S. - Japan Fusion Collaboration Program

" Resonance effects in electron - ion collisions :
A new contribution of A & M processes to fusion"

September 1 - 2, 1986
Institute of Plasma Physics, Nagoya University,
Nagoya 464

September 1

9:30 - 10:00 Registration

10:00 - 12:00 Y.Sugie (JAERI) (30 min.)
Diagnostics of JT - 60 and impurity measurements

S.Morita (IPP) (15 min.)
X-ray spectroscopy of highly ionized atoms

M.Nakai (ILE, Osaka Univ.) (30 min.)
Spectroscopic measurement of non-local transport in laser-produced plasma

12:00 - 13:00 lunch

13:00 - 15:00 R.Phaneuf (ORNL) (30 min.)
Indirect mechanisms in electron impact ionization of multiply charged ions

H.Suzuki (Sophia Univ.) (30 min.)
Recent activities of electron- ion collision experiments in IPP/Nagoya and Sophia University

Y.Itikawa (ISAS) (30 min.)
Distorted-wave -method caculation of innershell excitation

15:00 - 15:30 coffee break

15:30 - 17:30 R.Henry (Louisiana State Univ.) (30 min.)
Resonance effects in electron-ion excitations

S.Nakazaki (Miyazaki Univ.) (15 min.)
Cross sections for electron excitation of O^{3+}

T.Fujimoto (Kyoto Univ.) (30 min.)
Decrease and disappearance of the resonance contribution to the excitation cross section of ions in plasma

Y.Hahn (Univ. Connecticut) (15 min.)
Resonance effects in electron capture and ionization

September 2

9:00 - 10:30 Y.Kim (NBS) (30 min.)
Relativistic effects in electron-ion excitation

T.Kagawa (Nara Women's Univ.) (30 min.)
Energy levels and transition probabilities of multiply charged ions

10:30 - 11:00 coffe break

11:00 - 12:30 G.Dunn (JILA) (30 min.)
Tuneable resonances : dielectronic recombination

K.Sakimoto (ISAS) (30 min.)
Effects of electric fields on dielectronic recombination

12:30 - 13:30 lunch

13:30 - 15:00 H.Griem (Univ. Maryland) (30 min.)
Collisional rate coeeficients for highly charged ions from transient plasmas

T.Kawamura (IPP) (30 min.)
Evaluation and assessment of atomic data and surface interaction data for boundary plasma modelling

15:00 - 17:00 Discussion on future U.S.-Japan collaboration

Please note that 5 - 10 min. discussion time is reserved after each talk.

Appendix 6

Data Centers on Atomic Spectroscopy at the National Bureau of Standards

I. Atomic Energy Levels Data Center
W.C. Martin, Director

A. Progress Report

Our new energy-level compilations for the 235 spectra of the iron-group elements potassium through nickel (Z=19-28) were published in a one-volume supplement to the J. Phys. Chem. Ref. Data.

We completed and published the most extensive compilation of data for (forbidden) magnetic-dipole transitions ever carried out. The data include 1660 predicted wavelengths and transition probabilities (10nm to 26mm) for atoms and ions of the element beryllium through molybdenum. These tables should be very useful for diagnostics and analysis of radiation from tokamak plasmas.

Two joint compilation efforts with Japanese scientists from JAERI for ionized Ni and Mo spectra are almost completed. Critically evaluated tables of the Ni ions Ni^{8+} through Ni^{27+} containing wave-lengths, energy levels and transition probabilities as well as energy level diagrams have been completed, and similar tables for the spectra of Mo^{5+} through Mo^{41+}, but without transition probabilities and energy level diagrams, are almost ready for submission for publication.

B. Future plans

We are starting to critically review and compile data on energy levels for the spectra of sulfur and chlorine. The results of new calculations, theoretical interpretations, and measurements stimulated by our reviews are being included in these compilations.

We monitor the literature on atomic energy levels, wavelengths, wavefunctions, etc., and the resulting reference files and published bibliographies are used by wide clientele. We plan a fourth supplement to our Bibliography on Atomic Energy Levels and Spectra, covering the period from January 1984 through December 1987.

II. Data Center on Atomic Transition Probabilities

W.L. Wiese, Director

A. Progress Report

Critical evaluations and tabulations of atomic transition probabilitiy data for the iron group elements, scandium through nickel, have continued. The research activity in this field is very strong, mainly propelled by interests of astrophysicists and the fusion community. This has meant that new and revised data are continually becoming available, and we attempt to include this material to the greatest extent possible, revising and adding to existing data tables. This influx of new data has slowed the pace of our work, but we are making steady progress. During the past year, we have completed the evaluation of both allowed and forbidden lines for all ions isoelectronic with sulfur, phosphorus, silicon, aluminum, and magnesium. Tabulations of the forbidden lines of neutral and low ionization stages of the elements Sc through Ni have been completed, as have the forbidden lines of ions in the oxygen, fluorine and neon sequences.

Work is in progress on a volume in the new Oak Ridge Red Book series, which will contain spectroscopic data for the elements titanium, chromium and nickel through all stages of ionization. The material is largely selected and updated from recent NBS-NSRDS compilations, and the new volume will contain wavelengths, energy levels, ionization energies and transition probabilities, both of electric dipole (allowed) and magnetic dipole (forbidden) lines.

B. Future Plans

We shall continue and soon complete our work on the compilation of transition probabilities for Fe-group elements. We shall also attempt to complete within the next year the "Red Book" on spectroscopic data for Ti, Cr and Ni.

We shall also continue the presently slowed-down work on database development and we shall keep up the monitoring and collection of new literature on atomic transition probabilities and shall supply reference material to IAEA in regular intervals.

Recent Publications

J.Sugar and C. Corliss, "Energy Levels of the Elements of the Iron Group, Potassium through Nickel", J. Phys. Chem. Ref. Data 14, Suppl.2 (1985).

V. Kaufman and J. Sugar, "Forbidden Lines in ns^2 - np^k Ground Configurations of Beryllium through Molybdenum Atoms and Ions", J. Phys. Chem. Ref. Data 15, 321 (1986).

W.C. Martin, R. Zalubas, and A. Musgrove, "Energy Levels of Phosporus, PI through PXV," J. Phys. Chem. Ref. Data 14, 751 (1985).

K. Mori, W.L. Wiese, T. Shirai, Y. Nakai, K. Ozawa and T. Kato, "Spectral Data and Grotrian Diagrams for Highly Ionized Titanium, TiV-Ti XXII," Atom. Data and Nucl. Data Tables 34, 79 (1986).

T. Shirai, K. Mori, J. Sugar, W.L. Wiese, Y. Nakai, and K. Ozawa, "Spectral Data and Grotrian Diagrams for Highly Ionized Nickel, Ni IX - Ni XXVII," Atom. Data and Nucl. Data Tables (in press).

CONTROLLED FUSION ATOMIC DATA CENTER
Oak Ridge National Laboratory

Progress Report

September 5, 1986

1. The categorized bibliographic files are up to date, and installments continue to be sent quarterly on magnetic tape to the IAEA and IPP-Nagoya. The 1985 Bibliography has been published and distributed as ORNL-6287.

2. Work on Volume 5 of the new "Redbook" series of recommended data, entitled "Collisions of Carbon and Oxygen Ions with Electrons, H, H_2 and He" is 95% complete, and will be published before the end of 1986.

3. Work on Volume 1 of the new "Redbook" series of recommended data, entitled "Collisions of H, H_2, He and Li Atoms and Ions with Atoms and Molecules" is roughly 50% complete, and publication is planned during 1987.

4. A subset of Volume 5 of the new "Redbook" series, entitled "Recommended Cross Sections for Electron Capture and Ionization in Collisions of C^{q+} and O^{q+} with H, He and H_2" has been prepared for submission to Atomic Data and Nuclear Data Tables for publication.

5. An evaluation and parametrization has been completed of experimental and theoretical data for charge-exchange collisions of Fe^{q+} with H, H_2 and He. The recommended data have been parametrized in terms of a single analytic function and a draft report has been prepared. This contribution will be included in the Report of the Advisory Group on Atomic Data for Fusion Plasma Modelling, to be coordinated by J.G. Hughes and published in Nuclear Fusion.

6. An evaluation of experimental and theoretical data for electron-impact ionization of Fe^{q+} ions has been completed and a draft report prepared. This contribution will be included in the Report of the IAEA Advisory Group on Atomic Data for Fusion Plasma Modelling, to be coordinated by J.G. Hughes and published in Nuclear Fusion.

Appendix 8

Orsay, 5 September 1986

Recent Numerical Data Activities at the Atomic Data Centre GAPHYOR

Konstantinos Katsonis, Centre de Donees Atomiques GAPHYOR
Laboratoire de Physique des Plasmas, CNRS and Université Paris-Sud, 91405 Orsay CEDEX, France

This report is relating only to activities subsequent to the Fifth Meeting of the Atomic and Molecular Data Centre Network held at Palo Alto, California, in July 1985.

The system used for storage and retrieval of numerical data is currently being developed to become also usable with working stations based in commonly used personal computers (mini or microcomputers) working under the DOS operating system. After this implementation is completed, data handling and transfer under standard ASCII format files contained in floppy disks will become straightforward.

Numerical data included in the Belfast-Daresbury data bank are now available at the main computing facility of the Paris region (CIRCE). In collaboration with the Astrophysical Laboratory at Meudon, the whole data bank of Belfast-Daresbury will be installed at CIRCE and eventually merged with the GAPHYOR numerical bank. This activity is supported by the French Atomic Energy Authority (CEA) and the National Centre for Scientific Research (CNRS).

GAPHYOR is participating in the organization in the UK of an atomic data workshop in August 1987, which will be a satellite meeting to the XV ICPEAC to be held at Brighton. GAPHYOR is also planning a CODATA workshop on the management of data banks directly after the atomic data workshop. During this CODATA meeting actual data bank managers will discuss technical details concerning data exchange and data bank architecture.

Calculation and evaluation of atomic data is the subject of a collaborative programme with the Royal Holloway College, University of London and the Institute of Physics of the University of Belgrade. A review report has been prepared to present the recent achievements in atomic data measurement, calculation and evaluation. This report is mainly reflecting the work produced under the Coordinated Research Programme (CRP) on "Atomic Collision Data for Diagnostics of Magnetic Fusion Plasmas" conducted by the Atomic Data Unit of the IAEA and includes all its conclusions and recommendations, as suggested by the IFRC A+M Data Subcommittee. In order to keep pace with the fast development in this field, subsequent work has also been included. Although the typing is still under way, a draft copy of the report was presented at the meeting.

Numerical calculation of charge transfer cross section for Ar and Fe ions are also on progress. The necessary numerical code CTMC for Monte Carlo type calculations developed by M.R.C. McDowell and G. Peach has been successfully run on the CRAY computer of the Polytechnical School.

OPERATION DE RECHERCHE N° 7

BANQUE DE DONNEES GAPHYOR

Nom	Cadre	Ne	Equipe
ASSAL W.	*ING.CNRS*	-	*J.L. DELCROIX*
BRIQUIN R.	*SECRETAIRE*	-	*J.L. DELCROIX*
CLAUDON E.	*SECRETAIRE*	-	*J.L. DELCROIX*
COTTE P.H.	*STAG.MIL*	*0.46*	*J.L. DELCROIX*
DELCROIX J.L.	*ENS.SUP*	*0.66*	*J.L. DELCROIX*
KATSONIS K.	*ING.CNRS*	*0.5*	*J.L. DELCROIX*
LEPRINCE C.	*ING.CNRS*	-	*J.L. DELCROIX*
		1.62	

Experts : M. AUBES, Maître de conférence, Toulouse - J.M. BARONNET, Professeur, Toulouse - G. CHAMBAUD, Maître de conférence, E.N.S. Paris - J.L. DELCROIX, Professeur, Orsay - A.M. DIAMY, Chargée de recherche, Paris VI - P. GAUCHEREL, Chargé de recherche, Nice - G. GOUSSET, Chargé de recherche, Orsay - K. KATSONIS, Ingénieur de recherche, Orsay - L. HOCHARD, Maître de conférence, Orsay - C. LALO, Chargée de recherche, Paris VI - J. MAFTOUL, Chercheur, E.S.E., Gif-sur-Yvette - J. MASANET, Chargée de recherche, Paris VI - J.M. MERMET, Directeur de recherche, Lyon - J. RAKOWITZ, Proviseur, Limoges - P. RANSON, Chargé de recherche, Orléans - A. RICARD, Directeur de recherche, Orsay.

1) Présentation générale

Rappelons que GAPHYOR est une banque de données bibliographiques, factuelles et partiellement numériques, consacrée aux propriétés des atomes, des molécules et des gaz neutres ou ionisés. Les molécules doivent être relativement petites et simples (pas plus de 8 atomes, et de quatre éléments différents). Les propriétés couvertes sont classées en 5 sections (SE) et 112 processus (PR) comme indiqué dans le Tableau 1.

Au 15 Mars 1986, le fichier principal de GAPHYOR comprenait environ 175 000 fiches réparties comme suit :

Systèmes à ·	1 élément	2 éléments	3 éléments	4 éléments	Totaux
Propriétés des atomes et des molécules	25 393	34 396	13 446	2 583	75 818
Collisions photoniques	5 336	4 361	1 796	393	11 886
Collisions électroniques	8 909	3 622	537	51	13 119
Collisions atomiques et moléculaires	5 677	26 510	13 660	3 641	49 488
Propriétés macroscopiques des gaz	3 938	5 676	2 037	618	12 269
Totaux	49 253	74 565	31 476	7 286	162 580

TABLEAU I

Section 1. Propriétés des atomes et molécules
EN Niveaux d'énergie, fonctions d'onde
CP Profils Compton
DP Moments dipolaires
MP Moments multipolaires
PE Polarisabilité électrique (ou magnétique)
VR Courbes de potentiel, structure des molécules
TR Probabilités de transition, durées de vie radiatives
IN Autoionisation
DT Autodétachement
DS Autodissociation
XX Changement d'excitation (transitions non radiatives)

Section 2. Collisions photoniques
AN Absorption vraie
SN Absorption apparente, diffusion totale
SC Diffusion angulaire (scattering)
EL Diffusion élastique (Thomson, Rayleigh)
FF Transition free-free
EX Photoexcitation
ER Emission de raie
DX Photodésexcitation (émission stimulée)
XX Changement d'excitation
DO Dépolarisation, changement de polarisation
IN Photoionisation
DT Photodétachement
DS Photodissociation
P2 Interaction à 2 photons
P3 Interaction à 3 photons
P4 Interaction à 4 photons
PN Interaction à plus de 4 photons
NL Effets non linéaires
PR Produits indéterminés

Section 3. Collisions électroniques
SN Sections efficaces totales et de transport
SC Diffusion angulaire (scattering)
EL Collision élastique
EX Excitation
ER Emission de raie
DX Désexcitation
XX Changement d'excitation
DO Désorientation, changement d'orientation
IN Ionisation
RC Recombinaison (mécanisme non précisé)
RR Recombinaison radiative
RE Recombinaison e-e-i
RO Recombinaison e-i-o
RD Recombinaison diélectronique
RS Recombinaison dissociative
AT Attachement
DT Détachement
DS Dissociation
BS Bremsstrahlung
PR Produits indéterminés

Section 4. Collisions entre atomes et/ou molécules
SN Sections efficaces totales et de transport
SC Diffusion angulaire (scattering)
EL Collision élastique
EN Energie ou enthalpie de réaction
EX Excitation
ER Emission de rayonnement
DX Désexcitation (quenching)
XX Changement d'excitation
DO Désorientation, changement d'orientation
TE Transfert d'excitation
IN Ionisation
DT Détachement
RI Recombinaison ion-ion
10 Transfert de charge 1 → 0 (A^{+}, B → A, B^{+})
20 Transfert de charge 2 → 0 (A^{2+}, B → A, B^{2+})
LN Transfert de charge L → N (partic. rap.) ($A^{\ell+}$, B^{m+} → A^{n+})
MP Transfert de charge M → P (partic. clb.) ($A^{\ell+}$, B^{m+} → B^{p+})
LP Transfert de charge LM → NP ($A^{\ell+}$, B^{m+} → A^{n+} ; B^{p+})
IR Réaction d'échange (d'atome ou de groupe d'atomes)
AS Association
DS Dissociation
IH = EN + IR
AH = EN + AS
DH = EN + DS
KE Constante d'équilibre chimique
PR Produits indéterminés

Section 5. Propriétés macroscopiques
PV Compressibilité, équation d'état
FT Fonctions thermodynamiques
VR Amplitude de vibration
ZT Fonctions de partition
CO Corrélations
DN Diffusion
VI Viscosité
CT Conductivité thermique
TD Diffusion thermique
PE Constantes diélectriques et magnétiques
EN Largeurs et déplacements de raie (effets collisionnels)
DM Diffusion de métastables
RW Relaxation dans les gaz neutres
FE Fonctions de distribution électronique
CE Conductivité électrique
ME Mobilité électronique
DE Diffusion des électrons
PI Premier coefficient de Townsend
AT Attachement
DT Détachement
PC Puissance échangée par collisions électron-neutre
FI Fonction de distribution ionique
MI Mobilité ionique
DI Diffusion des ions
DA Diffusion ambipolaire
RC Recombinaison (mécanisme non précisé)
RR Recombinaison radiative
RE Recombinaison radiativo-collisionnelle et e-e-i
RO Recombinaison e-i-o
RD Recombinaison diélectronique
RS Recombinaison dissociative
RI Recombinaison ion-ion
PD Post-décharges
LA Laser à gaz
MD Température caractéristique électronique (D/μ)
ST Statistique de niveaux

2) Descripteurs, langages, interrogations

Une fiche GAPHYOR contient à l'heure actuelle les descripteurs suivants :

Familles de Mendeleev : FA, FB, FC, FD / Informations : INFO
Eléments dans les familles : AA, BB, CC, DD / Année de publication : AN
Section : SE / Références bibliographiques : JO, VO, PAGE
Etat initial : M1, M2, M3 / Premier auteur : AU
Processus : PR / Lieu d'exécution : NA, ST, CI
Etat final : M4, M5, M6

On peut interroger sur tous ces descripteurs (sauf la page). Les valeurs des descripteurs sont écrites dans l'ordinateur dans un langage très compact appelé "mode interne". A l'interrogation et pour l'édition des résultats les utilisateurs parlent ou lisent un langage physico-chimique naturel dans deux variantes appelées respectivement "mode d'interrogation" et "mode d'édition". L'écriture des divers processus traitée dans GAPHYOR se perfectionne régulièrement par le travail du groupe des experts qui se réunissent deux fois par an pour définir les méthodes de travail. Suite à ces réunions, un important document de synthèse a été rédigé sous forme de rapport interne en 1985. On y voit que des améliorations récentes rendues nécessaires par l'évolution de la science ont été introduites pour mieux décrire les sujets suivants :

Ions multichargés	/ Transferts de charge
Atomes et molécules exotiques	/ Séquences isoélectroniques et homonucléaires
Interactions gaz-solide	/ Thermodynamique statistique

Le logiciel d'interface SYGAL créé en 1979 a été perfectionné en permanence. Il a pour but d'effectuer les traductions entre les langages utilisés et de fournir en ligne des aides automatiques aux utilisateurs.

GAPHYOR est implanté au CIRCE et en terme d'informatique, ses fichiers ont les volumes suivants :

- Fichiers (données, listes inverses, gestion) : 66 Mb
- Logiciels annexes (Sygal, corrections automatiques, édition): 14 000 lignes de PL1

L'interrogation de GAPHYOR en ligne peut se faire 24h/24 et 7 jours/7 à travers les réseaux de transmission de données. Grâce au logiciel SYGAL le mode d'interrogation est à la fois très simple, très rapide et très efficace (bruit et manque pratiquement nuls).

Exemple : Excitation vibrationnelle de CO par collisions électroniques.

L'utilisateur pose la question selon le schéma suivant :

M1 = E M2 = C101 M4 = C101/V FIND

3) Publications

GAPHYOR publie régulièrement deux types de documents imprimés :

- GAPHYOR UPDATE (série bleue : fascicules trimestriels rassemblant les nouvelles entrées) ;
- GAPHYOR COLLECTION (série rouge : index cumulatifs classés par familles chimiques).

Tous ces documents sont en langage chimique naturel.

La publication de la totalité de GAPHYOR COLLECTION par un grand éditeur scientifique international est en cours de négociation. Grâce à une nouvelle présentation "à la française" (Tableau 2) elle pourrait se faire sous forme d'une série de trois gros volumes :

- Systèmes à 1 élément : 450 p. (1986)/ - Systèmes à 2 éléments : 700 p. (1987)/
- Systèmes à 3 ou 4 éléments, généralités : 350 p. (1988)

Tableau 2

AA	BB	CC	DD	E	M1	M2	M3	PR	M4	M5	M6	INFO	AN	JO	VO	PAGE	AU	GEOG
* H = H D T * 4A = C Si Ge Sn Pb * 5A = N P As Sb Bi * 6A = O S Se Te Po *																		
H	C	N	O	3	é	HCNO		DS	e	H	CNO	J	E	84	315	89	51	IOKUE I	JAPOKU
H	C	N	O	3	e	HCNO		DS	e	HN •	CO		E	84	315	89	51	IOKUE I	JAPOKU
H	C	N	O	3	e	HCNO		DS	HN •	CO		J	E	77	44	81	1252	FUKUI K	JAUSID
H	C	N	O	3	e	H3CNO2		SC					E	79	20	60	518	FLICKER W	USCAPA
H	C	N	O	3	e	H3CNO2		EX	e	H3CNO2 •		S	E	79	20	60	518	FLICKER W	USCAPA
H	C	N	O	3	e	H3CNO2		EX	n	H3CNO2 •			VE	80	30	72	2488	FLICKER W	USCAPA
H	C	N	O	3	e	H4C	H2O	A1	HO -			M	L E	77	47	90	6471	SMIT A L C	USMYNY
H	C	N	O	3	e	H6C2	H2O	A1				KM	L E	78	30	68	2757	SHIMANDRI	USIMND
H	C	N	O	3	e	H6C2	H2O	A1	H5C2	HO -	N2	KM	L E	79	30	70	1137	SHIMANDRI	USIMND
H	C	N	O	4				1Q	H2C2 +	NO		K	L E	80	09	236	492	VIGGIANO A	USCUBO
H	C	N	O	4	hv	H4C	H2DD	IR	CN				L E	82	30	77	1677	ANDERSON W	USINAB
H	C	N	O	4	hv	H4C	H2O	IR	CHO				L E	82	30	77	1677	ANDERSON W	USINAB
H	C	N	O	4	hv	H4C	H2DD	IR	C2 •				L E	82	30	77	1677	ANDERSON W	USINAB
H	C	N	O	4	elec. fld	H3N	H2CO r	AX	H2CO r			K	L E	83	28	44	1149	CHARDON J	FR2SDE
H	C	N	O	4	H	CO	N2	AS	HCO	N2		K	L E	78	48	74	316	CAMPBELL I	UKENLE
H	C	N	O	4	H	CNO		1R	HO	CH		K	L E	80	258	84	835	ROTH P	DUNNDS
H	C	N	O	4	HO	CO	HO	AS	HNO2	CO		K	L E	79	48	75	2048	CAMPBELL I	UKENLE
H	C	N	O	4	HO	CO	NO2	AS	HNO3	CO		K	L E	79	48	75	2048	CAMPBELL I	UKENLE
H	C	N	O	4	HO	CO	N2	IR	H	CO2	N2	K	L E	84	30	80	259	PANASKEVOP	CDDNDT
H	C	N	O	4	HO	CO2	NO2	AS	HNO3	CO2		K	L E	77	258	81	22	ERLEN K	DUNSGD
H	C	N	O	4	HO	CO2	NO2	AS	HNO3	CO2		K	L E	83	49	79	111	DUNNDS S J	UKENDX
H	C	N	O	4	HO	CN		1R	HCN	O		K	LNR	80	6731	67		WESTLEY F	USDCNA
D	C	N	O	4	OD	C2	CO	PR				K	LNE	82	646	12	124	PANASKEVOP	CDDNDT
H	C	N	O	4	HN r	CO		1R	H	CHO •		K	LNE	80	30	72	288	ADAMS N G	UKENDI
H	C	N	O	4	HN r	CO		1R	HCO •	H		K	LNE	80	30	72	288	ADAMS N G	UKENDI
H	C	N	O	4	HN •	CO		UK				K	L E	76	250	80	1354	ZETSCH C	DUNNDC
H	C	P	O	4	HP •	CO		DX				K	L E	79	20	63	86	LENZI M	ITLAND
H	C	P	O	4	HP •	CO		DX				S	L E	81	30	75	4912	MARGANI A	ITLAND
H	C	N	O	4	HN •	CO2		DX				K	L E	76	258	80	1354	ZETSCH C	DUNNDC
H	C	N	O	4	HN •v	CO		DX					L E	75	20	36	238	GELERNT B	CUONUC
H	C	N	O	4	HN •	CO2		1R	HNO •	CO		K	LNE	80	30	72	288	ADAMS N G	UKENDI
H	C	N	O	4	HN •	CO2		1R	HCO	NO •		K	LNE	80	30	72	288	ADAMS N G	UKENDI
H	C	N	O	4	HN •	CO2		1R	HCO2 •	H		K	LNE	80	30	72	288	ADAMS N G	UKENDI

4) Développements en cours

a) Améliorations de détails

L'amélioration permanente des méthodes d'analyse scientifique, de classification et de codage sera poursuivie. Nous envisageons par exemple de créer pour chacun des descripteurs tel que M1 décrivant le processus chimique, des descripteurs partiels M1(struct.) et M1(ion.,exc.) décrivant séparément la formule brute d'une molécule et les états d'excitation et d'ionisation. Cela faciliterait certaines interrogations sur des ensembles de molécules ayant en commun un état d'ionisation ou d'excitation (p.ex. : relaxation vibrationnelle).

b) Utilisation des CD-ROM : traitement local

L'apparition des disques optiques compacts (CD-ROM) comme nouveau support informatique pourrait créer une révolution dans les banques de données. Ces disques (non-effaçable = ROM) permettent de stocker 500 Mb. Sur un tel disque on pourrait stocker tout le fichier GAPHYOR ainsi que les logiciels d'utilisation . Les questions posées sont alors les suivantes : pourrait-on

une fois par an (ou plus souvent ?) éditer un tel disque et le vendre aux utilisateurs ? Peut-on adapter les logiciels pour que l'utilisateur puisse travailler en local sur un microordinateur ? Une expérience démarre en ce moment avec une petite entreprise spécialisée pour étudier la faisabilité technique et économique de ce nouveau mode de diffusion.

c) Mode videotex (MINITEL)

En liaison, ou non avec l'opération précédente nous essaierons de développer un mode d'interrogation et d'édition en ligne de GAPHYOR utilisant le mode videotex.

5) Données numériques

Le développement à partir du troisième trimestre 1984 d'un projet relatif à des données numériques ajoute à GAPHYOR des activités indispensables pour un centre de données atomiques. GAPHYOR fait partie d'un réseau de centres de données animé par l'Agence Internationale à l'Energie Atomique de Vienne (AIEA), orienté vers les applications des données atomiques à la fusion contrôlée.

Les données numériques font l'objet des activités suivantes :

a) Addition d'un fichier numérique annexe à la banque de données GAPHYOR incluant des valeurs numériques évaluées. La structure factuelle de GAPHYOR a permis l'adjonction directe d'un tel fichier avec un minimum de modifications conformes à des décisions émanant de réunions internationales. Cette partie est déjà opérationnelle.

b) Création d'ensembles de données évaluées pour inclusion au fichier numérique GAPHYOR.

Le premier de ces ensembles est basé sur les résultats d'un programme de collaboration internationale conduit par l'AIEA sous la responsabilité d'un des membres de l'équipe GAPHYOR. Ces résultats seront publiés prochainement (K. KATSONIS et R. JANEV, "Recent developments in Atomic Data for Fusion, an IAEA Coordinated Research Programme" en préparation).

D'autre part, un projet d'évaluation et ensuite de calcul et de mesure de données numériques sur l'argon est en cours de développement. Il concerne les sections efficaces d'excitation, d'ionisation et de transfert de charges de tous les états (Ar I à Ar XVIII) ainsi que la recombinaison diélectronique et l'autoionisation. Le projet sera mené en collaboration avec plusieurs laboratoires français et européens. La partie d'évaluation débute en avril 1986 avec l'arrivée de M. M.R.C. McDOWELL pour une visite

de quatre mois. De même, M. R. JANEV fera partie de l'équipe GAPHYOR pour trois mois à partir de juin 1986.

Cette partie des activités de GAPHYOR fait l'objet d'une proposition de collaboration avec le CEA de Fontenay-aux-Roses (Cadarache) dans le cadre du programme CNRS-IRF-MRT sur le confinement magnétique des plasmas de fusion. Il a été convenu que des ingénieurs du CEA participeront aussi à ce projet.

c) Collaboration internationale sur la coordination et le développement de la production (mesure, calcul), l'évaluation et le traitement (collecte, stockage, distribution) des données atomiques. Cette activité inclut une collaboration avec l'AIEA et avec CODATA.

Progress Report of the A+M Data Unit
September 1986
A. Lorenz

1. IAEA A+M Data Programme Review

On the request of the IFRC, the Agency's A+M Data Programme is currently undergoing a review by the IFRC Subcommittee on A+M Data for Fusion. The final recommendations of this review will be submitted to the IFRC at its meeting in November 1986.

2. Staff

In addition to the administrative and supervisory function of the Nuclear Data Section, (which amounts to approximately 0.25 man-years), the IAEA A+M Data Unit has at the present time one full time position at the P-3 level, one full-time data entry clerical position and one part-time secretary. As a result of the unexpected recall of John Hughes (who occupied the P-3 post) by his home organization, the only full time professional post of the A+M Data Unit remained vacant for six months. On 1 April 1986, this post was filled by James Smith, atomic physicist and programmer, who was employed by the IAEA Safeguards department prior to joining the A+M Data Unit.

The attempt to acquire an additional professional post for the A+M Data Unit has not succeeded; the request was turned down at the highest IAEA administrative level. The reason given for this was the compliance of the whole Agency to strict zero growth.

3. Programme

Bibliographic Data

The International Bulletin on A+M Data for Fusion continued to be published on schedule during the six-month non-occupancy of the A+M Data Unit post by hiring John Hughes as a consultant for one week at the time of the Bulletin preparation in December 1985 and March 1986.

The publication of the CIAMDA index to the literature on A+M collision data, which had been scheduled for this year, is proceeding as planned. James Smith is formulating a new publication format. Suggestions as to its layout have been distributed to the A+M Data Centres network. The status of the CIAMDA publication will be presented at the meeting.

Numerical Data

Work has started on the formulation of a numerical data index, listing the content of all numerical data which are stored in the A+M EXFOR system at the IAEA. The data which are considered to be "recommended" are flagged. A preliminary draft copy of this index was also sent out to the Data Centres. This index is proposed to be distributed to the fusion research and atomic physics communities in the form of a report.

Work has also started on the formulation of a compendium of "recommended" numerical atomic collision data. This compendium is proposed to be produced in a loose-leaf form, and contain only "recommended" data. The data will be presented in tabular and graphical format, and could also be available on

magnetic tape. It is planned that James Smith will visit the Culham and JET laboratories, as well as the computer department at Queen's University at Belfast, to discuss the fusion user requirements for numerical atomic data so as to maximize the usefulness of the planned compendium and the services provided to the fusion research community by the IAEA.

4. A+M Data Meetings

An advisory group meeting on "Atomic Data for Fusion Plasma Modelling" was held at IAEA Headquarters in September 1985. The meeting reviewed the status of the atomic data available for electron impact excitation and ionization, recombination and charge exchange, with an emphasis on iron and its ions. The meeting was attended by 12 experts. It was recommended that the meeting summary report and the resultant recommended data be published in the Nuclear Fusion journal.