International Atomic Energy Agency

INDC(NDS)-202/GA

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

SEVENTH MEETING OF THE

ATOMIC AND MOLECULAR DATA CENTRE NETWORK

Oak Ridge National Laboratory, Oak Ridge, Tennessee
9-11 November 1987

SUMMARY REPORT

Prepared by J.J. Smith

Febraury 1988

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

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Abstract

Summary report of the Seventh A+M Data Centre Network Meeting convened by the IAEA at the Controlled Fusion Atomic Data Centre, Oak Ridge National laboratory, Oak Ridge, Tennessee, 9-11 November 1987. The meeting was attended by twelve representatives of centres from six Memeber States concerned with the coordination of the international management of atomic and molecular data pertinent to controlled fusion research and technology.

Reproduced by the IAEA in Austria
February 1988

88-01038

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A. Meeting Summary

1. Introduction

The Seventh A+M Data Centre Network (DCN) Meeting was convened by the IAEA Nuclear Data Section at the Controlled Fusion Atomic Data Centre, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 9-11 November 1987. The meeting was attended by twelve representatives of data centres from six Member States, concerned with the international coordination of atomic and molecular data pertinent to controlled fusion research and technology. The meeting was chaired by J.J. Smith.

The participants 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 establishment of a single international A+M collision data base was stressed to be the short term priority for the data centre network. All data centres agreed to cooperate in a joint effort to provide the fusion community with the required numerical data.

- The participants reviewed the outcome of the Specialists' Meeting on "Atomic and Molecular Data for Plasma Edge Studies" and fully endorsed the proposal for the formation of a coordinated research programme on the production and evaluation of A+M data for plasma edge studies as a means of generating the needed data for fusion.

- The participants discussed the recent publication of "Recommended Data on Atomic Collision Processes Involving Iron Ions" published as a special supplement to the Nuclear Fusion journal, 1987, and urged that the A+M data unit should complete and issue the appropriate numerical data files. The A+M data unit was asked to investigate the possibility of providing data covering recombination processes for iron ions which were not included in the recommended data base.

- The programme of the A+M Data Unit was considered. The participants agreed that a meeting covering the A+M and fusion data base interface was timely and is an important topic to maximise the efficient usage of the A+M collision data base. The convening of a Specialists' Meeting on C^{q+} and O^{q+} collision data was also discussed. It was felt that the meeting should be held if a substantial improvement in the data base could be expected, over that available in "Collisions of Carbon and Oxygen Ions with Electrons, H, H_2 and He" published in ORNL-6090. This is dependent on the amount of new or more accurate data which could be expected by May 1988.

- It was proposed that the A+M Data Unit should fully address the problem of discrepancies within the recommended collision data base. If necessary, it was suggested that relevant members of the data centre network could meet before following data centre meetings to attempt to resolve or propose follow-up actions necessary to resolve the discrepancies and report to the full data centre meeting.

3. Next A+M Data Centre Meeting

The next meeting of the A+M Data Centre Network was proposed to be held at the Institute of Atomic Energy, Chinese Nuclear Physics Division, Beijing, The People's Republic of China in early 1989. It was suggested that the IAEA send official announcements of the meeting by mid 1988.

B. Meeting Proceedings

1. Progress Reports

On the first day of the meeting each data centre reported on their progress and future plans. During or subsequent to the meeting the following written reports have been provided.

1.1 Progress Report of the Controlled Fusion Atomic Data Centre (presented by R.A. Phaneuf), Appendix 4

1.2 Progress Reports of the Data Centres on Atomic Spectroscopy at the National Bureau of Standards (presented by W.L. Wiese), Appendix 5.
I. Atomic Energy Levels Data Centre
II. Data Centre on Atomic Transistion Probabilities

1.3 The JAERI Activities on A+M Data for Fusion, Status Report, November 1987 (presented by Y. Nakai), Appendix 6.

1.4 Progress Report of Atomic Data Group, IPP/Nagoya, 1986-1987 (presented by H. Tawara), Appendix 7.

1.5 Progress Report of the Atomic and Molecular Data Centre at the Queen's University of Belfast (presented by J.G. Hughes), Appendix 8.

1.6 Summary of the Progress Report 1986-1987 of the GAPHYOR Data Centre, 1986-1987 (presented by J.L. Delcroix), Appendix 9.

1.7 The present status of A+M Data Research in China (presented by Zhou En Chen), Appendix 10.

1.8 Activities in the A+M Data Centre at ENEA Bologna, Italy (presented by G.C. Panini), Appendix 11.

1.9 Progress Report of the IAEA A+M Data Unit, and the IAEA A+M Data Unit Programme for 1988 (presented by J.J. Smith), Appendix 12.

No written report from Dr. Gallagher, from the Joint Institute for Laboratory Astrophysics (JILA), has been produced, but from her oral report the recent work and future activities can be summarised as given in Appendix 13.

2. The A+M Collision Data Base

The A+M collision data base was extensively discussed during the course of the meeting, and the following summaries the major conclusions and actions relating to this topic.

2.1. It was agreed that the numerical data package of collision data from recommended data for iron and its ions (Nucl. Fusion - Special Supplement 1987) should be completed and distributed to plasma physicists, for use in modelling and diagnostic applications, and also to all data centres. [Action 1].

2.2. The data base should be modified to allow for textual information, i.e. notes accompanying recommended data that describe the methodology used in producing the recommended values. Also allowance should be made for lists of references. After this is completed all the recommended A+M collision data should be included in the files and distributed. [Action 2].

2.3. With regard to 2.2., all data centres should send both numerical and textual data making up recommended data to the Agency in as structured and computer readable form as possible, [Action 3]. It was stressed that with the limited manpower the conversion of the data into the Agency's formats should be undertaken by the A+M Data Unit. With regard to this, the A+M data unit should consider the problem of exchange formats on input to the data base. [Action 4].

2.4. When appropriate, all data centres should be informed of changes being made to the status of the collision data. Before any publication of IAEA compendia of recommended A+M collision data all data centres should receive copies to allow for comments.

2.5. In due course, the Agency should inform physicists in other areas of the existence of the data base. [Action 5].

2.6. From the experience gained by the network in evaluating and recommending data, it was stressed that the majority of papers, both experimental and theoretical, do not contain significant information describing the procedures used, uncertainties involved etc. that allow the data to be intercompared. Dr. Phaneuf agreed to draft a letter which should be sent to the editors of leading journals in the field to address the problem of publishing standards. [Action 6]. It was felt that this letter should be sent from the head of the A+M data unit of the IAEA.

2.7. In recommending analytic fitting functions to represent cross sections or reaction rates, if possible, consistent use should be made of expressions that physically describe both threshold and asymptotic behaviour correctly.

2.8. Both cross sections and reaction rate coefficients should be included in the data base when both are available.

3. Establishment of Spectroscopic and Plasma-wall Interaction Data Bases

The establishment of both spectroscopic and plasma-wall (surface interactions) data bases was discussed. In the case of spectroscopic data, there is no current computer data base which contains the required data in a computer usable form. At NBS there is a significant amount of the data published by NBS held as "page images" which are processed into

the final reports using a photocomposition system. This data being stored on computer files could be transferred into a structured spectroscopic data base via translation programs.

Dr. Wiese pointed out that there is a significant difference in the uses of a collisional data base compared to a spectroscopic data base. Modelling calculations can require large inputs of collisional data for the study of particle transport, impurity behaviour and other topics. Spectroscopic data on the other hand is used primarily as basic reference data, little as such is used in bulk calculations, although the number of fusion physicists requiring such data is probably greater than collisional data. The establishment of a spectroscopic data base therefore requires careful consideration. The IFRC Subcommittee should consider this application and give advice on the role and future work on this topic.

It was suggested that the list of reports containing recommended structure and spectra data should be regularly published in the International Bulletin on Atomic and Molecular Data for Fusion. The A+M data unit and Dr. Wiese should cooperate on this matter. [Action 7].

Regarding a surface interactions data base, there are a vareity of groups studying surface interaction processes. However, the available collected data is scattered and there is no coherent data base addressing the complete scope of processes. It was felt that with the requirement for both collision and surface interaction data for studies of the plasma edge it would be appropriate to investigate recommending and establishing a surface interactions data base.

4. Bibliographic Data

1. Prof. Delcroix was asked to provide some selected retrievals for fusion relevant species and reactions for comparison with the IAEA bulletin data base. [Action 8].

2. The A+M Data Unit should distribute in the bulletin definitions of reactants and processes considered for selection of data. [Action 9].

3. The A+M Data Unit should plan for the next publication of the CIAMDA Series.

5. Matters Regarding IFRC-Subcommittee

1. The IFRC Subcommittee should be contacted to help define the specific topic on which the network could work on co-operatively.

2. It was asked that at the next meeting of the IFRC Subcommittee the position on data requirements for inertial fusion and ion-beam applications should be addressed.

6. Publication of the "Recommended Data on Atomic Collision Processes Involving Iron and Its Ions"

The A+M Data Unit should consult Dr. Summers on the possibility of him providing a recommended set of data for recombination processes involving Iron Ions. It was considered that this could be submitted to

the Nuclear Fusion Journal as a regular article. Dr. Hughes stated that there could be some collaboration on this topic between Dr. Summers and a member of the Belfast data centre.

7. Use of Computer Networks

There was an appreciable interest in using computer networks to distribute letters, draft versions of papers and numerical data between data centres. Each data centre was asked to supply all information such that data can be transmitted to a particular person. [Action 10].

To access the IAEA computer the following notes are provided.

The IAEA host computer can be accessed via two packet-switching networks, DATEX-P and TYMNET via Radio Austria (of the Austrian PTT). There are also direct dial-up ports at 300 Baud available.

The ID of the Austrian DATEX-P is 2322, and the IAEA computer Host-ID is 6221047. The ID of the Austrian TYMNET Node is 2329 and then the Host-ID is 11507701. The telephone number for direct calling is Vienna (222) 23-55-75.

A TSO Logon ID has been established for users wishing to access the IAEA mainframe: RN2. The password is NDSUSER. The TSO SEND command can be used to send a message (send the message to user RNG, James Smith).

In case you have an IBM 3274 (or equivalent) connected to your Public Packet Switching Network, please tell us your IDBLK and IDNUM in advance, so we can define your cluster to VTAM. In this case you can use SPF (full screen support)- a Mailbox system is available (send the message to user RNGMAIL).

At present, the IAEA Nuclear Data Section (and the A+M Data Unit) has access (via Radio-Austria) to the TRANSPAC network in France and the ITT-UDTS, MCII/WUI, TIMNET, TRT, IPST, ACCUNET, CONNECT and various other networks on a test basis in the USA, as well as various other networks in other countries. We are in the process of establishing access to the EARN and BITNET networks via IEZ (Austrian Inter-university EDP Center).

8. Miscellaneous

1. If possible, future data centre meetings should be arranged after or before Agency Consultants, Specialists or other meetings to reduce travel costs.

2. Each data centre was asked to send all experimental and theoretical basic collision data to the A+M data unit for incorporation into the EXFOR data base. [Action 11].

Appendix 1

Seventh Atomic and Molecular Data Center Network Meeting

9-11 November 1987

Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

List of Participants

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Appendix 2

Seventh Meeting of the

Atomic and Molecular Data Centre Network

Oak Ridge Atomic Data Centre
Oak Ridge National Laboratory, Tennessee, USA
9-11 November 1987

Adopted Agenda

Introductory and Preliminary Items and Review of Actions from the 1986 Meeting.

1. Reports of A+M Data Centres and Groups

2. Reports of the A+M Data Unit

3. Numerical Data

   3.1. Status of the A+M data base.
   3.2 Recommendation of data for A+M data base.
   3.3. Review of Exchange formats for numerical data.
   3.4. Review of EXFOR index and dictionaries.
   3.5. Comparison of formats for representation of reaction rates and cross section.

4. Bibliographic Data

   4.1. Status of IAEA A+M bibliographic data base.
   4.2. Production of the A+M data bulletin.

5. A+M Meetings and Publications

   - Publication of Recommended Data on Atomic Collision Processes involving Iron and its Ions.

   - Outcome of the Specialists Meeting on Atomic and Molecular Data for Plasma Edge Studies.

   - Proposal for next A+M Data Centre Meetings.

Appendix 3

Actions

1.	IAEA	Distribute numerical data package of collision data from recommended data for iron and its ions to plasma physicists and data centres.
2.	IAEA	Modify data base to allow for textual information and add all recommended collision data.
3.	Network	Send recommended data to the A+M data unit in as structured a format as possible.
4.	IAEA	Devise a format for inputting data into the recommended data base.
5.	IAEA	When appropriate, inform physicists in other application areas of existence of recommended collision data base.
6.	Dr. Phaneuf	Draft a letter addressing the problems of publishing standards.
7.	IAEA Dr. Wiese	Define list of reports containing recommended structure and spectra data. This list should be published in the International Bulletin on Atomic and Molecular Data for Fusion.
8.	Prof. Delcroix	Provide selected retrievals from the GAPHYOR data base for comparison with Bulletin data base.
9.	IAEA	Distribute in the bulletin a list of reactants and processes covered in the bulletin.
10.	Network	Each data centre should provide all information necessary to allow communication between members of data centres via computer networks.
11.	Network	Each data centre should send the "raw" experimental and theoretical data for inclusion in the EXFOR data base.

CONTROLLED-FUSION ATOMIC DATA CENTER

Oak Ridge National Laboratory

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H. B. Gilbody[2]
D. C. Gregory
C. C. Havener
H. T. Hunter
M. S. Huq[3]
R. K. Janev[4]
M. I. Kirkpatrick
E. W. McDaniel[5]
F. W. Meyer
T. J. Morgan[6]
R. A. Phaneuf
M. S. Pindzola[7]
J. K. Swenson[3]
E. W. Thomas[5]

Progress Report
IAEA Atomic and Molecular Data Center Network Meeting, ORNL
November 9-11, 1987

The primary task of the Controlled-Fusion Atomic Data Center (CFADC) is to collect, review, evaluate, and recommend numerical atomic collision data of interest in controlled thermonuclear fusion research. The CFADC operates with an equivalent of 1.5 full-time staff members, as well as a number of expert consultants from the research community, upon which it depends heavily.

Participants in the ORNL program in experimental atomic physics for fusion also each contribute a small fraction of their time to literature searches and categorization of relevant publications. The major activities of the data center are threefold:

- the maintenance of up-to-date bibliographies of fusion-related publications on atomic collision processes in computer files for on-line searching and publication.
- the preparation and publication of compilations of recommended atomic collision data for fusion research.
- the handling of user requests for specific data or information about relevant atomic processes.

The data center actively participates in cooperative agreements with the Atomic Data Center for Fusion at the Institute for Plasma Physics (IPP) of Nagoya University, Japan, the Atomic and Nuclear Data Center of the Japan Atomic Energy Research Institute (JAERI), and the Atomic and Molecular Data Unit of the International Atomic Energy Agency (IAEA) in Vienna. Our staff continues to participate in the IAEA International Atomic and Molecular Data Center Network and to advise the IAEA data center on their activities. Our bibliographic updates are sent to these centers every six months and form the basis for the semi-annual IAEA *International Bulletin on Atomic and Molecular Data for Fusion.*

Our data center also maintains a close cooperation with the Atomic and Molecular Processes Information Center at the Joint Institute for Laboratory Astrophysics in Boulder, Colorado, and with the NBS Data Center on Atomic Spectral Lines and Transition Probabilities in Gaithersburg, MD.

During this reporting period, a major effort continued to be directed toward the preparation of an updated and expanded version of the 1977 two-volume compilation of recommended tabular and graphical data, entitled *Atomic Data for Controlled Fusion Research,* and published as ORNL-5206 and -5207 (commonly referred to as the "Redbooks"). The new multiple-volume series is entitled *Atomic Data for Fusion,* and will consist of five volumes (ORNL-6086 through ORNL-6090). These volumes, with their (expected) publication dates, are as follows:

- Volume 1: Collisions of H, H_2, He and Li Atoms and Ions with Atoms and Molecules (publication expected in early 1988).
- Volume 2: Collisions of Electrons with Atoms and Molecules (publication expected in 1989).

- Volume 3: Particle Interactions with Surfaces (published 2/85).
- Volume 4: Spectroscopic Data for Iron (published 2/85).
- Volume 5: Collisions of Carbon and Oxygen Ions with Electrons, H, H_2 and He (published 2/87).

All tabular and graphical data for the new "Redbook" series are computer-generated in publication-ready format. A computer code calculates Maxwellian rate coefficients from the cross sections, and produces Chebyshev polynomial fits to both the cross sections and rate coefficients. This will facilitate our plans to eventually place these recommended collision data in internationally accessible files on the National Magnetic Fusion Energy Computer Center (NMFECC) network.

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 accepted for publication in *Atomic Data and Nuclear Data Tables*.

In addition, two data-base assessments have been prepared for collision processes involving iron ions, in coordination with the IAEA Data Center. These are currently in press and will form part of a supplementary issue of *Nuclear Fusion*. These articles contain recommended and parametrized data, and their titles are as follows:

- "Electron-Impact Ionization Data for the Fe-Isonuclear Sequence," M. S. Pindzola, D. C. Griffin, C. Bottcher, and H. T. Hunter.
- "Charge Exchange Processes Involving Iron Ions," R. A. Phaneuf, R. K. Janev and H. T. Hunter.

A similar data-base assessment for heavy-particle processes specific to the edge plasma of magnetic-confinement devices has also been prepared for a

recent IAEA Specialists Meeting on Atomic and Molecular Processes in the Plasma Edge.

Another major accomplishment of this reporting period has been the development of a new data-base management system for the CFADC's bibliographic files, and the transfer of approximately 20,000 existing records to this advanced personal-computer system. These current files are now available for instant on-line retrieval according to collision process, reactants or authors.

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1. Consultant, ORNL.
2. Consultant, Queen's University, Belfast, Northern Ireland.
3. ORAU Postdoctoral Research Associate.
4. Consultant, Institute of Physics, Belgrade, Yugoslavia.
5. Consultant, Georgia Institute of Technology, Atlanta, Georgia.
6. Consultant, Wesleyan University, Middletown, Connecticut.
7. Consultant, Auburn University, Auburn, Alabama.

Data Centers on Atomic Spectroscopy at the National Bureau of Standards

I. Atomic Energy Levels Data Center

W. C. Martin, Director

A. Progress Report

A compilation of energy levels for all 42 spectra of molybdenum (Mo I-Mo XLII) has been completed and has been submitted for publication. A separate compilation of wavelengths and their energy-level classifications for the spectra Mo VI through Mo XLII has just been published; this latter compilation was carried out in collaboration with Japanese scientists from JAERI. We also participated in the recently completed JAERI-NBS compilation of wavelengths, energy-level classifications, transition probabilities, and Grotrian diagrams for the nickel spectra Ni IX - Ni XXVIII.

As part of our new program on atomic wavelengths, we have critically reviewed the scandium line lists and energy-level classifications and compiled these data for all Sc spectra, Sc I -Sc XXI. These tables will be submitted for publication during 1988.

We combined extensive theoretical and experimental results now available for He I to obtain very accurate values for the complete system of energy levels and thus for all predicted wavelengths of the spectrum. In addition to its spectroscopic-data usefulness, this work is of basic interest in, for example, confirming predicted two-electron QED energy contributions.

B. Future Plans

We have begun a critical compilation of energy levels for all the copper spectra, Cu I - Cu XXIX. We expect during the next year to complete this work for most of the copper ions and also to make substantial progress on our energy levels compilation for the sulfur spectra S I through S XVI.

In collaboration with JAERI we will complete a critical compilation of wavelengths, energy-level classifications, and other data for lines of the chromium spectra Cr VI through Cr XXIV. We will also begin compilation of

wavelengths for lines of calcium spectra, Ca I - Ca XX. We want our data base for atomic spectra to include complete line lists and have begun this project with the iron-group elements.

We plan to have a new Bibliography on Atomic Spectra covering the 4-year period January 1984 through December 1987 ready for publication during 1988.

II. Data Center on Atomic Transition Probabilities

W. L. Wiese, Director

A. Progress Report

Critical evaluations and tabulations on atomic transition probability data for the iron group elements, scandium through nickel, have been completed and the final proofreading is in progress. During the past year, we completed the evaluation of both allowed and forbidden lines for all outstanding ions, particularly those isoelectronic with helium, lithium, beryllium, and boron.

Work is continuing on a volume in the 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 plan to complete within the next year the "Red Book" on spectroscopic data for Ti, Cr and Ni, and we intend to do preliminary evaluations on light elements and all their ions.

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

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).

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).

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 37, 235 (1987).

G. A. Martin, J. R. Fuhr, and W. L. Wiese, Atomic Transition Probabilities, Vol. III, Scandium through Nickel--A critical data compilation (submitted to J. Phys. Chem. Ref. Data Supplement Series).

T. Shirai, K. Ishii, J. Sugar, K. Mori, Y. Nakai and K. Ozawa, "Spectral Data for Highly Ionized Molybdenum, Mo VI - Mo XLII, J. Phys. Chem. Ref. Data 16, 327 (1987).

W. C. Martin, "Improved ^{4}He I 1snℓ Ionization Energy, Energy Levels, and Lamb Shifts for 1sns and 1snp Terms," Phys. Rev. A 36, 3575 (1987).

J. Reader and C. H. Corliss, Line Spectra of the Elements, in Handbook of Chemistry and Physics, 68th edition, CRC Press, E201-E327 (1987).

Appendix 6

The JAERI Activities on A+M Data for Fusion
Status Report, November 1987

Yohta Nakai and Toshizo Shirai

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1. Atomic Collision Data

Experimental data of the cross sections of atomic collision processes mainly on charge transfer, ionization and excitation processes relevant to fusion researches have been compiled and some of them are already evaluated in the form of empirical formulas.

Part of the results of compilations has been published in JAERI-M Report series. Up to present about 50,000 data points of experimental cross sections have been stored in the Atomic and Moleculare Data Storage and Retrieval System (AMSTOR) of JAERI.

(1) Charge Transfer of Hydrogen with Atoms and Molecules [1)]

The total cross sections for electron capture and loss in collisions of hydrogen atoms and ions with atoms and molecules have been complied and given by the analytical formulas.

(2) Charge Transfer of Hydrogen with Metal Vapors [2)]

The same cross sections as described above for the targets of metal vapors have been compiled and given by the analytic formulas.

(3) Charge Transfer of Helium with Atoms and Molecules [3)]

The total electron capture and loss cross sections in collision with rare gas atoms and H_2, N_2, O_2 and carbon containing molecules are cpmplied and given by the analytic formulas.

(4) Single Electron Capture of Multi Charged Ions [4)]

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

(5) Electron Capture of Protons into the Excited States from Atoms and Molecules

The Processes: $H^{+} + B - H(nl)$, where B's are H, H_2, N_2, O_2, He, Ne, Ar, Kr and Xe, are being compiled and fitted with analytic formulas.

2. Atomic Structure Data

Spectroscopic data for the ions of following elements are subjects of our compilations and evaluations: Ti, Cr, Mn, Fe, Co, Ni, Cu and Mo.

Since 1984, the cooperation program between National Bureau of Standards and JAERI for the compilation and evaluation of atomic structure data has been continued as a part of the US-Japan Fusion Cooperation Programs.

(1) Ti Data [5]

Wavelengths, energy levels, level configurations, Oscillator strength, and radiative transition probabilities for the titanum ions Ti V to Ti XXII are critically reviewed and tabulated. Grotrian Diagrams are also presented to provide a graphycal overview.

(2) Mo Data [6]

Wavelengths, intensities, and classifications for the molybdenum ions Mo VI to Mo XLII are compiled. A short review of the work on each stage of ionization is included. The data are critically evaluated and the best results, in our judgement, are quoted.

(3) Ni Data [7]

New compilation critically evaluated on the atomic spectra of Ni IX - Ni XXVII with their energy level classifications and the Grotrian diagrams has been recently completed. The report has been published in Atomic Data and Nuclar Data Tables in this November.

(4) Fe Data

The first report of the compilation of the spectroscopic data with Grotrian diagrams for the iron ions Fe VIII - Fe XXVI was published by Mori et al in Atomic Data and Nuclar Data Tables 23 195 (1979); however, many revisions were necessary. The new compilation for Fe ions has been completed and will be published by April 1988.

(5) Cr Data

New compilation of the spectroscopic data for Cr V - Cr XXIV is now in progress and will be completed by March 1988.

(6) Other Atomic Data

Compilations of spectroscopic data for Cu, Co and Mn have been started from 1987.

All the compiled data for collision and atomic structure are now stored in our computer system by our own formats. They are available to interested users on magnetic tapes on their requests as well as other

informations related to those data compilations. We will go on to compile other data which are urgently needed and requested by fusion community.

References

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(2) T. Tabata, R. Ito, Y. Nakai and T. Shirai: Cross Sections for Charge Transfer of Hydrogen Atoms and Ions Colliding with Metal Vapors, submitted to Nucl. Instr. Methods (1987)

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Progress Report of Atomic Data Group, IPP/Nagoya 1986 - 1987

H. Tawara

1. AM Working group

1.1 A critical data compilation of the ionization data by electrons including neutral atoms, ions and some molecules (H_2, D_2, N_2, O_2) was finished and published[1]. On the other hand, the up-dating of these data is being continued.

1.2 Data were compiled for important atomic and molecular collision processes relevant to edge plasmas[2]. Addenda to this report was published[3] where the main topics are concerned with the survey of important features of hydrogen atoms and ions produced through dissociative ionization or dissociative excitation of hydrogen molecules by electrons.

1.3 The present theoretical situation is surveyed on the final state distributions, that is, the (n,ℓ) distributions of ions followed electron capture of multiply charged ions in collisions with neutral atoms and theoretical values for typical collision systems ($C^{3+}(1s^2 2s) + H \rightarrow C^{2+}(1s^2 2\ell n\ell') + H^+$ and $C^{6+} + H \rightarrow C^{5+}(n\ell) + H^+$) are compared with available experimental data. Generally speaking, those for the dominant electron capture processes are in good agreement with each other but those for less dominant processes show some significant discrepancies[4].
Further, a quick compilation has just been finished on partial cross sections of the (n,ℓ) distribution of C^{q+} and O^{q+} ions, typical impurity ions in plasma apparatus, in collisions with H, H_2 and He.[5]

1.4 The wavelengths and energies of K-X-rays of iron ions in all ionization stages are compiled and published[6].

1.5 A critical compilation and evaluation of the excitation cross sections and rate coefficients of helium-like ions by electrons has been finished and is ready for publication[7].

1.6 Some important theoretical models of atomic structures in hot, dense plasmas have been reviewed and is ready for publication[8].

2. PWI working group

2.1 New empirical formulas for sputtering of monatomic solids by ion impact are proposed and found to reproduce the observed data better than our previous empirical formulas. In particular, the agreement near threshold and low energy region is improved[9].

2.2 Data are being surveyed for sputtering of compound materials where the segregation processes play a role.

2.3 A review is being continued on synergistic effects in plasma wall interactions. A phenomenological model has been developed for chemical sputtering of graphites and found to be satisfactory in understanding some behavior of hydro-carbon molecules and ions observed in hydrogen bombardment experiments and in hydrogen plasmas. This will be published in IPPJ-AM report.

2.4 Some calculations are being made on the reflection (or backscattering) of very low energy ((10 eV) light ions from solids based upon the embedded atom model (EAM).

3. On-going and near future activities

3.1 AM processes of hydro-carbon molecules (C, CH, CH_2, CH_3, CH_4) --- relevant to plasma apparatus with carbon coating/graphites

a) collision data (cross sections for ionization, excitation, dissociation, formation/destruction, photon-emissions,...)

b) Spectroscopic data

3.2 Collisions of molecules with surfaces (neutralization, dissociation)

3.3 Improvement of (n, ℓ) distribution data of C^{q+}, O^{q+} ions in collisions with H, H_2 and He

3.4 Sputtering of compound materials (segregation, etc.)

3.5 Backscattering of low energy (less than 10 eV) ions from solid

3.6 Synergistic effects-phenomenological model

3.7 Desorption processes

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The Atomic and Molecular Data Centre at Queen's University Belfast

Progress Report

Prepared by
John Hughes, November 1987

In January 1987, the data centre received renewed support from the UK Atomic Energy Authority, Culham Laboratory which allowed us to employ one full-time physicist (D.S. Elliott). The work carried out during the past year has consisted of

(i) an extension and revision of our previous work on electron impact ionization of atoms and ions, and

(ii) new work on ionization processes involving molecules relevant to plasma edge studies.

The following is a summary of work recently completed or in progress.

1. "Recommended Data on the Electron Impact Ionization of Atoms and Ions: Fluorine to Nickel", M.A. Lennon, K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston, M.J. Murray, and F.J. Smith.
   - to be published in the Journal of Physical and Chemical Reference Data (early 1988)
   This paper contains data and recommendations from Culham Report R270 brought up to date (August 1987).

2. "Electron Excitation Rates for Iron Ions", A.E. Kingston and M.A. Lennon
   - to be published in Nuclear Fusion (Special Issue, early 1988).
   This paper contains a compilation and assessment of excitation rates for Fe I - Fe XXVI. Recommended Maxwellian rate coefficients are presented in the form of polynomial fit coefficients, together with estimates of reliability. A full bibliography for each ion is also included.

   A more extensive version of this work, containing tabulated rate coefficients over a wide range of temperatures together with estimates of radiative power loss, will be published as a Culham report in early 1988.

3. "Recommended Data on Electron Impact Ionization of Atoms and Ions: Copper to Uranium"
   - in preparation. To be published as a Culham report in 1988.

4. "Recommended Data on Electron Impact Ionization of Molecules in the Plasma Edge", M.A. Lennon, A. Crowe, D.S. Elliott, J.G. Hughes, and F.J. Smith
   - in progress. A preliminary report on this work was presented by M.A. Lennon at the IAEA Specialist Meeting on Atomic and Molecular Data for Plasma Edge Studies, Vienna, July 8-10, 1987.

Appendix 9

GAPHYOR DATA CENTER

Progress Report 1986-1987

J.L. DELCROIX, K. KATSONIS.

Centre de Données GAPHYOR, Université de Paris-Sud, Bâtiment 212

91405 ORSAY CEDEX, FRANCE

1. FACTUAL DATA BASE

1.1. Some statistics

As of the 1st of October 1987, the number of entries in the files were distributed as follows :

a) Number of elements and sections

Table 1

Section / File	1 structure	2 hν col.	3 e col.	4 heavy part. col.	5 macro. prop.	Totals
1 element	30 245	5 896	10 372	6 214	4 081	56 808
2 elements	39 685	4 668	3 862	29 840	6 555	84 610
3 elements	16 818	2 010	611	15 839	2 239	37 517
4 elements	3 281	380	66	4 214	656	8 597
Totals	90 029	12 954	14 911	56 107	13 531	187 532

.../...

1.2. Gas-Phase Chemical Physics data base (Elsevier end of 1987)

The whole data base is presently beeing published by Elsevier North-Holland. The publication is planned for the end of 1987 in three volumes. The table of contents and the general introduction of these books are shown in appendix 1. This introduction provides a detailed description of the present state of GAPHYOR.

1.3. Recent technical developments

a) New processes (or reactants)

To take in account the recent developments in the field of atomic and molecular physics, GAPHYOR has improved the description of some reactants and introduced a few new processes. The most important are the following :

Shell structure description

ELEMENTS AA	S E	MOL1	INITIAL STATE MOL2	MOL3	PR	MOL4	FINAL STATE MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* 8A = Fe Co Ni *															
Fe	2	hν	Fe		IN	e	Fe k+	2-7-10-8	S	:T	86	IPPJ	REPT	AM48	MANSON S T	USGAAT
Fe	2	hν	Fe 3+		IN	e	Fe k+	2-7-10-5	S	:T	86	IPPJ	REPT	AM48	MANSON S T	USGAAT
Fe	2	hν	Fe 6+		IN	e	Fe k+	2-7-10-2	S	:T	86	IPPJ	REPT	AM48	MANSON S T	USGAAT
Fe	2	hν	Fe 10+		IN	e	Fe k+	2-7-8	S	:T	86	IPPJ	REPT	AM48	MANSON S T	USGAAT
Fe	2	hν	Fe 13+		IN	e	Fe k+	2-7-5	S	:T	86	IPPJ	REPT	AM48	MANSON S T	USGAAT

Neutral or ionized clusters

ELEMENTS AA	BB	CC	DD	S E	MOL1	INITIAL STATE MOL2	MOL3	PR	MOL4	FINAL STATE MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* H = H D T * 4A = C Si Ge Sn Pb * 5A = N P As Sb Bi * 7A = F Cl Br I At *																		
H	C	N	I	1	/I-/H3C2N/n	n=01-03		EN	/I-/H3C2N/n	n=00-02		8	R	86	552	15	1011	KEESEE R G	USPAUP
H	C	N	F	1	/F-/H3C2N/n	n=01-05		EN	/F-/H3C2N/n	n=00-04		8	R	86	552	15	1011	KEESEE R G	USPAUP
H	C	N	Cl	1	/Cl-/H3C2N/n	n=01-06		EN	/Cl-/H3C2N/n		n=00-05	8	R	86	552	15	1011	KEESEE R G	USPAUP
H	C	N	Cl	1	/N2+/H3CCl/n/H3C/n			EN	H3CCl			8	R	86	552	15	1011	KEESEE R G	USPAUP

Molecules adsorbed on a surface

ELEMENTS AA	BB	CC	S E	MOL1	INITIAL STATE MOL2	MOL3	PR	MOL4	FINAL STATE MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
* H = H D T * 4A = C Si Ge Sn Pb * 8B = Ru Rh Pd *																	
H	C	Ru	1	(Ru)H2C2			EN				/E	86	48	82	3197	EGAWA C	JATKBU
H	C	Ru	1	(Ru)H4C2			EN				/E	86	48	82	3197	EGAWA C	JATKBU
H	C	Ru	4	H2C2	(Ru)		PR				L/E	86	48	82	3197	EGAWA C	JATKBU
H	C	Rh	4	H4C	(Rh)		PR				L/E	86	30	84	4163	RETTNER C	USCASJ
H	C	Ru	4	H4C2	(Ru)		PR				L/E	86	48	82	3197	EGAWA C	JATKBU

b) Sections and processes (see appendix 1 paragraph 6 for process code)

Table 2

1 structure		2 hν col.		3 e col.		4 heavy part. col.		5 macro. prop.	
EN	50 059	AN	1 548	SN	967	SN	966	PV	905
CP	252	SN	491	SC	386	SC	444	FT	1 333
DP	2 482	SC	260	EL	1 445	EL	731	VR	146
NP	692	EL	156	EX	3 741	EN	1 355	ZT	94
PE	2 074	FF	84	ER	418	EX	2 210	CO	104
VR	22 838	EX	1 121	DX	175	ER	983	DN	519
TR	9 093	ER	386	XX	347	DX	6 631	VI	622
IN	584	DX	94	DO	39	XX	1 993	CT	698
DT	172	XX	61	IN	3 779	DO	265	TD	248
DS	1 146	DO	72	RC	174	TE	1 882	PE	249
XX	25	IN	4 274	RR	122	IN	5 514	EN	2 276
EA	612	DT	413	RE	85	DT	765	DM	56
		DS	2 384	RO	60	RI	424	RN	933
Tot.	90 029	P2	368	RD	309	10	4 516	FE	315
		P3	173	RS	467	20	184	CE	152
		P4	62	AT	1 237	LN	2 948	ME	554
		PN	866	DT	44	MP	112	DE	168
		NL	108	DS	788	LP	3 019	PI	479
		PR	33	BS	195	IR	11 469	AT	429
		Tot.	12 954	PR	133	AS	3 348	DT	69
				Tot.	14 911	DS	2 073	PC	60
						IH	742	FI	12
						AH	157	MI	834
						DH	72	DI	178
						KE	492	DA	40
						PR	2 279	RC	219
						IA	65	RR	84
						ID	468	RE	21
								RO	7
						Tot.	56 107	RD	3
								RS	0
								RI	4
								LA	868
								MD	77
								ST	875
								Tot.	13 631

.../...

Isoelectronic series

ELEMENTS AA	S E	INITIAL STATE MOL1	MOL2	MOL3	PR	FINAL STATE MOL4	MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
****** * 10 * ******															
	1	AA(N=16)+	Z=16-28		TR	AA(N=16)	Z=16-28		UI R	86	10	35	185	FAWCETT B	UKENRU
	1	AA(N=15)+	Z=15-28		TR	AA(N=15)	Z=15-28		UI R	86	10	35	203	FAWCETT B	UKENRU
	1	AA(N=05)+	Z=18-36		TR	AA(N=05)	Z=18-36		UI T	86	10	35	319	BHATIA A K	USMDGR
	1	AA(N=06)+	Z=12-28		TR	AA(N=06)+	Z=12-28		UI :R	86	10	34	215	FAWCETT B	UKENRU
	1	AA(N=05)+	Z=18-36		TR	AA(N=05)+	Z=18-36		UI T	86	10	35	319	BHATIA A K	USMDGR
	1	AA(N=04)+	Z=18-36		TR	AA(N=04)+	Z=18-36		UI T	86	10	35	449	BHATIA A K	USMDGR

Homonuclear sequences

ELEMENTS AA	S E	INITIAL STATE MOL1	MOL2	MOL3	PR	FINAL STATE MOL4	MOL5	MOL6	INFO	AN	JO	VO	PAGE	AU	GEOG
********** * R = He Ne Ar Kr Xe Rn * **********															
NeAr	1	AA n+*	n=01-06		EN				Q FR	86	552	15	321	KAUFMAN V	USMDGA
Ar	1	Ar n+*	n=09-14		EN				Q FR	86	552	15	321	KAUFMAN V	USMDGA
Ar	1	Ar n+*	n=09-13		TR	Ar n+	n=09-13		PQ FR	86	552	15	321	KAUFMAN V	USMDGA
Ar	1	Ar n+*	n=10-12		TR	Ar n+*	n=10-12		PQ FR	86	552	15	321	KAUFMAN V	USMDGA

b) New automatic methods of error detection

The publication of the book mentioned above has led the GAPHYOR team to develop new methods of computer aided detection of errors. The most important features in this field are the following :

- Programme "EQUILIBRE" - This is a programm who tests the correct balance, between initial and final state, of the total number of atoms of a given element and of the total electric charge.

- The method of "SQUELETTES" - This is based on a software who is able to produce the list of all the different skeletons included in the data base together with a statistics of the number of entries per skeleton. A skeleton is a structure of process not including the value of the elements (for example e, A_2/IN/e, A^+, A). The number of different skeletons is at present time shown in table 3.

Table 3

File	Number of skeletons	Entries per skeleton
1 element	5 773	9.8
2 elements	14 902	5.9
3 elements	13 429	2.8
4 elements	4 960	1.7
Total	39 064	5.7

By comparing the totals of table 1 and 3, one sees that at present time one skeleton represent on the average 5.7 entries. This is however somewhat misleading because there are many skeletons who have been considered as different in spite of their similarity.

Example : e, A^{2+}/IN/e, e, A^{3+}
e, A^{3+}/IN/e, e, A^{4+}
.....

1.4. On-line retrieval

GAPHYOR can be consulted on-line 7 days/week and 24 hours/day (except for a few maintenance interruptions) from everywhere in the world (through data networks). In France, and soon in some neighbour countries, this consultation can be made easily at home, through the French VIDEOTEX system using the so called MINITEL (about 3 millions homes presently equipped).

2. NUMERICAL DATA ACTIVITIES

2.1. Numerical data files

A system for storage and retrieval of numerical data was implemented for IBM compatible microcomputers. The bibliographic part of it is contained in three files compatible with the mainframe implementation of GAPHYOR. These files are using the new four-letters periodical code and all the GAPHYOR system conventions, as implemented in its recent North-Holland edition. This part of the system is currently being used in the Astrophysical Laboratory at Meudon for creating a bibliographic file for photoionization to be subsequently used for the needs of the international astrophysical project opacity. The numerical data file of the system comprise for the moment being evaluated charge transfer cross sections of ions colliding with H and He. The standard commercial data base system Rbase System V has been used as a basis for this implementation. Consequently, data handling and transfer under standard ASCII format files or other common commercial form files (e.g. .DB) is straightforward.

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 of Meudon the procedural part of the data bank of Belfast-Daresbury has been installed at CIRCE and part of the numerical values contained will eventually be merged with the GAPHYOR numerical bank. This activity has been supported by the French Atomic Energy Autority (C.E.A.) and the National Centre for Scientifique Recherche (C.N.R.S.).

.../...

2.2. Oxford and Abingdon meetings

GAPHYOR participated in the organization of an atomic data worshop (1st and 2 August 1987) in Oxford, U.K., a satellite meeting to the XV ICPEAC held at Brighton. The next meeting of this series has been scheduled to be held in Meudon in July 1988.

GAPHYOR was the organizer of a CODATA worshop on the management of data banks held in August 3 and 4 at Cosener's House, Abingdon, U.K., directly after the atomic data worshop. This meeting was sponsored by CODATA and the US National Bureau of Standards. During the meeting data bank managers discussed technical details concerning data bank implementations and architectures and data exchange. The need for a unified atomic data consideration for the main application fields (astrophysics, fusion, arcs, materials in contact with cold plasmas) and the advantages of extensive microcomputer use for related data bases were thoroughly addressed. Detailed information on these subjects will be included in the meeting's minutes, available as a GAPHYOR report.

2.3. Theoretical data production

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, to be published in Nuclear Fusion in a special issue, is mainly reviewing 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 I.A.E.A. under Dr. Katsonis responsibility ; it includes all the conclusions and recommendations of the CRP, 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 in the report.

Numerical calculations of charge transfer cross sections for Ar and Fe ions are also on progress. The necessary numerical CTMC code for Monte Carlo type calculations developed by M.R.C. McDowell and G. Peach has been successfully run on the CRAY computer of the french Polytechnic School and adapted to work in a Definicon acceleration board for IBM-compatibles based on MC68020 CPU and MC68881 FPU running SVS Fortran under a DOS compatible kernel. Preliminary results for Fe and Ar ions have been obtained.

TABLE OF CONTENTS

INTRODUCTION

The present book is a printed version of the full GAPHYOR factual and bibliographic data base which as of July 1st, 1987 contains more than 180 000 records covering the 1970-1986 period.

GAPHYOR (GAz-PHYsique-ORsay) is a data bank on properties of atoms, small molecules and gases. It includes excited and ionized states. The chemical systems described by GAPHYOR includes from 1 to 4 chemical elements and molecules of less than 9 atoms. The sorting of the data is based first on the number of elements involved :

- Systems with 1 element (Volume 1)
- Systems with 2 elements (Volume 2)
- Systems with 3 elements (Volume 3 pp. -)
- Systems with 4 elements (Volume 3 pp. -)

Within each of these chapters, the data sorting is based on the Mendeleev families order and on five sections :

1 - Properties of the atoms and molecules
2 - Photon collisions
3 - Electron collisions
4 - Collisions and reactions between atoms and molecules
5 - Macroscopic properties of gases

Each data line correspond to a well defined process ; thanks to the condensed description used, all the information in a data line is written along one computer listing line.

EXPLANATION OF DATA

1. LIST OF GAPHYOR DESCRIPTORS

The structure of a GAPHYOR record is shown on Figure 1.

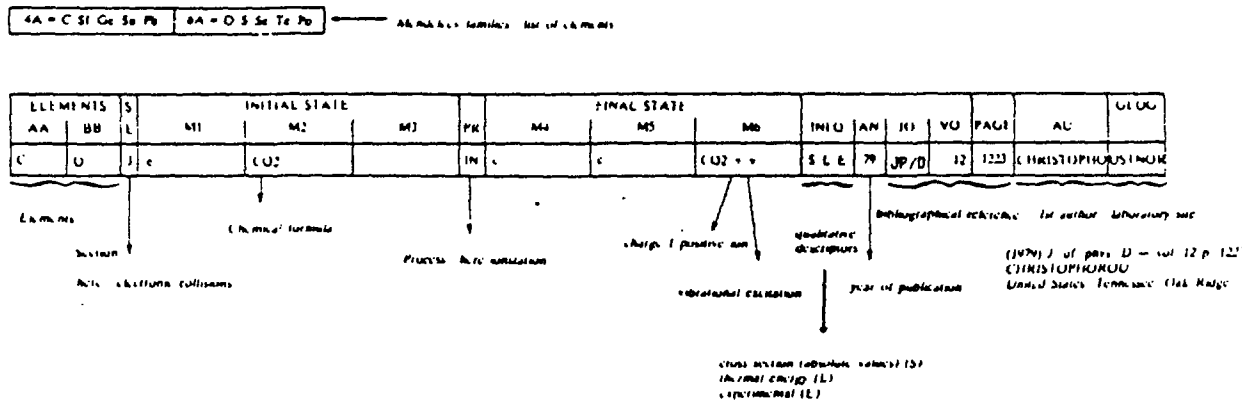

Figure 1 : Structure of a GAPHYOR line

It is based on the following descriptors :

Mendeleev families : FA, FB, FC, FD.
Elements in families : AA, BB, CC, DD.
Section : SE
Initial state : MOL1, MOL2, MOL3.
Process : PR
Final state : MOL4, MOL5, MOL6.
Informations : INFO
Year of publication : AN
Bibliographical references : JO, VO, PA.
First author : AU
Geographical laboratory site : NA, ST, CI.

The conventions used to write the values of those various descriptors and to sort the data file are described below.

2. THE MENDELEEV FAMILIES (FA, FB, FC, FD)

The chemical system analysed must be composed from 1, 2, 3 ou 4 elements (examples : He, H_2O, H_2N + CO_2 but not H_3N + CF_3Br). The elements are classified by family according to the following code :

R = He Ne Ar Kr Xe Rn
H = H D T

1A = Li Na K Rb Cs Fr
1B = Cu Ag Au
2A = Be Mg Ca Sr Ba Ra
2B = Zn Cd Hg
3A = B Al Ga In Tl
3B = Sc Y La Ac
4A = C Si Ge Sn Pb
4B = Ti Zr Hf
5A = V Nb Ta
6A = O S Se Te Po
6B = Cr Mo W
7A = F Cl Br I At
7B = Mn Tc Re
8A = Fc Co Ni
8B = Ru Rh Pd
8C = Os Ir Pt
9A = Cc Pr Nd Pm Sm
9B = Eu Gd Tb Dy Ho
9C = Er Tm Yb Lu
9D = Th Pa U Np Pu Am Cm Bk Cf Es ...
10 = unspecified elements, isolelectronic series
EE = Positronium (Ps), Muonium (Mu)

The Mendeleev families are the basis of the first sorting criterion of the file. The data base is composed of 4 files according to the number of chemical elements in the process. The first file (Volume 1) is concerned with chemical systems constituted of one element only. The above list order is the sort order, that is to say that the volume begins with rare gases properties and continues with properties of hydrogen, alkalines,... The next volumes are concerned with systems made of two (Volume 2), three or four elements (Volume 3). In every case the families (FA, FB, FC, FD) are written at the top of the page and sorted according to the above order.

Examples : H_2O –> FA = H FB = 6A
$N_2 + O_2$ –> FA = 5A FB = 6A

.../...

3. ELEMENTS CONCERNED IN EACH FAMILY (AA, BB, CC, DD)

The elements are represented by their standard chemical notation. They are not used to sort the file.

Lines relating to different elements of the same family can be merged into one single line which is then grouping results relating to these different elements : in this case the concerned elements are printed together in the ELEMENTS(1) columns (example : He Ar) and they are written collectively as AA, BB, CC or DD in the reaction scheme.

4. SECTION (SE)

A number from 1 to 5 defines the section according to the following code :

1 - Properties of atoms and molecules
2 - Photon collisions
3 - Electron collisions
4 - Collisions and reactions between atoms and/or molecules (including ions)
5 - Macroscopic properties

This descriptor is the second sorting criterion of the file : for each family group the processes are classified according to the section order.

.../...

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(1) Special notations - if space is lacking in the ELEMENTS columns, one uses the following notations :

2 3 5 = elements number 2, 3 and 5 of the family (Ne, Ar, Xe for rare gases)

1...5 = elements number 1 through 5 of the family (He, Ne, Ar, Kr, Xe for rare gases)

THE PRESENT STATUS OF A+M DATA RESEARCH IN CHINA

———THE INTRODUCTION OF CRAAMD

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I. GENERAL SITUATION OF CRAAMD.

CRAAMD IS A WORKING GROUP OF THE WHOLE COUNTRY FOR ATOMIC AND MOLECULAR DATA. IT WAS FORMALLY ESTABLISHED IN BEIJING IN FEBRUARY THIS YEAR. CRAAMD IS SUBORDINATE TO NUCLEAR DATA COMMITTEE OF CHINA AND TO CODATA CHINESE COMMITTEE AS WELL. THERE ARE TEN RESEARCH INSTITUTIONS JOINING CRAAMD SO FAR. THEY ARE:

1. INSTITUTE OF APPLIED PHYSICS AND COMPUTATIONAL MATHEMATICS (BEIJING)
2. DEPARTMENT OF MODERN PHYSICS, FUDAN UNIVERSITY (SHINGHAI)
3. INSTITUTE OF LOW ENERGY PHYSICS AND DEPARTMENT OF PHYSICS, BEIJING NORMAL UNIVERSITY (BEIJING)
4. NUCLEAR PHYSICS DIVISION OF INSTITUTE OF ATOMIC ENERGY (BEIJING)
5. INSTITUTE OF HIGH TEMPERATURE AND HIGH PRESSURE PHYSICS, CHENGDU UNIVERSITY OF SCIENCE AND TECHNOLOGY (CHENGDU)
6. INSTITUTE OF PHYSICS, ACADEMIA SINICA (BEIJING)
7. INSTITUTE OF ATOMIC AND MOLECULAT PHYSICS,JILIN UNIVERSITY (CHANG CHUN)
8. CENTER OF BASIC PHYSICS, CHINA UNIVERSITY OF SCIENCE AND TECHNOLOGY (HE FEI)
9. INSTITUTE OF ENVIROMENTAL FEATURES (BEIJING)
10. DEPARTMENT OF APPLIED PHYSICS, CHANG SHA UNICERSITY OF SCIENCE AND TECHNOLOGY.

THERE ARE FOUR WORKING GROUPS IN CRAAMD:

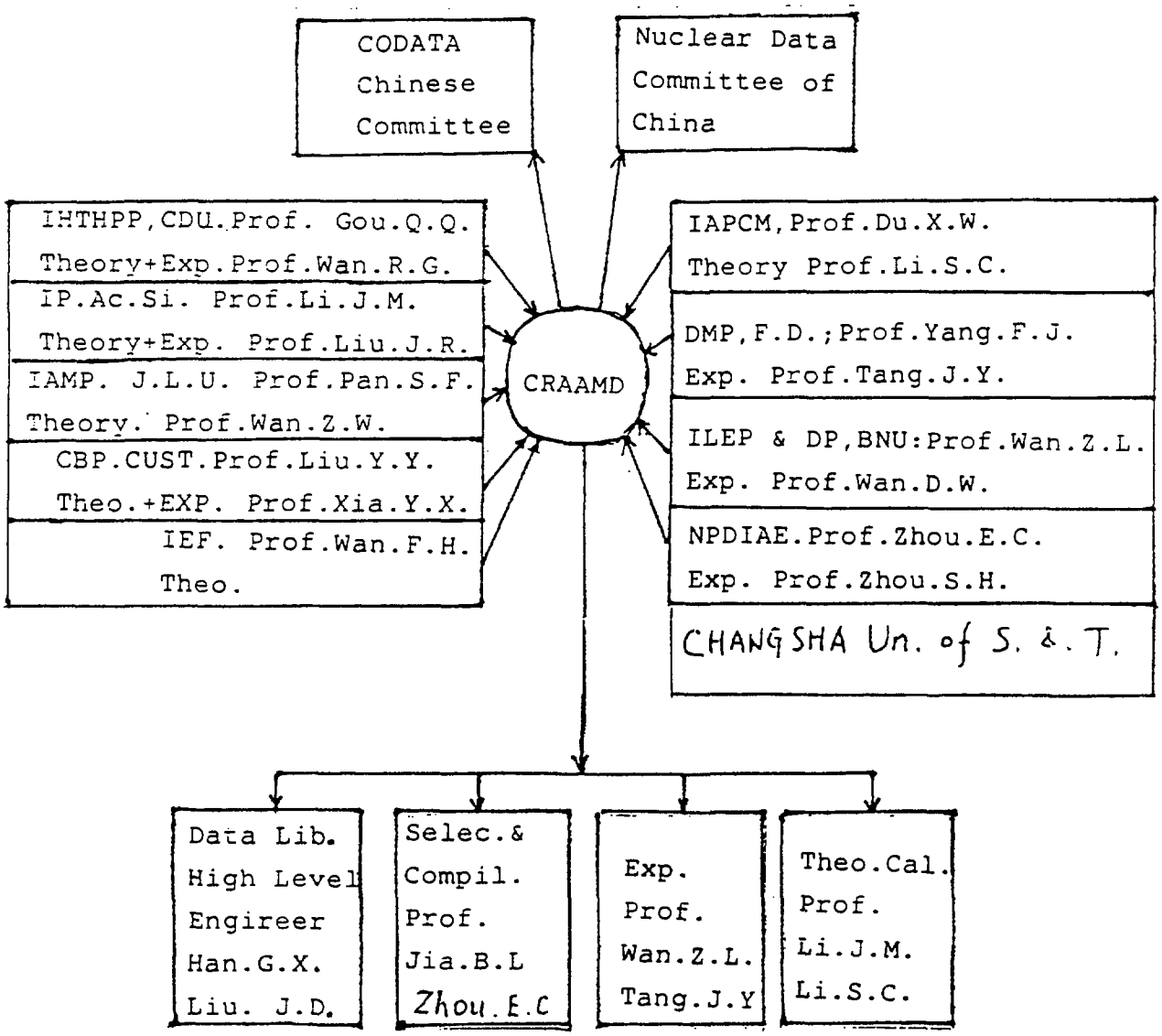
A. THE GROUP OF TJEORETICAL CALCULATIONS;

B. THE EXPERIMENTAL GROUP;

C. THE GROUP OF SELECTIONS AND COMPILATIONS;

D. THE DATA LIBRARY.

The Sketch of CRAAMD



THE EXECUTIVE DUTIES OF CRAAMD ARE HANDLED BY THE LEADING GROUP OF THREE PERSONS:

SUN YONGSHENG (HEAD OF THE GROUP, IAPCM, BEIJING)

TANG JIAYONG (VICE HEAD OF THE GROUP, FUDAN UNIVERSITY)

WANG ZHONGLE (VECE HEAD OF THE GROUP, ILEP, BEIJING NORMAL UN.)

THE IAPCM IS IN CHARGE OF THE ROUTINE OF CRAAMD.THE ROUTINE WORKING BODY OF SRAAMD IS SET UP IN IAPCM.

DR. DU X. W. AND ZHOU E. C. OF NDCC ARE RESPONSIBLE FOR THE WORK OF ITS A+M WORKING GROUP ——CRAAMD.

II. DUTIES OF CRAAMD

THE DUTIES OF CRAAMD ARE TO CALCULATE, MEASURE, COLLECT, COMPILE AND EVALUATE A+M DATA. OUR PURPOSE IS AS FOLLOWS: THE LIBRARY OF ATOMIC AND MOLECULAR DATA AND THE LIBRARY OF COMPU TATIONAL SOFTWARES WILL BE PROGRESSIVELY SET UP IN ORDER TO SATISFY THE NEEDS OF SOME MAJOR FIELDS OF SCIENCE AND TECHNOLOGY (FOR EXAMPLE: THE CONTROLED FUSION RESEARCH, THE LASER RESEARCH ETC.) ALL ATOMIC SCIENTISTS IN THE INSTITUTIONS JOINING CRAAMD WILL UNITEDLY MAKE THEIR PLANS AND COORDINATE THEIR RESEARCH WORKS ON ATOMIC AND MOLECULAR DATA.

AT PRESENT, WE ARE ENGAGED IN SEVERAL TOPICS SUCH AS:

(1) THE ENERGY LEVELS AND THEIR WIDTHS OF ATOMS AND IONS;

(2) ELECTRON IMPACT EXCITATION AND IONIZATION;

(3) DIELECTRONIC RECOMBINATION PROCESS;

(4) ATOMIC (ION) PHOTOELECTRIC EFFECT;

(5) CHARGE EXCHANGE PROCESS

AND SO ON.

MEANWHILE, WE ARE ALSO ENGAGED IN RESEARCH OF THE METHODS OF THEORETICAL CALCULATIONS AND OF EXPERIMENTAL MEASURMENTS, WE ALSO DEVELOP COMPUTATIONAL SOFTWARES, CALCULATE DATA, DO SOME MEASURMENTS, EXTENSIVELY COLLECT AND COMPILE A+M DATA.

III. ACADEMIC EXCHANGES

CRAAMD WOULD LIKE TO SUPPORT AND DEVELOP ACADEMIC EXCHANGES IN A+M FIELDS. RECENTLY—FROM AUGUST 26 TO SEPTEMBER 1ST WE HELD AN ACADEMIC SYMPOSIUM ON A+M DARA OF THE WHOLE COUNTRY IN QINHUANGDAO (HE BEI). MORE THAN 100 PEAPLE ATTENDED THIS SYMPO SIUM. THE PAPERS RECEIVED IN THE CONFERENCE WERE MORE THAN 80. THESE PAPERS WERE DIVIDED INTO THREE CATEGORIES:

A. THEORETICAL CALCULATIONS;

B. EXPERIMENTAL MEASUREMENTS;

C. SELECTIONS AND COMPILATIONS.

THE FAMOUS SCHOLARS—PROF. LI. Z. W, PROF. GOU. Q. Q, PROF. LI. J. W. AND OTHERS GAVE THEIR REPORTS IN THE CONFERENCE. THE DIGEST OF THE ABSTRACTS OF CONTRIBUTED PAPERS HAVE BEEN PUBLI SHED IN CHINESE, BUT NOT IN ENGLISH.

INTERNATIONALLY, WE HAVE ALREADY INFORMED NDS OF IAEA THAT CRAAMD WAS FORMALLY ESTABLISHED. THEY MAILED US CIAMDA, 87 AND A+M NEWSLETTER IN THE MIDDLE OF THIS YEAR. AT THE SAME TIME, WE ALSO INFORMED INTERNATIONAL CODATA THAT CRAAMD WAS ESTABLISHED.

WE WOULD LIKE TO ESTABLISH VOCATIONAL RELATIONS WITH ALL OF THE A+M RESEATCH CENTERS IN THE WORLD.

THANK YOU VERY MUCH!

ACTIVITIES IN THE A+M DATA AT ENEA BOLOGNA, ITALY

November, 1987

ACTIVITIES IN THE A+M DATA AT ENEA BOLOGNA, ITALY

MONTECARLO SIMULATION OF NEUTRAL TRANSPORT

E.Cupini, A.De Matteis

Starting from the available formulas, analytical expressions for the calculation of atomic and molecular data for Monte Carlo simulation of neutral particle transport in the plasma edge have been selected and implemented in the NIMBUS(+) code.

The computed reactions include: electron impact ionization, ion impact ionization, charge exchange; the neutral of interest are H, D, T and He. Ion impact ionization and dissociation on H_2 molecule have also been considered. The work has been performed in the framework of the ENEA/JET and ENEA/NET agreements.

(+) E.Cupini, A.De Matteis and R.Simonini: NIMBUS - Monte Carlo Simulation of Neutral Particle Transport in Fusion Devices. Part One: Physical Model and Numerical Method. NET Report 9, EUR XII-324/9(1983)

PLASMA IMPURITY

P.L.Ottaviani

In the framework of the ENEA-JET agreement for the development of impurity transport codes, atomic data packages were organized for the following impurity atoms: beryllium, carbon, nitrogen, oxygen, neon, iron and nickel.

Only electron collision processes were considered: electron impact ionization, radiative and dielectronic recombination, collisional excitation.

Most part of the work rely upon theoretical calculations or semi-empirical formulas coming from a relative small number of experiments.

The data packages have been built taking into account the most widely used expressions for the calculation of the rate coefficients, in order to asses the sensitivity of the results to their variations.

Sets of recommended data coming from recent critical compilations on electron impact excitation and ionization were included.

Work is in progress to investigate the excitation rate coefficients for the iron ions. All the relevant calculations and experiments up to late 1986 were collected and organized on magnetic media; we intend to bring up-to-date this file with more recent data. The goal is to generate a set of reliable coefficients to be used at low temperatures (< 30 ev) where large uncertainities it is known to exist.

Activities in the A+M data at ENEA Bologna, ITALY

Appendix 12

Progress Report of the A+M Data Unit

November 1987

J.J. Smith

Staff

Dr. Ratko Janev replaced Dr. Alex Lorenz as Head of the Atomic and Molecular Data Unit during September 1987. Dr. Janev was previously at the Institute of Physics, Belgrade, Yugoslavia. The other members of the section are Mr. James Smith (Physcisicst/Programmer) and Mr. Khalid Sheikh (Documentation Clerk/Typist).

Programe

Bibliographic Data

The computerized index to Atomic and Molecular Collision Data for Fusion, CIAMDA 87 was completed and published in February 1987. Over 1,000 copies of the publication where sold and distributed. The International Bulletin on Atomic and Molecular Data for Fusion has been continued to be published, with new publication schedule of two bulletins per year. Volume 36 is completed and will be distributed in November.

Numerical Data

A large effort has been devoted to the establishment of a data base and auxcillary supporting software for the storage, exchange and publication of recommended atomic collision data. A data base has been established using the commercial data base management system ADABAS. All relevant data fields for the representation of cross sections and reaction rates by analytic formulae with fitting coefficients have been established. The recommended data to appear in the Nuclear Fusion Supplement for iron has been introduced into the files. Examples of the data index and output are available. Computer software for the generation of linearly interpolable tables from fitting parameters and the derivation of reaction rate coefficients from cross section data have been completed and are available. Generalised plotting software has been developed.

The programme of work and meetings for the Atomic and Molecular Data Unit is provided for information.

IAEA A+M Data Unit Programme for 1988

(As prepared by the A+M Data Unit staff in consultations with Drs. J.J. Schmidt and A. Lorenz, the head and deputy head of the IAEA Nuclear Data Section).

(1) Specialist Meeting on the A+M Data Base and Fusion Application Interface

The development of the IAEA/NDS A+M data base system (computer software for handling the data) is approaching the stage of completion. At the same time, a certain amount of evaluated data has become available from different data centres and are now being stored in the IAEA A+M data base. The crucial problem in the further development of the data base system, and in particular its interface with the plasma users and data centres producing evaluated data, is the establishment of a unique accepted format (or formats) for the presentation of the data by these three interacting groups. An agreement has also to be reached on the unification of A+M data base files used by different plasma users groups (which presently is not the case), by continuous up-dates and the acceptance of the A+M data files recommended by A+M Data Centre Network.

It is, therefore, deemed extremely useful to convene a three day Specialist Meeting at the IAEA, Vienna next year with the task to settle these problems. Representatives of all major plasma user groups (Princeton, Oak Ridge, San Diego, Culham, JET, Garching, Jülich, Cadarache, Kurchatov Institute, Nagoya, JAERI), as well as of the Data centres (Oak Ridge, Belfast, Nagoya, JAERI) would be invited to participate. (Note that Specialist meetings are held at no cost to the IAEA). An up-date of the A+M data needs for fusion (mostly core-plasma) modelling should also be done at that meeting. The meeting is suggested to be held in the Spring (April, May), 1988, in conjunction with another Specialist Meeting on C^{q+}, O^{q+} data (see below).

(2) Specialist Meeting on C^{q+}, O^{q+} Collision Data

Besides the data for iron, the evaluated data base for C^{q+}, O^{q+} colliding with electrons, H, H_2 and He is virtually (at least for the ground-state targets) complete (ORNL Red Book vol. 5, the Belfast data on ionization, the ORNL-Nagoya Report on excitation). Nevertheless, there are still gaps in the data base (for instance, there are no data for charge exchange of C^+ on He, no data for the processes involving excited states, dissociative processes, dielectronic recombination, etc) and in some cases there are differences between the recommended data from different groups (excitation and ionization by electron impact).

In order to eliminate these differences, and to complete the data base for C^{q+} and O^{q+} ions, a small specialist meeting is suggested to be organized with evaluators from ORNL, Belfast and Nagoya, and the producers of new data on dielectronic recombination (DR) (e.g. Lebedev Institute/Moscow, NBS/Washington, Meudon/France, ORNL/USA, etc.) and possibly some other processes. The producers of new data will be contacted in due time, so that they would bring their data to the meeting for evaluation. For instance, Pindzola and / or Roszmann will be asked to perform the DR calculations, ORNL and Nagoya for the missing ion-atom cross sections, etc. The meeting should

endorse the final form of the recommended data for these ions, which then will be stored in the Agency's A+M Numerical Data Base, and published in the IAEA series on A+M Data for Fusion (see point (4) below). The meeting is proposed to be held immediately after Specialist's Meeting (1) discussed above.

(3) Proposal for a Coordinated Research Programme on the Production and Evaluationof A+M Collision Data for the Plasma Edge

Following the conclusions of the July 1987 Specialist Meeting on A+M Data for Plasma Edge Studies, the IAEA A+M Data Unit intends to initiate early in 1988 a CRP with the above title. The project will concentrate on the production of needed data as identified by the 1987 SM, with a parallel work in the Data Centres on data evaluation. It is hoped that the proposed CRP will initiate and encourage (with modest Agency support) data production work in many laboratories. The relevant experimental and theoretical groups would be invited to participate in this project.

The CRP should be constituted by March/April 1988, and the first working meeting (Research Coordination Meeting) of its participants would be convened in 1989. At each such meeting the CRP participants would critically evaluate their accomplishments during the preceding period and the completed subsets of data would be introduced in the IAEA A+M Data Base and made available to interested users. The final results of the CRP effort would be published in a special volume of the planned IAEA Series on A+M Data for Fusion (see below).

(4) IAEA Series on A+M Data for Fusion

In the course of 1988, the A+M Data Unit will initiate the publication of a special series on A+M Data for Fusion, each volume containing a separate and comprehensive subset of recommended A+M data.

The general philosophy of this series is similar to that of the ORNL Red Books, but there will be much more emphasis on the internationally adopted recommended data and on their completeness (i.e. inclusion of accurate theoretical data, use of physically well-founded inter-and extrapolation procedures, etc).

The place of this series within the IAEA publication programme is still being discussed (as well as its budgeting and format). It is suggested that these publications form separately identifiable series in the framework of the Agency's Nuclear Fusion publications. The preliminary plan of publication (based on the availability of recommended data) is proposed to be the following:

Vol. 1 : e^-, H^+ collisions with H, H_2, He, and their ions (1988).

Vol. 2 : C^{q+} collisions with e, H, H_2, He, and their ions (1988).

Vol. 3 : O^{q+} collisions with e, H, H_2, He, and their ions (1988).

Vol. 4 : Fe^{q+} collisions with e, H, H_2, He, and their ions (1989).

Vol. 5 : Ni^{q+} collisions with e, H, H_2, He, and their ions (1990 ?).

The data content of each volume will also be stored in a complete file as part of the IAEA A+M Numerical Data Base.

(5) Coordination of the Compilation and Evaluation Work in Data Centres and Fusion Laboratories on Plasma-Wall Interaction (PWI) Data for Fusion and its Incorporation in the IAEA A+M Data Unit Activity

Plasma-surface interaction data have been and are being compiled by the A+M Data Centres (ORNL, Nagoya, JAERI and others?); some evaluation work on them has also been done (ORNL Red Book vol. 3), and compendia have been published by the IAEA A+M Data Unit (Nucl. Fusion, special issue, 1984) and Nagoya Data Centre (IPPJ-AM-32 and 41). The bibliography on plasma-surface interaction processes is also being covered by the IAEA Bulletin on A+M Data for Fusion. However, it is felt that the activity on data evaluation for PWI processes is not adequately organized on an international level, nor do internationally recommended data for these processes exist.

The IAEA A+M Data Unit during 1988 intends to undertake steps in improving the situation in this data area by trying to reach an agreement among the PWI data producers and users for the creation of an international file of recommended data on PWI processes, and initiate a systematic evaluation activity in this field. An attempt will be made to organize an Specialist's Meeting during 1988 or 1989 on this subject, with involvment of the A+M Data Centres. At the same time, the necessary work will be done on adapting the IAEA A+M data base system to incorporate PWI data.

The necessity of the link between the gas-phase A+M and PWI data bases is particularly evident in modelling and diagnostics of tokamak edge plasmas. It is also felt that for a stronger implementation of PWI problems in the Agency's A+M programme, the IFRC Subcommittee should be adjusted to allow representation from the PWI community (e.g. R. Behrisch (Garching), G. McCracken (Culham), R. Langley (Oak Ridge), etc).

Appendix 13

Progress and Future Activities at the Joint Institute for Laboratory Astrophysics (JILA)

Recently completed studies

1. Comparison and evaluation of orientation and alignment parameters. Report is to be published in the journal of Physics Reports.

2. Data for photoionization and fragmentation of molecules has been analysed. Results will be published shortly.

Ongoing and planned activities

1. The most important fusion related project relates to the publication of the recommended data for electron collisions with atoms and molecules, planned as volume 2 of the atomic data for fusion, ORNL series. The relevant data from the literature has been input into the computer data base at JILA but no recommendations as yet have been performed.

2. Collision strengths for electron impact excitation and photoionzation cross sections are being evaluated for some heavy elements not studied as part of the international opacity project.

3. Swarm data are being collected and evaluated.