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**INTERNATIONAL NUCLEAR DATA COMMITTEE**

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FIFTH MEETING OF THE  
ATOMIC AND MOLECULAR DATA CENTRE NETWORK  
Stanford University, Palo Alto, California  
22-23 July 1985

SUMMARY REPORT

Prepared by A. Lorenz

January 1986

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



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### Abstract

Summary report of the Fifth A+M Data Centre Network Meeting convened by the IAEA at Stanford University, Palo Alto, California, 22-23 July 1985. 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.



## A. Meeting Summary

### 1. Introduction

The fifth A+M Data Centre Network (DCN) meeting was convened by the IAEA Nuclear Data Section at Stanford University, Palo Alto, California, 22-23 July 1985. 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 A. Lorenz.

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

- Decided to include current activities of the A+M data centres in the Work in Progress section of the IAEA Bulletin.
- Decided to defer the publication of CIAMDA 85 to the middle of 1986 to allow additions to be included from all centres.
- Decided on a concerted effort by the data centre to identify all A+M collision data sets considered to be evaluated or recommended and publicize this list in the Nuclear Fusion journal.
- Performed a periodic review of the A+M EXFOR dictionaries.
- Initiated an effort to compile a list of processes in atomic interactions and their definitions.

### 3. Next A+M Data Centre Meeting

It was recommended that the next meeting of the network take place in conjunction with the meeting of the IFRC Subcommittee. The DC meeting should consist of a 2-day meeting and a 1-day workshop. One of the 2-day meetings should overlap with the IFRC Subcommittee meeting. The date for this next meeting was suggested to be 8-13 September. It was suggested that IAEA send official announcement of the meeting before the end of 1985.

## B. Meeting Proceedings

### 1. Progress Reports

- 1.1. W.L. Wiese (U.S. National Bureau of Standards), Appendix 4.
- 1.2. S. Fivozinsky (U.S. National Bureau of Standards), Appendix 5.
- 1.3. H. Tawara (Inst. for Plasma Physics, Nagoya University), Appendix 6.  
(See also distributed report "RIC-Users Instruction Manual", May 1985).
- 1.4. J.W. Gallagher (JILA Data Center, University of Colorado),  
Appendix 7.
- 1.5. R.A. Phaneuf (Oak Ridge National Laboratory), Appendix 8.
- 1.6. Y. Nakai (JAERI).
- 1.7. F.J. Smith (Queen's University of Belfast).
- 1.8. J.L. Delcroix (Laboratoire de Physique des Plasmas, Orsay),  
Appendix 9.
- 1.9. K. Katsonis (Laboratoire de Physique des Plasmas, Orsay),  
Appendix 10.

### 2. Bibliographic Data

- 2.1. In discussions of the bibliographic input to the IAEA bibliographic data base (A+M/BDB), which emphasized the need to have as complete a coverage of the literature as possible, it was agreed that the GAPHYOR data centre will send quarterly to the Oak Ridge data centre a print-out of current bibliographic references, where it would be checked against the Oak Ridge data base. The journals would be sorted by volume, number, page. The Oak Ridge data centre would send the equivalent input to the Gaphyor data centre for cross-checking. The timing for the exchange of this information is to be arranged by the two centres concerned (presumably it would correspond with the IAEA Bulletin deadlines of January, April, July and October). In this context it was requested that the GAPHYOR centre be included in the list of centres contributing to the input of the IAEA Bulletin. (Action 1).
- 2.2. The IAEA Bulletin should be used to advertise work that is being done at the various centres, and that reports from centres be included under the "Work in Progress" section of the Bulletin. The centres were asked to send periodic information for the "Work in Progress" section of the IAEA Bulletin (Action 2). It was suggested that the IAEA centre prompt such contributions by reminding the centres when such contributions are expected.
- 2.3. Delcroix was asked to include all data centres on the distribution of the GAPHYOR quarterly bulletin. (Action 3).



- 2.4. Wiese informed the meeting that a new bibliographic compilation on atomic structure data was to be published in June 1985.
- 2.5. With regard to CIAMDA 85, the centres urged IAEA to insure that this compendium be as complete as possible, and suggested that information from GAPHYOR and the Oak Ridge data base be merged with the IAEA A+M/BDB. In the effort to assure completeness, the IAEA was asked to send a draft copy of CIAMDA 85 with a cut-off date of 31 December 1985 to all data centres as soon in 1986 as possible. (Action 4). To allow for the centres to respond, and their input included, the publication date of CIAMDA was agreed to be postponed to mid-1986.

### 3. Numerical Data

- 3.1. General discussion of "evaluated" and "recommended" data: participants pointed out the need for the IAEA centre to produce a list of those data sets which are considered to be evaluated and/or recommended; in this context it was suggested that IAEA publicize in the Nuclear Fusion journal and in the Bulletin those data which are available at the IAEA as recommended data.
- 3.2. The data centres were asked by IAEA to send to the IAEA centre a list of those data sets which are considered to be "evaluated" or "recommended". (Action 5).
- 3.3. It was suggested that only "evaluated" data be stored in the IAEA numerical (EXFOR) data base, unless only "experimental" data existed for any given reaction/species.
- 3.4. It was decided by the network that only cross sections were to be stored in the IAEA (EXFOR) A+M/BDB; reaction rates are to be excluded as they are condition specific and can be calculated for any given application by the users.
- 3.5. It was also suggested by the network that all collision data compiled in the IAEA (EXFOR) A+M/BDB should be given in standard units.
- 3.6. In the discussion regarding the process of "recommending" data, there was general agreement that the A+M Data Centre network is in the position to act as the body to "recommend" data.

### 4. Review of EXFOR Dictionaries

The following changes/corrections were made:

#### Journals (Diction. 2)

- Add JPCS (after JPCR) = J.Phys.Chem.Ref. Data Supplements
- Change JPO to JPFR
- JPOC to JPFC
- JPOL to JPFL

#### Reports (Diction. 3)

- Eliminate all addresses in this dictionary
- Spell all acronyms used in this dictionary

- Correct Boulder in JILA entry
- Add Japan to the description of JAERI

#### Reactant Codes (Diction. 10)

- Change the location of TiC
- add SiC

#### Quantity Codes (Diction. 12)

- change SGV to RAT

#### Quantity Modifiers (Diction. 13)

- add total: TOT

#### Data Heading Codes (Diction. 14)

- Smith was asked to reduce this dictionary to a reasonable size (Action 6)

#### Data Units (Diction. 15)

- replace SP by CM/SEC
- replace DEG K by KELVIN
- Phaneuf was asked to reduce this dictionary to basic units limited to those which would be used to transmit data (Action 7)

#### Data Centres ID (Diction. 16)

- All centres were asked to send to IAEA the expansion of their centre's postal address (Action 8)

#### Keywords (Diction. 17)

- Add: ABSTRACT
- Correct: corporate under AUTHORS

### 5. Terminology

Reflecting a concern expressed at the previous (May 1984) meeting, about the need for a common terminology in describing the physics processes in atomic interactions, the participants agreed on the following:

- 5.1. Katsonis agreed to formulate a list of surface effects phenomena and their definitions, and to circulate this list to the network. (Action 9).
- 5.2. Delcroix agreed to formulate a list of atomic collision processes (in the form of initial and final states) and the names proposed for these processes, and to circulate this list to the network (Action 10).
- 5.3. Katsonis and Delcroix are to send their network-reviewed lists to the IAEA centre in the beginning of 1986, and IAEA is to distribute the proposed terminologies to the network before the next (1986) A+M data centre meeting.
- 5.4. After a common terminology is agreed upon it was suggested that an article be written for publication by members of the network to advertise it to the community at large.

Meeting on the A+M Data Centre Network

Stanford University, Palo Alto, California  
22-23 July 1985

List of Participants

Dr. Crandall, D.H.	ER-542, MS G-226, GTN U.S. Department of Energy Washington, D.C. 20545 U.S.A.
Prof. Dr. Delcroix, J.L.	Laboratoire de Physique des Plasmas Université de Paris XI (Paris-Sud) 15, Rue G. Clemenceau F-91405 Orsay Cedex
Dr. Fivozinsky, S.P.	Manager Physical Data Program Office of Standard Reference Data National Bureau of Standards Gaithersburg, Maryland 20899 U.S.A.
Dr. Gallagher, J.W.	JILA Data Center Campus Box 440 University of Colorado Boulder, Colorado 80309 U.S.A.
Dr. Katsonis, K.	Laboratoire de Physique des Plasmas Université de Paris XI (Paris-Sud) 15, Rue G. Clemenceau F-91405 Orsay Cedex
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Research Information Centre  
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Fifth Meeting of the

Atomic and Molecular Data Centre Network

CERAS Bldg., Room 204, Stanford University, California, USA  
22-23 July 1985

Adopted Agenda

Introductory and Preliminary Items and Review of Actions from the 1984 Meeting.

1. Reports of A+M Data Centres and Groups
2. Report of the A+M Data Unit
3. Bibliographic Data
  - 3.1. Status of IAEA A+M Bibliographic Data Base
  - 3.2. Status of IAEA Quarterly Bulletin
  - 3.3. Next publication of CIAMDA data index
  - 3.4. Terminology and definition of processes
  - 3.5. Surface effects
4. Numerical Data
  - 4.1. Exchange of Numerical Data
  - 4.2. EXFOR Index (distribution)
  - 4.3. Review of A+M EXFOR Dictionaries
  - 4.4. Graphical representation of data
  - 4.5. Distribution of numerical data to users
  - 4.6. On-line access of data

List of Actions

1. IAEA  
Include GAPHYOR in introduction to the IAEA Bulletin as one of the contributing centres to the IAEA Bulletin.
2. All Centres  
Send to IAEA for inclusion in the IAEA Bulletin contributions to the "Work in Progress" section describing what specific work is being done.
3. Delcroix  
Include all centres on the distribution of the GAPHYOR Bulletin.
4. IAEA  
Send to all centres a draft copy of CIAMDA 85 for review as soon in 1986 as possible.
5. All Centres  
Send to IAEA a list of data sets which are considered to be "recommended" or "evaluated".
6. Smith  
Reduce the EXFOR Dictionary 14 on "Data Heading Codes" to a reasonable size and send it to the IAEA.
7. Phaneuf  
Reduce the EXFOR Dictionary 15 on "Data Units" to a reasonable size and send it to the IAEA.
8. All Centres  
Send to IAEA correct expansion of their centres' address for inclusion in EXFOR Dictionary 16.
9. Katsonis  
Formulate a list of surface effects and their definitions and circulate it to the network.
10. Delcroix  
Formulate a list of atomic collision processes and their definitions and circulate it to the network.

Spectroscopic Data Centers at the National Bureau of Standards

I. ATOMIC ENERGY LEVELS DATA CENTER

W. C. Martin, Director

A. Recent Accomplishments

We completed our critical compilation of the energy levels for phosphorous (P I through P XV), and the paper on these data has been accepted for publication in the Journal of Physical and Chemical Reference Data (JPCRD). We have begun a similar compilation for the sulfur spectra. A JPCRD supplement with our energy-level compilations for the iron group elements ( $z = 19-28$ ), including 235 spectra) is in press. Supplement 3 of our Bibliography on Atomic Energy Levels and Spectra, July 1979 through December 1983, has been published recently (June 1985). A report on atomic spectroscopic data of astrophysical interest was submitted for publication in the Transactions of the Internal Astronomical Union.

We have begun building a data base on atomic spectral wavelengths with their energy-level classifications. Substantial progress was made on an extensive list of predicted and observed forbidden lines as the first such project. We have postponed work on energy-levels compilations for the Mo spectra to allow extra effort on this wavelengths project.

B. Future Plans

We expect to complete our compilation of predicted and observed M1 (forbidden) lines. It will include about 1300 lines from 294 different spectra of 39 elements (Be through Mo). We will also compile lines due to allowed transitions (wavelengths, energy-level classifications, etc.) for selected spectra for our data base.

We plan to begin evaluation and compilation of data on the spectra of molybdenum-energy levels and wavelengths. It is likely that work on the classified lines of Mo will be carried out in collaboration with workers at the Japan Energy Research Institute, Tokai-mura.

We expect to complete the major part of our energy-levels compilation for sulfur during 1986. This work is part of our longer-range project of compilations for the elements Na through Ar ( $z = 11 - 18$ ).

II. DATA CENTER ON ATOMIC TRANSITION PROBABILITIES

Director: Dr. Wolfgang L. Wiese

A. Recent Accomplishments

Significant progress has been made on the design and development of computerized databases which will facilitate the storage, retrieval, and updating of critically evaluated numerical atomic spectroscopic data. Data elements pertinent to tables of energy levels, wavelengths, transition probabilities, and lifetimes have been identified and

characterized; extensive documentation of requirements and specifications for energy-level tables has been completed, as well as partial documentation for tables of wavelengths and transition probabilities. Compilations of atomic transition probability data continued for the spectra of the Fe-group elements scandium through nickel. Tabulations of allowed lines of neutral or weakly ionized atoms where the principal data sources are experimental have been completed, and work on the evaluation and compilation of data on forbidden lines of Fe-group elements is progressing.

Two critical reviews of Stark widths and shifts of spectral lines of both neutral and ionized atoms have been published in the Journal of Physical and Chemical Reference Data. A spectroscopic data book, which includes transition probabilities as well as energy levels and wavelengths, has been completed for the element Fe and has been published as a volume in the new Oak Ridge "Red Book" series. Work is now being started on a second volume, which will contain data for the elements titanium and nickel. A compilation of spectroscopic data on titanium, including energy level diagrams and transition probability data, was completed. This work was done in collaboration with several scientists from major Japanese fusion facilities.

#### B. Future Plans

We shall continue our work on the tabulation of Fe-group transition probabilities. Also we will assemble the next volume of spectroscopic data tables for the fusion research community in the "Red Book" series of Oak Ridge. This new volume, as stated above, will consist of the two metals titanium and nickel, and the material will be taken largely from recent NSRDS compilations and will contain not only transition probabilities but also energy levels and wavelengths of spectral lines. We shall also continue the work on database development and will continue to monitor, collect, and classify the literature on atomic transition probabilities.

#### Recent Publications

1. Musgrove, A., and Zalubas, R., "Bibliography on Atomic Energy Levels and Spectra, July 1979 through December 1983," Nat. Bur. Stand. (U.S.), Spec. Publ. 363, Suppl. 3 (June 1985).
2. Martin, W. C., and Zalubas, R., "Energy Levels of Phosphorus, P I through P XV," J. Phys. Chem. Ref. Data 14, 751 (1985).
3. Sugar, J., and Corliss, C., "Energy Levels of the Elements of the Iron Period, Potassium through Nickel," J. Phys. Chem. Ref. Data 14, Suppl. 2 (1985).
4. N. Konjević, M. S. Dimitrijević, and W. L. Wiese, "Experimental Stark Widths and Shifts for Spectral Lines of Positive Ions (A Critical Review and Tabulation of Selected Data for the Period 1976 to 1982)", J. Phys. Chem Ref. Data 13, 649-686 (1984).
5. N. Konjević, M. S. Dimitrijević, and W. L. Wiese, "Experimental Stark Widths and Shifts for Spectral Lines of Neutral Atoms (A Critical Review of Selected Data for the Period 1976 to 1982)", J. Phys. Chem. Ref. Data 13, 619-648 (1984).
6. W. L. Wiese, editor, "Spectroscopic Data for Iron", Vol. IV of the series "Atomic Data for Controlled Fusion Research", ORNL-6089 (1985).



The Physical Data Program in the Office of Standard Reference Data

S. P. Fivozinsky  
National Bureau of Standards  
Gaithersburg, MD 20899, USA

Current activities in the National Bureau of Standards (NBS) Standard Reference Data program are carried out in 25 data centers and approximately 30 short-term projects located in the technical divisions of NBS and in academic and industrial laboratories. Each of these activities undertakes the collection and evaluation of the available data on a specified set of properties and substances. The activities are aggregated into three discipline-oriented program areas:

Physical Data - Includes data on atomic, molecular, and nuclear properties, and spectral data utilized for chemical identification.

Chemical Data - Covers primarily kinetic, thermodynamic, and transport properties of substances important to the chemical and related industries.

Materials Properties Data - Includes structural, electrical, optical, and mechanical properties of solid materials of broad interest.

The Physical Data Program was created last year as the result of a change in the technical management structure within the Office of Standard Reference Data (OSRD). The old programmatic areas, Energy and Environmental Data, and Industrial Process Data were reorganized to reflect a disciplinary content rather than application areas. As a result, the new Physical Data Program is concerned with atomic, molecular, nuclear, and those spectral databases used heavily in analytical chemical instrumentation.

The following data centers are associated with the Physical Data Program:

- \* Atomic Collisions Cross Section Data Center
- \* Atomic Energy Levels Data Center
- \* Atomic Transition Probabilities Data Center
- \* Fundamental Constants Data Center
- \* Molecular Spectra Data Center
- \* Photon and Charged Particle Data Center

These data centers are long-term activities which develop, maintain, and disseminate a major database in these areas. The Physical Data Program also supports a number of short-term projects whose efforts lead to specific one-time outputs. The following projects have been active during the past year:

- \* Critical Compilation of Mass Spectral Data
- \* Compilation of Atomic Wavelengths below 2000 Å
- \* K shell Ionization by Hydrogen and Helium Ions
- \* Digitization of the Coblenz Society Infrared Database
- \* Soft X-ray Interactions with Matter
- \* Medical Physics Data Book, 2nd edition

Through the combination of data centers and short term projects the Physical Data Program addresses the most critical needs for databases with a combination of NBS and other-agency funding. More detailed descriptions of the data centers, the short-term projects, and their current activities and future plans, are found later in this report.

While most outputs of the Program are in printed form, an increasing number of computer-readable databases are being designed and disseminated. In the future, internal operations of data centers, evaluation techniques, and dissemination will involve heavy utilization of modern computer technology.

Because of considerable increased pressure from user communities for greater support of these programs and availability of evaluated atomic and molecular data, a major effort will be made next year to develop new funding sources for this work and to draw increased attention to NBS as the primary national source for evaluated databases of atomic and molecular data.

### Highlights of Recent Activities

The Physical Data Program has been very active during the last year. Two new projects have begun with a combination of NBS and other-agency funding. The first expands the Photon and Charged Particle Data Center to carry out a pilot project to evaluate soft x-ray cross sections. A quantitative knowledge of low energy x-ray interactions with matter has many applications in understanding the effects of radiation on living tissues, in material science, and in microcircuitry.

The second new project will expand the activities of the Atomic Energy Levels Data Center to include the compilation of wavelengths of atomic transitions. These are used heavily in identification of the specific atomic ions giving rise to a set of measured spectra. Initially the Data Center will compile magnetic dipole transitions since they are the ones primarily observed by astronomers, and measured during diagnostics of nuclear fusion plasmas.

The Atomic Energy Levels and Atomic Transition Probabilities Data Centers are presently working on the development of a computer-readable database. There has been considerable interest in the availability of such a system expressed by the scientific community through, for example, the NAS/NRC Committee on Line Spectra of the Elements, and members of the NAS Board on Assessment for the National Bureau of Standards.

The Fundamental Constants Data Center will publish the latest "Least Squares Adjustment of the Fundamental Constants." This effort represents the primary source of information in the world on the values of the fundamental physical constants. The new set of recommended values will be published as a CODATA Bulletin. The full details of the adjustment will be submitted for separate publication during 1985.

This year the Atomic Collisions Cross Section Data Center at JILA in Boulder, Colorado, will begin preparing a computerized database of electron collision cross sections for atoms, ions, and molecules. These data are important in modeling gas discharges and plasma systems such as those describing nuclear fusion processes and interstellar atmospheres.

The Photon and Charged Particle Data Center has had a long and successful history of providing photon and electron interaction cross sections for

varied applications in medicine, health physics, and national defense. This year the Center is releasing two computer-readable databases, EPSTAR, providing electron and positron stopping power data for 285 materials, and XGAM, an interactive system which calculates photon interaction cross sections on whatever substance the user inputs.

Other agency funded activities will lead this year to a major compilation of atomic wavelengths below 2000 A, a digitized database of reference condensed-phase infrared spectra, and a compilation of K shell ionization data. The Program continues to support the generation of new spectra for the Mass Spectral Database, which is widely disseminated. Plans are underway to develop a specific interagency agreement for future development of this database and other important spectral substance-identifying database systems.

The following Data Centers and projects are associated with the Physical Data Program. The descriptions reflect their scope, activities and future plans:

#### Data Centers

##### ATOMIC COLLISION CROSS SECTION DATA CENTER

Jean W. Gallagher, Director  
University of Colorado  
Boulder, CO 80309  
Telephone: (303) 492-7801

The Center's aim is to compile, evaluate, and disseminate data concerning electron and photon collisions with atoms, simple molecules, ions, and low energy heavy particle collisions. Emphasis is given to electron-collisional excitation and ionization, heavy-particle energy transfer, photoionization, photodetachment, and photofragmentation.

In the past year the Center has collaborated with a number of visiting scientists and JILA staff members to produce evaluated data publications. Articles on (1) collisional energy transfer rates and lifetimes for diatomic halogens and (2) theoretical charge transfer cross sections for non-hydrogenic atoms and ions appeared in this year's issues of the Journal of Physical and Chemical Reference Data. An update to the Multiphoton Bibliography for 1981-82 was completed. Articles on proton impact ionization of gaseous targets and on charge transfer for hydrogen and deuterium atoms and ions with metal vapors are nearing completion. An article on partial-channel photoionization of molecules is in progress. Collision strengths for electron impact excitation of ions are being compiled for a report on that subject which will be particularly useful to the astrophysics community.

A database management system has been designed for the storage and retrieval of the bibliographic and numerical data of interest to this Center. The bibliographic data has been loaded, and loading of the numerical data has begun.

## ATOMIC ENERGY LEVELS DATA CENTER

W. C. Martin, Director  
National Bureau of Standards  
Gaithersburg, MD 20899  
Telephone: (301) 921-2011

The Center compiles, evaluates and disseminates data on energy levels and spectral lines of atoms and atomic ions. Reliable atomic spectroscopic data are essential in such areas as plasma diagnostics, laser physics and astronomy.

A major updating and extension of energy-levels compilations for the 235 spectra of the iron-group elements K through Ni (Z=19-28) was completed and submitted for publication as a supplement to the Journal of Physical and Chemical Reference Data. An energy-levels compilation for the 15 phosphorus spectra is almost complete. A supplement to the Bibliography on Atomic Energy Levels and Spectra covering the period July 1979 through December 1983 is in press.

Work on compilations of energy levels of phosphorus and sulfur will continue as part of our project covering the Na-Ar row (Z=11-18). Such work will be extended to the elements copper through molybdenum (Z=29-42), beginning with molybdenum. Future efforts will also include a compilation of forbidden spectral lines of interest for plasma physics and astronomy; this work will be the first of a series of planned compilations of atomic spectral lines (wavelengths and energy-level identifications).

## ATOMIC TRANSITION PROBABILITIES DATA CENTER

Wolfgang L. Wiese, Director  
National Bureau of Standards  
Gaithersburg, MD 20899  
Telephone: (301) 921-2071

The Center's purpose is to compile, evaluate, and disseminate data on atomic transition probabilities and lifetimes of excited levels of atoms and atomic ions. Interpretation of fusion plasma diagnostic techniques is highly dependent on the availability of these data.

Revision and updating of atomic-transition-probability data for allowed lines in the elements scandium through nickel is nearly complete, and work on evaluating data on forbidden transitions in these elements is in progress. Critical reviews of Stark widths and shifts in neutral and ionized atomic species were processed for automatic typesetting and are in press. A computerized database of bibliographic information on atomic energy levels, atomic transition probabilities, and atomic line shapes and shifts was designed; much of the implementation of input capability, as well as very limited retrieval and output capability, was completed in collaboration with the staff of OSRD.

Future plans call for completing the compilation of transition probabilities for scandium through nickel, at which point the major effort will be focused on the light elements hydrogen through neon, as well as selected heavy elements (such as Kr and Zr). It is also planned to complete work on both input and output capability for the bibliographic database system. Input of references on atomic transition probabilities

Will be initiated. Long-range plans include the design and development of a computerized database of critically evaluated data on atomic spectroscopic quantities.

#### FUNDAMENTAL CONSTANTS DATA CENTER

Barry N. Taylor, Director  
National Bureau of Standards  
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Telephone: (301) 921-2701

The Center provides a centralized source of information on the fundamental physical constants and on closely related precision measurements. It participates in the periodic development, under the auspices of CODATA, of sets of "best" or recommended values of the fundamental physical constants by means of least-squares adjustments. The self-consistent best values of the constants resulting from an adjustment are required for computational purposes and often are the basis for other data compilations. The Center also publishes a quarterly preprint and reprint newsletter entitled "Preprints on Precision Measurement and Fundamental Constants" or PMFC; participates in the organization of conferences relating to the precision measurement-fundamental constants (PMFC) field; administers the NBS Precision Measurement Grant program; and participates in the work of various committees in the PMFC field.

The major activity of the Center during 1984 involved working towards the completion of the 1983 least-squares adjustment of the constants. The set of best values resulting from this adjustment will replace the now nearly obsolete set resulting from the 1973 adjustment. The 1983 effort, like its 1973 predecessor, is being carried out by B. N. Taylor in collaboration with E. R. Cohen and under the sponsorship and guidance of the CODATA Task Group on Fundamental Constants. The Task Group met in August 1984 to review the progress made to date by Cohen and Taylor and to offer its suggestions regarding the new adjustment.

The principal focus of the Center during 1985 will be the completion and publication of the 1983 least-squares adjustment. It is expected that a CODATA Bulletin giving the new set of recommended values will be published in 1985 and that the lengthy paper giving the details of the adjustment will be submitted for publication before the end of the year.

#### MOLECULAR SPECTRA DATA CENTER

Frank J. Lovas, Director  
National Bureau of Standards  
Gaithersburg, MD 20899  
Telephone: (301) 921-2023

The Center provides for the collection, evaluation, and dissemination of molecular spectral frequencies and other molecular constants. These are designed to aid in the analysis and identification of compounds and to permit assignment of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

A manuscript on "Recommended Rest Frequencies for Observed Interstellar Molecular Transitions in the Microwave Region" is nearing completion. The evaluation of microwave data for the "Microwave Spectral Tables of

Hydrocarbon Species" is nearly complete. Finally, an infrared spectral calibration atlas for the frequency range 500 to 720  $\text{cm}^{-1}$  is in progress and employs high resolution spectra of OCS,  $\text{N}_2\text{O}$  and  $\text{CO}_2$  .

Next year the "Recommended Rest Frequency" paper will be published. A manuscript on the spectra of hydrocarbons and on the infrared spectral atlas will be prepared.

#### PHOTON AND CHARGED PARTICLE DATA CENTER

M. J. Berger, Director  
National Bureau of Standards  
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Telephone: (301) 921-2685

The Center compiles, evaluates, and disseminates data on the interaction of ionizing radiation with matter. The data on photons and charged particles include single-scattering cross sections as well as transport data pertaining to the penetration of radiation through bulk matter.

Activities during the past year include the following: (a) Tabulations have been published of relativistic Hartree-Fock-Slater modified atomic form factors in all elements from  $Z = 1$  to 100. These results are applicable to the coherent scattering of photons and electrons; (b) Tabulations has been published of the density-effect correction for the stopping power of charged particles, as a function of particle velocity, for 278 materials; (c) A method has been developed for the synthesis of reliable bremsstrahlung cross sections, using various fragmented theoretical and experimental results. A systematic tabulation of the bremsstrahlung cross section is in progress for all elements,  $Z - 1$  to 100, at energies from 1 keV to 100 GeV; (d) Using a previously developed database of photon cross sections for scattering, absorption and pair production in elemental substances, software has been developed for calculating these cross sections in compounds of any specified composition, duly taking into account the absorption edges for all the atomic constituents. This software will be used for a planned set of tables of cross sections for compounds of interest in radiation dosimetry and metrology; (e) A magnetic tape containing electron stopping powers, ranges and bremsstrahlung yields has been delivered to OSRD, to be used as an NBS Standard Reference Database.

#### Projects

##### CRITICAL COMPILATION OF MASS SPECTRAL DATA

Martin G. Robiette  
Mass Spectral Data Centre  
Nottingham, England  
Source of Support: NBS

This project compiles, evaluates, and enters mass spectra into the Mass Spectral Database. The data are collected from the open literature and other sources, both public and private. Their quality is assessed through application of a quality index algorithm. The high-quality spectra are added to the database.

This year over 1500 new spectra have been delivered. They are combined with spectra from other sources such as the U.S. Environmental Protection

Agency, and disseminated on magnetic tape to individuals, laboratories, and online vendors. They are also periodically published through supplements to the NSRDS-NBS series of publications.

#### COMPILATION OF ATOMIC WAVELENGTHS BELOW 2000 ANGSTROMS

Raymond L. Kelly  
Spectroscopic Data Center, Naval Postgraduate School  
Monterey, California  
Source of Support: NSF

This project has completed a compilation of atomic spectral lines with wavelengths below 2000 Å. A manuscript is being prepared for publication as a major supplement to the Journal of Physical and Chemical Reference Data. The compilation will cover the elements hydrogen through krypton.

In the future, this type of work will be done within the NBS Atomic Energy Levels Data Center. Increased NBS and OA resources have been obtained to allow the expansion in the Data Center.

#### K SHELL IONIZATION BY HYDROGEN AND HELIUM IONS

Gregory Lapicki  
East Carolina University  
Greenville, North Carolina  
Source of Support: DOE

This project has been recently completed, and a preliminary manuscript entitled UK Shell X-ray Production by Hydrogen and Helium Ions in The Elements ( $Z= 4$  to 92)," has been delivered. The work presents x-ray production cross sections along with comparisons to theoretical results.

Present plans call for publication in the Journal, "Atomic Data and Nuclear Data Tables."

#### DIGITIZATION OF THE COBLENTZ SOCIETY INFRARED DATABASE

William Strauss  
Johns Hopkins Applied Physics Laboratory  
Columbia, Maryland  
Source of Support: EPA, NIH

This project has been established to digitize a printed database of 5000 evaluated reference infrared spectra of substances in the condensed phase. The purpose is to provide the beginning of a major computer-readable database of IR reference spectra.

A minicomputer-based digitization system at the Applied Physics Laboratory is being utilized to generate the spectra. APL personnel are also compiling the associated information which will accompany each digitized spectrum.

A magnetic tape containing the first few hundred spectra will be delivered shortly. This will provide a check on numerous aspects of the digitization process and general structure and usefulness of the system. The remainder of the database will be completed when the final tape format is approved.

## SOFT X-RAY INTERACTIONS WITH MATTER

Martin Berger

Center for Radiation Research, NBS

Source of Support: DOE, NBS

A pilot project has been established within the Photon and Charged Particle Data Center, to compile and evaluate soft x-ray cross sections (100 eV to 10 keV). Requirements for these photon cross sections exist, for example, in the following fields: Lithography in the manufacture of integrated circuits, EXAFS method for determination of atomic distributions in amorphous materials, trace element analysis by x-ray emission spectroscopy, design of x-ray lasers, and calculation of x-ray and particle beam radiation effects.

Plans are to analyze the available data for those elements where the data is most complete, compare with best available theory, and investigate the validity of additivity, that is of generating cross sections for compounds as linear combinations of cross sections for atomic constituents, and to estimate the corrections for departure from additivity.

## MEDICAL PHYSICS DATA BOOK (2nd edition)

Medical Physics Data Group, AAPM

Source of Support: AAPM, NBS

The American Association of Physicists in Medicine (AAPM) has requested that a second edition of the highly successful Medical Physics Data Book be produced for use by hospital physicists. The handbook which provides physical and chemical data related to radiologic and nuclear diagnostic and therapeutic techniques, will be expanded to include new information in all existing areas as well as subjects such as nuclear magnetic resonance (NMR) imaging.

Work is carried out by the Medical Physics Data Group of the AAPM. This group was constituted by the Association to monitor important data requirements and respond to them.



## Progress Report at RIC, IPP/Nagoya

H. Tawara and T. Kato

## 1. A &amp; M working group

1.1 Following evaluation and compilation of excitation cross sections and rate coefficients for carbon and oxygen ions by electron impact<sup>1)</sup>, a similar work for carbon-like isoelectronic sequence ions has been finished<sup>2)</sup>. A work for He-like ions is under way.

1.2 The up-dated data for total cross sections of charge transfer of ions in atomic and molecular hydrogens (up to mid-1984) have been published<sup>3)</sup>. We have begun to compile and evaluate data for partial cross sections of the state-selected electron capture processes which are quite important in applications to plasma diagnostics. Up to now there are some experimental and theoretical data available for the n-distribution (n: the principal quantum number) in electron capture processes and most of these are found to be in agreement with the classical model and quantal calculations. However, only few experimental results have been reported for the l-distribution (l: the angular momentum) though a number of the calculations are available. It should be noted that the l-distributions in electron capture processes are fairly different among theories in some cases.

1.3 Compilation of the cross sections for ionization of atoms and ions by electron impact has been published<sup>4)</sup>. These data, together with other numerical data of excitation, charge transfer, sputtering and backscattering, are stored in our data bank and have also been transferred to IAEA Datacenter.

1.4 Compilation has been finished on the charge distributions of ions ( $Z \geq 4$ ) after passing through foils<sup>5)</sup>. These data are useful in designing the targets for inertial fusion research.

1.5 A review on the energy loss of heavy ions in hot, dense plasmas has been made<sup>6)</sup>. Also a review on the atomic model in such hot, dense plasmas are under way.

1.6 The up-dating of bibliographic data on atomic processes in hot, dense plasmas (HIDENS) is also under way.

## 2. PSI working group

2.1 Compilation and evaluation for data on backscattering coefficients of light ions in normal and oblique incidence have been completed and published in a series of papers<sup>7)</sup>.

2.2 As it has been found that data for sputtering and backscattering at low energies (< 100 eV) and for synergistic processes are quite important in understanding the plasma behavior near the edges, we have decided to review data for the following processes:

- a) sputtering near threshold<sup>8)</sup>
- b) backscattering at very low energies
- c) sputtering of compound materials in particular metal/graphite system
- d) thermal and radiation-induced interface mixing in metal/graphite
- e) synergistic effects in hydrogen recycling

The particular emphasis is on graphite and its compounds because they are now believed to be one of the most promising materials for the inner wall of torus.

## 3. Plasma modelling and AM data

Investigation of the effects of AM data on the plasma modelling has started recently. Analysis and discussion on AM data necessary for modelling and those available are under way. Some results for the behaviors of Fe, O and other impurity ions in tokamak plasmas will be described in the forthcoming IAEA Advisory Group Meeting in September.

## 4. Data bases

The numerical databases developed at the Center can now be handled in a unified format and their users manuals (in Japanese and also English) have been prepared. These databases can be accessed through computer terminals.

- a) AMDIS (Atomic and Molecular Data Interactive System: data on excitation and ionization cross sections and rate coefficients for atoms and ions by electron impact).

data set number	exp.	theory
ionization	463	392
d ssociative ionization	11	
excitation	102	2294
<hr/>		
total	3213	

b) CHART (Charge Transfer (experimental) cross sections between ions and H/H<sub>2</sub> targets)

charge transfer	770
ionization	143
excitation	14
<hr/>	
total	927

c) SPUTY (Sputtering Yields of monatomic solids by ion impact)

exp.	722
------	-----

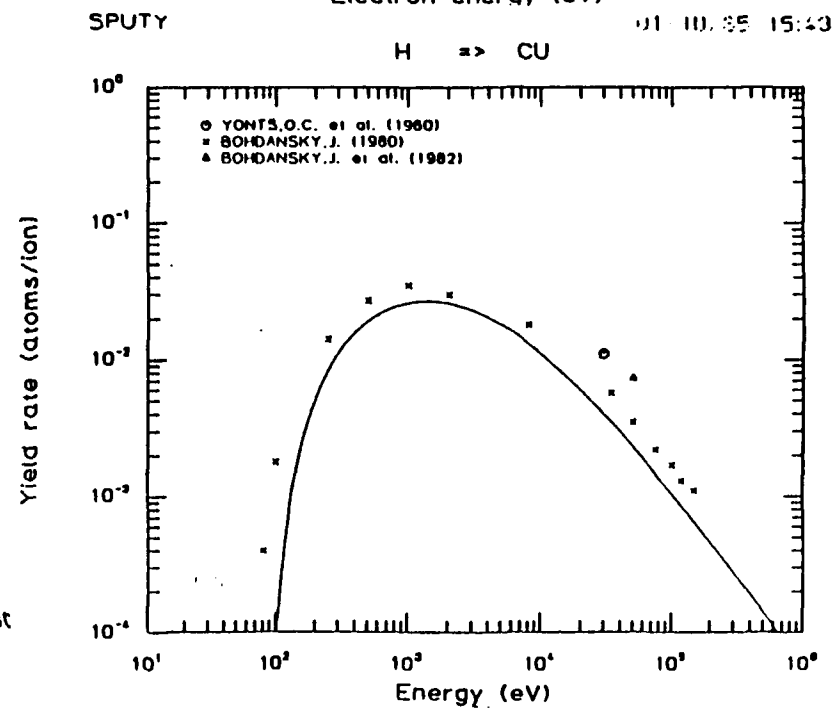
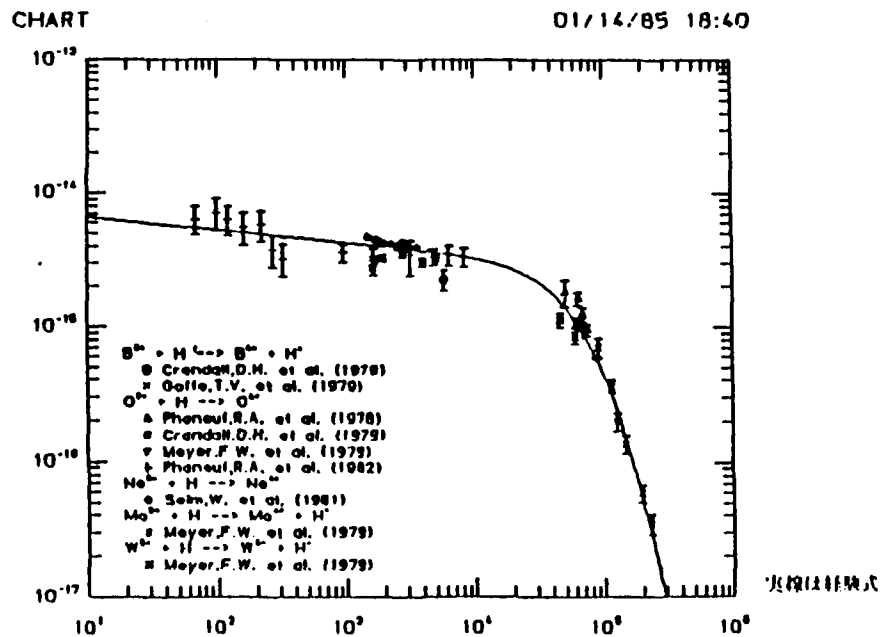
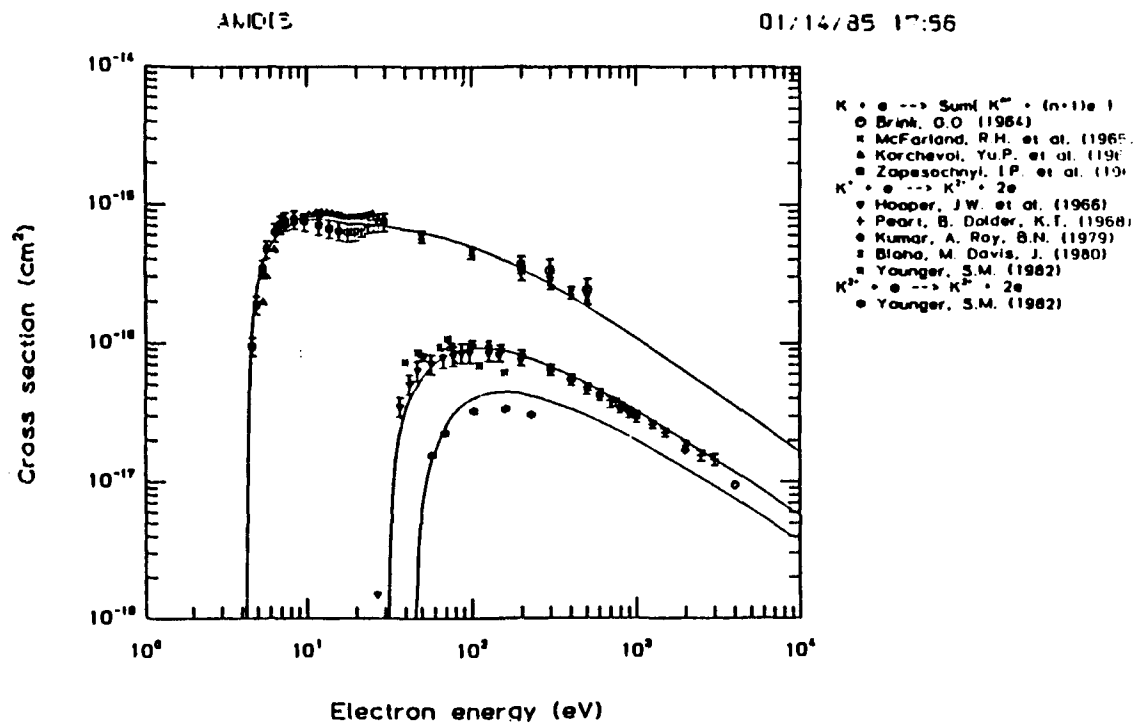
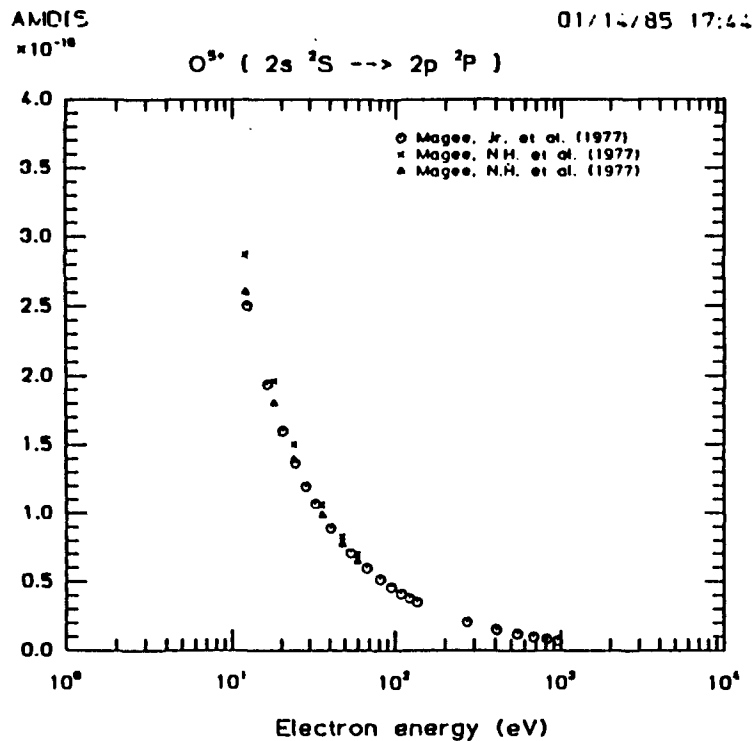
d) BACKS (Backscattering coefficients of light ions from solids for normal and oblique incidence)

exp.	87
simulation	24
<hr/>	
total	111

All these databases include the reference information such as the published journals and can be shown in the same format (see Fig. 1-4). Also the curves based upon empirical formulas can be shown in figures.

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6. S. Karashima et al., IPPJ-AM (to be published 1985).
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Joint Institute for Laboratory Astrophysics  
Atomic Collisions Cross Sections Data Center

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1. "Rate Coefficients for Vibrational Energy Transfer Involving the Hydrogen Halides," S. R. Leone, J. Phys. Chem. Ref. Data 11, 953 (1982).
2. "An Annotated Compilation and Appraisal of Electron Swarm Data in Electronegative Gases," J. W. Gallagher, E. C. Beaty, J. Dutton, L. C. Pitchford, J. Phys. Chem. Ref. Data 12, 109 (1983).  
"A Compilation of Electron Swarm Data in Electro-Negative Gases," J. W. Gallagher, E. C. Beaty, J. Dutton, L. C. Pitchford, JILA Data Center Report #22, (1982).
3. "Angular and Energy Distributions of Secondary Electrons from Helium. Slow Electrons Ejected by Electron Impact," Y.-K. Kim, Phys. Rev. A 28, 656 (1983).
4. "Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms," R. K. Janev, B. H. Bransden, J. W. Gallagher.  
"I. Hydrogen Atom-Fully Stripped Ion Systems," J. Phys. Chem. Ref. Data 12, 829 (1983).  
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"III. Non-Hydrogenic Target Atoms," J. Phys. Chem. Ref. Data 13, 1199 (1984).  
"Evaluated Theoretical Cross Section-Data for Charge Exchange of Multiply Charged Ions with Atoms," R. K. Janev, J. W. Gallagher, B. H. Bransden, JILA Data Center Report #25, (1984).
5. "Rate Data for Inelastic Collisions Processes in the Diatomic Halogen Molecules," J. I. Steinfeld, J. Phys. Chem. Ref. Data 13, 445 (1984).
6. "Scaling Laws for Inelastic Collision Processes in Diatomic Halogens," J. I. Steinfeld, Patricia Ruttenberg, JILA Data Center Report #23, (1983).
7. "Multiphoton Bibliography 1981-82," J. H. Eberly, N. D. Piltch, J. W. Gallagher, NBS Publication LP-92, Suppl. 4, January 1984.
8. "Electron Production in Proton Collisions: Total Cross Sections," M. E. Rudd, Y.-K. Kim, D. Madison, J. W. Gallagher, in press, Reviews of Modern Physics.
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10. "An Evaluated Compilation of Data on Charge Transfer of Hydrogen Ions and Atoms in Metal Vapors," T. J. Morgan, A. S. Schlachter, R. E. Olson, J. W. Gallagher, in press, J. Phys. Chem. Ref. Data.

11. "Anisotropic Scattering of Electrons by  $N_2$  and Its Effects on Electron Transport: Tabulations of Cross Section and Results," A. V. Phelps, L. C. Pitchford, JILA Data Center Report #26, (1985).
12. "Tabulations of Collision Cross Sections and Calculated Transport and Reaction Coefficients for Electrons in  $H_2$  and  $D_2$ ," S. J. Buckman, A. V. Phelps, JILA Data Center Report #27, (1985).
13. "Tabulations of Collision Cross Sections and Calculated Transport and Reaction Coefficients for Electron Collisions with  $O_2$ ," A. V. Phelps, JILA Data Center Report #28, (1985).

Work Currently in Progress:

1. "Collisional Alignment and Orientation in Outer Shell Excitation of Atoms," I. V. Hertel, N. Andersen, J. W. Gallagher.
2. "A Review of Cross Sections for Electron Impact Excitation of Atoms and Ions," D. W. O. Heddle.
3. "Atomic Data for Controlled Fusion Research. Vol. II. Collisions of Electrons with Atoms and Molecules," J. W. Gallagher, C. F. Barnett.
4. "Cross Sections for Photoionization of Molecular Targets. Theory and Experiment," P. W. Langhoff, C. E. Brion, J. W. Gallagher.

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ORNL Controlled-Fusion Atomic Data Center (CFADC)

Progress Report - November 14, 1985

Apart from its regular bibliographic activities, which form the basis for the IAEA Quarterly Bulletin, the CFADC has been engaged in the preparation of a revised and expanded series of "Redbook" compilations of recommended atomic data. These are being published as ORNL reports under the title Atomic Data for Fusion. The initial series consists of five volumes, listed below with their (expected) publication dates.

Volume 1 (ORNL-6086): "Collisions of H, H<sub>2</sub>, He, and Li Atoms and Ions with Atoms and Molecules," C. F. Barnett, editor - (10/86).

Volume 2 (ORNL-6087): "Collisions of Electrons with Atoms and Molecules," C. F. Barnett and J. W. Gallagher, editors - (3/87).

Volume 3 (ORNL-6088): "Particle Interactions with Surfaces," E. W. Thomas, editor - (2/85).

Volume 4 (ORNL-6089): "Spectroscopic Data for Iron," W. L. Wiese, editor - (2/85).

Volume 5 (ORNL-6090): "Collisions of Carbon and Oxygen Ions with Electrons, H, H<sub>2</sub>, and He," R. A. Phaneuf, R. K. Janev, and M. S. Pindzola, editors - (5/86).

Copies of Volumes 3 and 4 are still available, and additional reservations for the remaining volumes are being accepted. The person to contact is:

M. I. Kirkpatrick  
Controlled-Fusion Atomic Data Center  
Oak Ridge National Laboratory  
P. O. Box X, Bldg. 6003  
Oak Ridge, TN 37831, U.S.A.

In the experimental atomic collisions group, cross sections have recently been measured for electron-impact ionization of Fe<sup>5+</sup>, Fe<sup>6+</sup>, Fe<sup>9+</sup>, and Fe<sup>11+</sup> at energies ranging from the ionization thresholds to 1500 eV. Maxwellian rate coefficients have also been calculated from the cross sections. These yet-unpublished data may be obtained from D. C. Gregory at the above address. Plans are to extend these measurements to higher charge states in January, and to study Cr and Ni as well.





- PR est le processus et appartient à la catégorie de processus SE (section). Le classement de GAPHYOR distingue 108 processus différents. Les plus importants dans le cadre du présent symposium sont les suivants :

*Section 1 : Propriétés des atomes et des molécules (11 processus)*

EN Niveaux d'énergie, fonctions d'onde  
 DP Moments dipolaires  
 NP Moments multipolaires  
 PE Polarisabilité électrique ou magnétique  
 VR Courbes de potentiel, structure des molécules  
 TR Probabilités de transition, durée de vie radiatives  
 IN Autoionisation  
 .....

*Section 2 : Collisions photoniques (21 processus)*

EX Photoexcitation  
 IN Photoionisation  
 DT Photodétachement  
 DS Photodissociation  
 P2 Interaction à 2 photons  
 .....

*Section 3 : Collisions électroniques (22 processus)*

SN Sections efficaces totales et de transport  
 EX Excitation  
 IN Ionisation  
 RC Recombinaison  
 AT Attachement  
 DS Dissociation  
 .....

*Section 4 : Collisions entre atomes, molécules et réactions chimiques (28 processus)*

SN Sections efficaces totales et de transport  
 EN Energie ou enthalpie de réaction  
 EX Excitation  
 DX Désexcitation (quenching)  
 TE Transfert d'excitation  
 IN Ionisation  
 R1 Recombinaison ion-ion  
 IO Transfert de charge IO  
 IR Réaction d'échange (d'atome ou de groupe d'atome)  
 AS Association  
 DS Dissociation  
 KE Constante d'équilibre chimique  
 PR Produits indéterminés  
 .....

*Section 5 : Propriétés macroscopiques des gaz (35 processus)*

PV Compressabilité, équation d'état  
 FT Fonction thermodynamique  
 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  
 ME Mobilité électronique  
 MI Mobilité ionique  
 .....

- M1, M2, M3 sont les principaux composants de l'état initial. Par composant on entend des ions, des atomes, des molécules, des photons, des électrons ou des champs.  
De même, M4, M5 et M6 sont les produits de l'état final.
- La rubrique INFO regroupe au moyen d'un code à un chiffre ou à une lettre certains aspects importants de l'article. Dans l'exemple ci-dessus on a les informations suivantes :
  - E Données expérimentales
  - R Article de synthèse
  - S Sections efficaces (valeurs absolues)
  - L Energies thermiques ( $E < 10$  eV Système CM)
  - J Energies moyennes ( $10$  eV  $< E < 10$  keV Système CM)
  - N Effets nucléaires (isotopes, structure hyperfine, molécules exotiques...)
- AN est l'année de publication
- JO est le numéro de code du périodique. Ce code est fourni dans le manuel d'utilisation.
- VO est le numéro du volume ou le type de l'ouvrage
- PAGE est le numéro de la page
- AU est le nom du premier auteur suivi de l'initiale du ou des prénoms si la place le permet. Le nom est tronqué à droite s'il fait plus de 10 caractères.
- GEOG est la localisation géographique du laboratoire du premier auteur.  
Le pays est codé par les deux premiers caractères, la province par les deux suivants et la ville par les deux derniers.  
Exemple : USCARI (US = Etats-Unis, CA = Californie, RI = Riverside)  
Le code est fourni dans le manuel d'utilisation.

## 1.2. Interrogation

Elle consiste à sélectionner un sous-ensemble de la banque en imposant une ou plusieurs valeurs pour un choix de rubriques (FA, FB, FC, FD, XX, YY, etc...) parmi celles qui furent précédemment décrites, hormis la page.

Exemples : FA = 1A  
 XX = NA  
 M1 = NA1CL1  
 AN = 80 THRU 84  
 INFO = S AND E  
 SE = 4  
 PR = IN OR PP

La banque de données est composée de 4 fichiers concernant les processus impliquant respectivement la présence d'1, 2, 3 ou 4 éléments chimiques.

\* La première commande entrée par l'utilisateur doit correspondre à la sélection d'un de ces fichiers.

Exemple :

```
FILE 1
...commandes de recherche...
FILE 4
...commandes de recherche...
.....
```

\* Sélection sur les composants :

Il est conseillé d'interroger plutôt sur l'état initial, l'état final étant souvent omis lorsqu'il est évident.

Exemple : M 1 = NA1CL1/Z+/\*

Après chaque élément de la molécule il faut préciser le nombre d'atomes présents (ce qui permet de distinguer CO = cobalt et C1O1 = monoxyde de carbone).

Après une première barre de fraction (/) on peut spécifier l'état d'ionisation de la molécule et après une deuxième barre de fraction son état d'excitation.

La liste des valeurs possibles est la suivante :

*i = indice d'ionisation*

i = 0 ou blanc	atome ou molécule neutre
i = +	ion positif à 1 charge
i = 2+	ion positif à 2 charges
i = 3+	ion positif à 3 charges
i = 4+	ion positif à 4 charges
i = n+	ion positif à plus de 4 charges
i = -	ion négatif à 1 charge
i = 2-	ion négatif à 2 charges
i = n-	ion négatif à plus de 2 charges
i = k+	atome ou molécule ionisé(e) dans une couche profonde
i = 2k+	double ionisation en couche interne
i = k++	double ionisation, l'une en couche interne, l'autre en couche externe
i = ALL	tous états d'ionisation et tous états d'excitation

*x = indice d'excitation*

Modes d'interrogation ou de sortie

x = x ou blanc	état fondamental
x = r	excitation rotationnelle
x = v	excitation vibrationnelle
x = *	excitation électronique
x = s	atome ou molécule orienté(e)
x = *r	excitation électronique et rotationnelle
x = *v	excitation électronique et vibrationnelle
x = *s	excitation électronique et atome ou molécule orienté(e)
x = rv	excitation vibrationnelle et rotationnelle
x = *rv	excitation électronique et ro-vibrationnelle
x = l	interface liquide
x = w	interface solide
x = k*	promotion d'un électron interne sur une couche externe
x = **	double excitation électronique
x = ALL	tous états d'excitation

*Exemples :*

M 1 = H2            M 3 = H1CL1  
M 3 = C102/2-/ (2ème barre de fraction obligatoire)  
M 2 = N102/+/  
M 4 = N2//\*        (molécules non ionisée mais excitée)  
M 4 = N2/+/\*  
M 1 = S1F6/k+/\*RV  
M 1 = N1/ALL        (tous états d'ionisation et tous états d'excitation)  
M 1 = N1/+/ALL (tous états d'excitation)

- \* Une fois la sélection spécifiée, il est possible de lister les paramètres de sa requête à l'aide de la commande LIST.

Exemple :

```
FILE 1            XX = HE THRU XE NOT AR  
PR = IN.         SE = 3 OR 2  
LIST
```

On obtient la réponse :

```
GAPHYOR 1  
ELEMXX = "HE" THRU "XE" not "AR"  
PROCESS = "IN"  
SECTION = "3" OR "2"
```

- \* La recherche est déclenchée par la commande FIND

Le système répond par exemple : FIND : SET 1 : 4 RECORDS FOUND

Les résultats ont été groupés dans un ensemble (SET) dont le numéro, ici, est 1.

- \* Listage des résultats

Les résultats peuvent être sortis sur 1 ou 2 lignes par fiche selon le nombre de colonnes du terminal utilisé.

TYPE s : imprime l'ensemble s sur le terminal de l'utilisateur, en utilisant toute la largeur d'une ligne de GAPHYOR. Le terminal doit avoir une capacité suffisante pour recevoir au moins 132 colonnes.

SCREEN s : imprime l'ensemble s sur le terminal de l'utilisateur à raison de 2 lignes par fiche. Le terminal doit avoir une capacité suffisante pour recevoir au moins 80 colonnes.

- \* Aides automatiques à l'interrogation (options)

GAPHYOR fournit certaines aides automatiques appelées options. Ces options sont conçues pour aider les utilisateurs qui ne connaissent pas toutes les subtilités des codes GAPHYOR (comme par exemple les règles de classement). Au commencement d'une session, GAPHYOR fonctionne avec la liste d'options standard suivante :

```
ORDER (résolution automatique des problèmes d'ordre d'éléments,  
      de molécules, etc...)  
ALL    (résolution automatique des problèmes de permutations dans  
      l'écriture d'une réaction)  
EXASS (association automatique d'états d'excitation analogues)  
PRASS (association automatique de processus analogues)
```

## 2. Etat actuel et perspectives de développement

Au 15 mars 1985, le fichier principal de GAPHYOR comprenait environ 153 000 fiches réparties comme suit :

Systèmes à ->	1 élément	2 éléments	3 éléments	4 éléments	Totaux
Propriétés des atomes et des molécules	23 992	32 455	12 045	2 277	70 899
Collisions photoniques	5 106	4 163	1 645	382	11 308
Collisions électroniques	8 663	3 458	506	49	12 694
Collisions atomiques et moléculaires	5 511	24 983	12 545	3 305	46 347
Propriétés macroscopiques des gaz	3 741	5 586	1 975	595	11 906
<b>Totaux</b>	<b>47 013</b>	<b>70 645</b>	<b>28 716</b>	<b>6 608</b>	<b>152 982</b>

En termes d'informatique, les fichiers GAPHYOR avaient les volumes suivants :

- Fichier DATA (données)..... 22 Mb
- Fichier ASSO (listes inverses)..... 28 Mb
- Fichier WORK (travail ADABAS)..... 4 Mb
- Fichiers de gestion propre à GAPHYOR..... 12 Mb
- Logiciel SYGAL (interface d'interrogation) 8 000 lignes de PL1
- Logiciel CORRECT (corrections automatiques) 3 000 lignes de PL1
- Logiciels d'édition..... 2 800 lignes de PL1

GAPHYOR publie maintenant 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.

Le programme de GAPHYOR pour les années 1985 et 1986 comprend les développements nouveaux suivants :

- publication accélérée de GAPHYOR COLLECTION (voir le plan de publication ci-joint). Compte tenu des progrès techniques de nos systèmes informatiques, la vitesse de publication sera limitée essentiellement par les possibilités financières. La question se pose également d'améliorer la distribution commerciale de cette série.
- étude d'une version vidéotex permettant d'accéder à GAPHYOR par MINITEL. Ce produit pourra être un puissant moyen de diffusion de GAPHYOR en France, à vrai dire surtout comme "produit d'appel" vers la version professionnelle plus performante.
- création d'une banque de données numériques : il s'agit d'une banque de données atomiques et moléculaires pour la fusion nucléaire. Ce travail effectué par C. KATSONIS se place dans le cadre d'un programme de coopération internationale piloté par l'A.I.E.A. et associant 7 centres de données (Boulder, Oak Ridge et Washington aux U.S.A. ; Nagoya et JAERI au Japon ; Belfast et GAPHYOR en Europe).

PLAN DE "GAPHYOR COLLECTION"

Volume	Titre
1	GAZ RARES
2	HYDROGENE
3	METAUX MONOVALENTS (1A,1B)
4	METAUX DI ET TRIVALENTS (2A à 3B)
5	CARBONE..., TITANE... (4A,4B)
6	AZOTE..., VANADIUM... (5A,5B)
7	OXYGENE..., CHROME... (6A,6B)
8	HALOGENES, TRIADES, TERRES RARES, ACTINIDES (7A à 9D)
9	GAZ RARES + X1 (R-R,R-H)
10	GAZ RARES + X2 (R-1A à R-9D)
11	HYDROGENE + X1 (H-H à H-3B)
12	HYDROGENE + CARBONE... (H-4A,H-4B)
13	HYDROGENE + AZOTE... (H-5A,H-5B)
14	HYDROGENE + OXYGENE... (H-6A,H-6B)
15	HYDROGENE + HALOGENES... (H-7A à H-9D)
16	METAUX MONO, DI ET TRIVALENTS + X (1A-X à 3B-X)
17	CARBONE... + X (sauf oxygène) (4A-X,4B-X)
18	CARBONE... + OXYGENE... (4A-6A,4B-6A)
19	AZOTE... + X (5A-X,5B-X)
20	OXYGENE... + X (6A-X,6B-X)
21	HALOGENES... + X (7A-X à 9D-X)
22	GAZ RARES + X + Y (R-X-Y)
23	HYDROGENE + X1 + Y (H-H-Y à H-3B-Y)
24	HYDROGENE + CARBONE... + X (sauf oxygène) (H-4A-X, H-4B-X)
25	HYDROGENE + CARBONE... + OXYGENE... (H-4A-6A,H-4B-6A)
26	HYDROGENE + AZOTE... + OXYGENE... (H-5A-X à H-9D-9D)
27	SYSTEMES à 3 ELEMENTS (sauf R et H)
28	SYSTEMES à 4 ELEMENTS
29	GENERALITES, SERIES ISOELECTRONIQUES
30	ATOMES et MOLECULES EXOTIQUES

## RÉSUMÉ POUR "XVI ICPEAC, PALO ALTO, 1985"

GAPHYOR : AN ATOMIC AND MOLECULAR DATA CENTRE AT ORSAY

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An atomic and molecular data centre has been established at the Orsay campus of the Paris-Sud University, France. Activities at this centre named GAPHYOR (Gaz PHYsique ORsay) were initially oriented towards collection and handling of bibliographic data. These data are collected from the published papers, books, or reports by a team of fifteen scientists collaborating with this project. The arrangement of the data allows the user to obtain more information than the one provided by standard bibliographic patterns. The identification and sorting of data is based on a simple code for writing molecules and collision processes or chemical reactions instead of using keywords. Molecules including up to eight atoms of no more than four different elements can be coded, by indicating the chemical formula, the constituting elements, and the excitation and ionization stage. The sorting of the data file is based on the Mendeleev families order and on "second-level" descriptors arranged in five standard "first-level" categories :

- a) Properties of atoms and molecules.
- b) Photon collisions.
- c) Electron collisions.
- d) "Heavy particles" (i.e. atoms, molecules and their ions) collisions.
- e) macroscopic properties.

A handy interactive system called SYGAL (SYStem Gaphyor Language) developed for the user's convenience allows on-line retrievals worldwide through the existing data transmission networks in "natural" physicochemical language without using the internal code of GAPHYOR.

Activities at ORSAY were recently enlarged to include collection, evaluation and dissemination of numerical data pertinent to atomic processes encountered in common (e.g. astrophysical, thermonuclear, arc and laser) plasmas. In the development of numerical data files emphasis is given to unique sets of "recommended" data. Especially for applications (e.g. modelling, diagnostics etc) these are more convenient than files including all the available values. Moreover, the anticipated use of each file determines not only the output form to be selected (computer readable files, printed tables, graphs) but also its internal structure. The general lines followed in implementing "recommended" data files are described elsewhere <sup>1</sup>.

The computer system used for the storage (and possibly the exchange) and retrieval of numerical data is

closely related to AMDIS and EXFOR systems, previously developed in Nagoya and Vienna correspondingly. Special effort is paid to establish a system compatible with the aforementioned ones allowing straightforward exchange of data. In so doing the periodicals, processes, quantum states, units etc, dictionaries used in the system follow standards currently used in the field.

Another characteristic of the system is its close connection with the existing wider bibliographic data base. In fact, the bibliographic part and the retrieval of the data sets are based on the GAPHYOR software <sup>2</sup>.

International collaboration in data assessment and exchange is also part of the GAPHYOR data centre activities. In this context a proposal has been made to CODATA for standardisation and unification of atomic and molecular data currently used in various applications. The choice of evaluated data is initially oriented towards two well-known data sets obtained :

1. as a result of the IAEA Coordinated Research Programme on "Atomic collision data for diagnostics of magnetic fusion plasmas" run essentially from 1981 to 1984 <sup>3</sup>. The bulk of these data was recommended for fusion applications by the IFRC subcommittee for atomic and molecular data for fusion.
2. during the recent workshop on "atomic data for fusion and astrophysics" held in March 1985 at the Daresbury Laboratory, UK <sup>4</sup>. This set of data consists essentially of recommended data for electron impact excitation of atoms and ions.

Work in data evaluation is also carried out on charge exchange collisions parametrisation in collaboration with the University of Belgrade, Yugoslavia (Dr R. Janev). Also, promotion of astrophysical applications of atomic data was recently developed through collaboration with the Meudon Astrophysical Laboratory.

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