

NBS TECHNICAL NOTE **947**

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Critical Evaluation of Data in the Physical Sciences—

A Status Report on the National Standard Reference Data System

January 1977

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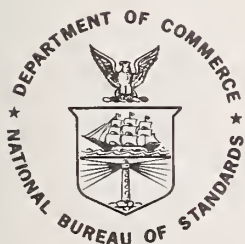
Critical Evaluation of Data in the Physical Sciences—

A Status Report on the National Standard Reference Data System, January 1977

t. Technical Note no 947

Stephen A. Rossmassler, Editor

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National Bureau of Standards
Washington, D.C. 20234



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P R E F A C E

The last report on the status of the National Standard Reference Data System appeared nearly two years ago. Since that time a number of new data projects have been started, and the management structure of the Office of Standard Reference Data has been substantially changed in order to focus more strongly on the use of reference data in the attack on important national problems. The progress of the system, the plans for the future, and the relationship of the National Standard Reference Data System to other organizations are summarized in this Status Report.

The National Standard Reference Data System is intended to provide a basic service to the entire scientific and technical community of the United States. The success of the program depends very critically on feedback from the users of the output. We welcome all comments, suggestions, and criticisms on the program.

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A B S T R A C T

This is a report on the status of the National Standard Reference Data System as of January 1977. Current activities and functions of the Office of Standard Reference Data are summarized. A complete list of data evaluation projects supported by the Office of Standard Reference Data during Fiscal Year 1977 is included; this list also includes projects which received financial support during the previous fiscal year, and which are still actively involved in some aspect of data compilation and evaluation. The list of projects includes continuing data centers in the United States whose activities fall within the scope of the system, but which are not formally affiliated with it. A list of publications resulting from the National Standard Reference Data program is provided.

Key words: Atomic and molecular data; chemical kinetics data; energy data; environmental data; industrial process data; materials utilization data; mechanical properties; nuclear data; physical science data; standard reference data; solid state data; thermodynamic data; transport properties.

CRITICAL EVALUATION OF DATA IN THE PHYSICAL SCIENCES
A STATUS REPORT ON THE NATIONAL STANDARD REFERENCE DATA SYSTEM

January 1977

I. GENERAL SURVEY

A. Origin of the National Standard Reference Data System

The formal existence of the National Standard Reference Data System dates from 1963, when the Federal Council for Science and Technology asked the National Bureau of Standards to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The text of the Federal Policy statement is given in Appendix IA. The program was conceived as a decentralized national effort, with financial support coming from a variety of Government and private sources, but with NBS responsible for the overall planning and coordination. The existing data compilation activities supported by NBS and other Government agencies were to be strengthened, new projects started in neglected technical areas, and the entire effort molded into a coherent program.

The technical scope of the program gives primary emphasis to well-defined physical and chemical properties of substances and systems which are well characterized. Also included are materials of commerce (alloys, ceramics, etc.) whose composition may vary only within clearly stated ranges. Materials of uncertain or widely variable composition are not included. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. While these definitions leave many borderline cases, the overall intent is to concentrate the effort on intrinsic properties that are clearly defined in terms of accepted physical theory and substances whose composition is so well known as to justify evaluation of the data. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

The major aim of the program is to provide critically evaluated numerical data to the scientific and technical community in a convenient and accessible form. Certain secondary outputs, such as annotated bibliographies and procedures for computerized handling of data, are also made available. A second aim is to provide feedback into experimental programs to help raise the general standards of measurement. That is, by communicating the experience gained in evaluating the world output of data in the physical sciences, NSRDS helps to advance the level of experimental techniques and improve the reliability of physical measurements.

B. Organization of NSRDS

When the National Bureau of Standards accepted the primary responsibility for the National Standard Reference Data System, the Office of Standard Reference Data (OSRD) was established at NBS to manage the program. This office is now located under the Associate Director for Information Programs. The OSRD performs several functions. It has the responsibility for allocating that part of the NBS budget which is spent on critical data evaluation, both within the NBS technical divisions and through contracts with outside groups. The staff of the office act as monitors for all projects which are supported. The management of the publications program of NSRDS is also in the hands of OSRD, and an information service is operated on a limited scale. In addition, OSRD maintains close contact with other data compilation activities, both in the United States and abroad. It attempts, both domestically and internationally, to avoid needless duplication and to improve coverage of all important technical areas. Finally, a small group within OSRD is engaged in research and development on computer handling of data and in application of automated procedures to the activities of data centers.

The actual compilation and evaluation of data takes place in many widely separated groups. It is these groups which form the components of the National Standard Reference Data System. The fact that these groups vary greatly in size, organizational structure, and source of financial support leads to a certain degree of diffuseness in the system. However, it is instructive to recognize two broad types of components in NSRDS. The first is the continuing data center, which has a charter (formal or informal) to cover a certain technical area on a continuing basis. Ideally, such centers have an assurance of stable long-term financial support. The task of a data center is to search the world literature on a regular basis, to retrieve and index papers within its scope of interest, to extract the numerical data, and to carry out critical evaluation leading to publication of tables or reviews. Many of the centers are highly mechanized and have large, computer-based files from which bibliographic citations and data can be retrieved. Generally, they are able to respond to requests for specific information from the scientific public.

The other type of component is the individual scientist (or small group of collaborators) who produces a "one-shot" compilation or critical review as a part of what he regards as his normal scientific activity. Many valuable data compilations have been produced in this way. Such individuals do not consider themselves part of a formal data center, and there is generally no commitment for continuity or updating. The rapid growth of the scientific literature makes it increasingly difficult for an individual to do this type of compilation. However, the continuing data centers can serve a useful function by providing bibliographic back-up for individual scientists in other locations who wish to write critical reviews or do critical compilations of limited scope.

In the pattern which has emerged, it is clear that both types of components are essential for the successful operation of the National Standard Reference Data System. The concentration of the bibliographic phase in a relatively small number of continuing data centers offers many advantages. While these centers carry out some of the critical evaluation of the data, they generally do not have the expertise on their own staff to cover every aspect of the field in question. By enlisting the help of specialists in other institutions for evaluations and critical reviews, the data centers can greatly increase the utilization of their resources.

One of the primary goals of the Office of Standard Reference Data is to establish continuing data centers in all technical areas which fall within the scope of the program. In addition, the office attempts to provide funds for individual compilations and critical reviews of well defined scope and duration. Since the resources of OSRD are limited, every effort is made to persuade other agencies and private organizations to participate in the support of these activities.

C. Organizational Structure of the Office of Standard Reference Data

For management purposes, the Office of Standard Reference Data originally divided the total scope of its technical program into seven areas on the basis of their discipline-related content. Those seven areas were: Thermodynamics and Transport Properties, Atomic and Molecular Data, Chemical Kinetics, Solid State Data, Nuclear Data, Colloid and Surface Properties, and Mechanical Properties.

Early in 1976, OSRD restructured its program along application lines rather than in accordance with scientific disciplines. Organizationally, the OSRD now consists of an overall management unit, four applications-related data programs, an information service activity, and a data systems design group. The four data programs are designated Energy and Environmental Data, Industrial Process Data, Materials Utilization Data, and Physical Science Data. Briefly, the programs have the following content:

Energy and Environmental Data - Projects dealing with data that have an important application in some aspect of energy R&D or environmental quality improvement. Projects in chemical kinetics, nuclear properties, spectroscopic data, and interaction of radiation with matter are currently incorporated in this program. The output of these projects is particularly important in R&D on new energy sources, environmental monitoring techniques, and prediction of the effects of pollutants introduced into air, water, or land.

Industrial Process Data - Projects dealing with thermodynamic, transport, colloid and surface, and physical properties of industrially important substances are included in this program. Such data have particular application to design of new processes in the chemical and metallurgical industries, optimization of currently used processes, and general productivity enhancement.

Materials Utilization Data - Properties required for material selection and R&D on new materials. The structural, optical, electric, magnetic, and mechanical properties of solid materials are included.

Physical Sciences Data - Projects which involve basic data of very broad applicability, or which are associated with an important frontier field of science, are included in this program. Examples are fundamental physical constants, data on fundamental particles, and data relevant to radioastronomy.

While the new organizational structure involves a substantial change in management emphasis, the basic disciplinary framework of NSRDS will be retained. The scientific expertise required for critical evaluation of data in a particular discipline can best be obtained through a data center focussed on that discipline. However, the priorities within a data center will be strongly influenced by the identified needs for data in the appropriate application areas; thus, the scheduling of tasks within the

disciplinary scope of each data center will reflect the priorities established for the application areas in the new OSRD organizational structure. In addition, more emphasis is being given by OSRD to the packaging of data in formats appropriate to the various areas of application.

Obviously, the technical output of many of the data centers is applicable to more than one (frequently to all four) of the program areas. The OSRD program managers maintain close communication with one another to assure that the full resources of the system are available as needed without any constraint which might arise from arbitrary dividing lines.

What the new organizational structure offers is a better, more readily identified match between the needs of outside users and the capabilities of NSRDS to supply reliable data relevant to major national problems. Taking full advantage of this match requires close interaction with data users, with Federal agency representatives who are working to solve these national problems, and with data programs in other countries. Such interaction is discussed in Section II of this Report.

D. Information Resources in OSRD

1. OSRD Library. The Office of Standard Reference Data has built a broad, although selective, collection of reference data compilations and ancillary publications within the scope of the NSRDS. A list of the holdings was published in September 1970 as NBS Technical Note 554, Annotated Accession List of Data Compilations of the NBS Office of Standard Reference Data. NBS Technical Note 554 listed about 1300 documents. The collection has continued to grow. As of September 1976, the OSRD Library housed about 3000 publications--one of the most extensive holdings of this scope in the world. This is not a lending library, but the use of the documents by visitors within the library is encouraged. In the summer of 1976, the OSRD Library was relocated physically as part of the main NBS Library. The data collection occupies its own separate set of shelves but is also treated as an integral part of the Library's reference material.

2. Inquiry Services. The Office of Standard Reference Data attempts to answer, within restrictions imposed by limited staff and time, inquiries concerning data in the physical sciences and engineering. Information and data are provided from NSRDS publications and other available sources. Inquiries may be referred to data centers and individual specialists in NBS and elsewhere. At times references are provided; if available and appropriate, copies of publications or excerpts therefrom containing the requested data are furnished. OSRD normally receives about 1000 requests and inquiries per year. Under the system-wide cost-recovery policy, custom services which require a substantial amount of time are billed to the requestor.

E. Data Systems Design Activities

The Data Systems Design Group devises computer techniques to enable the NSRDS data centers to automate their work in such a way as to reduce clerical costs, speed up publication, reduce errors, and reduce the cost of typesetting their output. Activities of the group are focussed on the design, implementation, and application of a number of general-purpose computer programs for storage and retrieval; file manipulation; and

computer-assisted text preparation, editing, and printing. In the latter area, the group is working in close collaboration with the Computer-Assisted Section of the NBS Office of Technical Publications in developing and applying a variety of computer-based systems for more effective use of the Electronic Composing System at the Government Printing Office.

Current Activities of the Data Systems Design Group include:

1. Design, Implementation, and Application of the NBS Typographic System

The text handling system based on the General Purpose Scientific Document Code (GPSDC) is used as the common data code of the NBS Typographic System. Interface programs have been written that permit information keyboarded on three different computerized text-editing systems to be converted to GPSDC. Another program is used to convert a GPSDC file into a Linotron driver tape used to typeset material on the Linotron 1010 Phototypesetter at the Government Printing Office (GPO). This allows the use of a Model 37 teletype or equivalent ASCII coded terminal with an on-line text-editing system to prepare material to drive the Linotron at GPO directly using the NBS Typographic System. For those without access to one of the accepted on-line text editors, provision is made for input from cards, paper tape, or ASCII coded magnetic tape.

The three on-line text editors that interface are: the ATS system that runs on IBM 360 or 370 computers; the EDTEXT system that runs on UNIVAC 1108's; and the RUNOFF system that runs on Honeywell and some Digital Equipment computers.

For cases where character size and page characteristics vary within a document, a set of commands keyboarded in red has been implemented. These special commands along with the formatting commands required by the on-line text-editing system are used by the NBS Typographic System to control the format of the phototypeset page.

Because editing of data and text files in the GPSDC system is cumbersome, a program was written and implemented to convert GPSDC files into ATS Archival form. In this form corrections and formatting or typesetting commands can be entered easily from a keyboard. This technique is now standard procedure for publications keyboarded in GPSDC format.

2. Automatic Typesetting and Composition of Data Tables

A major fraction of the effort in this area involves production of NSRDS publications from existing card files and computer tapes. The program SETLST with multiple table substitution has proved to be most versatile for handling fixed field information on data tapes. It is used to rearrange the data as desired and to insert typesetting codes required for input to the typography programs at the Government Printing Office. It is also used to convert data to the required form for input to the NBS Typographic System.

3. Source Automation of Technical Manuscripts

During the calendar years 1975 and 1976 over 20% of the pages published in the Journal of Physical and Chemical Reference Data were prepared for publication using automated procedures which feed more or less directly into computerized phototypesetting machines. During this same period 50% of all the publications of the Office of Standard Reference Data that were printed via the Government Printing Office were fully or partially automated.

4. Data Analysis and Retrieval System

The data analysis and retrieval system OMNIDATA (previously called TODARS) has been modified to improve its efficiency, and more modules have been added to enhance its capabilities. The general-purpose system has been used productively both interactively and in the batch mode to operate on a number of NSRDS files (including unusual data bases), NBS files, and files of users at other agencies. Examples of production uses include the correcting and updating of the crystal data files in preparation of NBS Magnetic Tape 9, the publication of the crystal data space-group tables, and the production of various types of indexes associated with JPCRD. It is presently operative not only at NBS, but on the 1108 computer at the Department of Housing and Urban Development. The final documentation for OMNIDATA is in process, a training course has been given, and several workshops and further training sessions have been planned.

Recent Data Systems Design Accomplishments

Productive uses of the OMNIDATA System include:

a. A portion of OMNIDATA in absolute form and expressly tailored to run on the computerized version of the crystal data files was demonstrated on-line as an adjunct to the following talks:

"The NBS Crystal Data File: On-Line and Off," Mighell, Ondik, and Breen, presented at the Tenth International Crystallographic Congress, Amsterdam, The Netherlands, August 1975.

"Crystal Data: On-Line Computer Search Capabilities," Mighell, Ondik, and Breen, presented at the American Crystallographic Association Winter Meeting, Clemson, South Carolina, January 1976.

b. The system was used extensively to analyze and update the crystal data files, in order to prepare them for sale as NBS Magnetic Tape 9.

c. The publication, "Crystal Data Space-Group Tables," Mighell, Ondik, and Molino (Breen), appears in Volume 6 of the JPCRD. Without the aid of many of the OMNIDATA modules, this publication would have been delayed a minimum of two years.

d. The module KWOC (Keyword Out of Context) is a powerful tool for indexing and has been used productively to prepare various indexes for the JPCRD. Included are an index of words in the title and one for keywords and properties. The module has the facility of putting in special flags, recognizing certain characters (i.e., a shift symbol), and outputting a file which can then be sent forward for typesetting.

e. OMNIDATA has also proved useful for handling other types of data bases, both at NBS and in other agencies, such as the Department of Housing and Urban Development. NSRDS Data Files Available for Distribution on Magnetic Tape

The Office of Standard Reference Data has made three additional magnetic tapes available for sale by the National Technical Information Service. They are:

NBS Magnetic Tape 8, EPA/NIH Mass Spectral Data Base 1975 Edition, contains about 11,300 mass spectra which were acquired by EPA and NIH for the Mass Spectral Search System.

NBS Magnetic Tape 9, Crystal Data Tape, Derived from the 3rd Edition of Crystal Data Determinative Tables, contains the cell parameters, Z, space group, measured density, X-ray density, formula, inorganic name, and determinative ratios for approximately 24,000 crystalline compounds.

NBS Magnetic Tape 10, Atomic Spectral-line Intensities, contains the intensity, character, wavelength, spectrum, and energy levels of 3900 lines in the spectra of 70 elements.

F. Standard Reference Data Legislation

The Standard Reference Data Program was established under the general enabling legislation of the National Bureau of Standards. In addition, in 1968 the Congress provided specific legislative authority for the program through passage of Public Law 90-396, the Standard Reference Data Act. The text of the Act is given in Appendix IB.

One of the principal features of PL 90-396 is the provision of authority for recovering some of the cost of the program through user charges. In order to make this possible, the Secretary of Commerce is authorized to copyright publications which result from the program and to assign this copyright to others. Several contracts have been negotiated under this authority. In particular, OSRD has contracted with the American Chemical Society and the American Institute of Physics to publish the quarterly Journal of Physical and Chemical Reference Data. This Journal has completed its fifth year of publication. With the appearance of the last issue of Volume 5, 88 data compilations have been disseminated to users through this medium; in addition, two major compilations have appeared as Supplements. Over 1200 subscriptions to JPCRD are now in force, including foreign subscriptions in 44 countries.* Subscription to the Journal and sales of Supplements and individual reprints have provided a useful financial return to the program.

Other channels for cost recovery have also been established. They include:

1. Sale of reports and magnetic tapes through the National Technical Information Service (NTIS).

2. A formal system by which Data Centers charge for custom information and data services.

3. A cooperative undertaking with Plenum Press in the publication of a series of NSRDS-derived bibliographies on specialized topics.

* Australia, Austria, Belgium, Brazil, Canada, Chile, Czechoslovakia, Denmark, Finland, France, German Democratic Republic, Federal Republic of Germany, Hong Kong, Hungary, India, Iran, Iraq, Israel, Italy, Japan, Korea, Malawi, Malaysia, Mexico, Netherlands, New Zealand, Nigeria, Norway, Philippines, Poland, Portugal, Romania, Singapore, South Africa, Spain, Sweden, Switzerland, Taiwan, Uganda, Union of Soviet Socialist Republics, United Kingdom, Venezuela, Yugoslavia, Zambia.

G. Advisory Mechanism

For good management, the NSRDS program must have reliable feedback from the scientific and technical community. Such feedback is provided on a formal basis by the NAS-NAE-NRC through the Numerical Data Advisory Board (NDAB). The scope of the NDAB includes numerical data of concern to all parts of science and technology. The NDAB also serves as a focus for coordination with certain other national information programs (such as the National Materials Advisory Board) and international programs parallel to NSRDS. In this latter role, NDAB has responsibility for the US National Committee for CODATA. International undertakings are described more fully in the following section of this report.

The NDAB administers advisory panels in several of the program areas of NSRDS. These panels meet periodically to discuss needs and priorities within each program area. The membership of the panels is drawn from industry, universities, and Government; an effort is made to achieve coverage of the major specialities within each area. The NDAB submits a report to OSRD after each panel meeting, in which the current activity is appraised and suggestions made for future emphasis.

In addition to the principal advisory panels, ad hoc subpanels are convened at the request of OSRD to discuss problems of a more specific nature. Subpanels of this type have been organized in fields such as Mossbauer spectroscopy, interatomic distances, electrical properties of solids, and thermodynamic properties of aqueous electrolyte solutions. Meetings of such groups have led to the establishment of new compilation projects or (in some cases) to the recommendation of procedures for obtaining and reporting experimental data in the particular field. The NDAB also serves as co-sponsor with OSRD of symposia and conferences on special topics when a broader level of professional interaction appears appropriate to a special subject.

In its broader responsibilities, NDAB is concerned with data outside the physical sciences and with data on less well-defined properties and substances.

II. RELATIONSHIPS WITH OTHER ORGANIZATIONS

The two specific authorities under which the NSRDS and the OSRD operate, a 1963 Federal Policy and the Standard Reference Data Act of 1968 (Appendix IA and IB), both identify the need for participation by other Federal agencies, as well as other appropriate non-Government activities. OSRD has pursued this objective vigorously. Changes made in 1976 to the organizational structure of OSRD, designed to match NSRDS capabilities and resources more accurately to the data needs inherent in major national problems, have brought into even sharper focus the importance of effective relationships between OSRD and others responsible for attacking and solving such problems.

A significant fraction of the work of OSRD staff is devoted to establishing, developing, and utilizing relationships with other individuals and organizations involved in data generation, data compilation and evaluation, and the application of data for the solution of problems.

While all of the professional staff members share in this responsibility, a specific focus has been created through the establishment of a new position - Special Assistant for Technical Liaison - set up in the fall of 1976. This Assistant will lead the efforts of OSRD to inform users more effectively of the data available through the NSRDS program and will strengthen efforts for determining what data are most needed.

Analyzed in the broadest practical terms, OSRD relationships can be considered in three classes -- with other Federal agencies, with private users and suppliers of data, and with foreign national and international organizations.

A. Relationship with Other Federal Agencies

The National Bureau of Standards has been charged with the administration of NSRDS; OSRD is the organizational unit of NBS set up for that purpose. As operator of a national system, OSRD welcomes formal or informal collaboration with data evaluation projects in any of the Federal agencies, but as a practical matter, adherence to the system by a specific activity must arise out of the explicit wish of the sponsoring agency. A number of Departments and other Executive agencies have found it appropriate to join forces with NSRDS in pursuit of common goals. The longest-standing and most extensive relationships have come about with the Department of Defense (and its three Service Departments) and with ERDA (also formerly with AEC) both of which sponsor their own information analysis centers on topics within the scope of NSRDS. Equally meaningful relationships exist with the Department of Health, Education, and Welfare, the Department of the Interior, the Department of Transportation, the Environmental Protection Agency, the National Aeronautic and Space Administration, and the National Science Foundation.

The kinds of relationships between NSRDS and other agencies vary widely, but fall into four broad categories:

1. Common planning to meet existing or anticipated data needs. Another agency may identify a present or new need for data, and may work with OSRD to determine what data are already available, what current data projects could supply data, what experts might assist, or how a new data project might be set up. A frequently used device for common planning is a conference or workshop under joint sponsorship.
2. Specific advice to agencies from OSRD. Another agency, or one of its internal information projects, may ask OSRD or NSRDS project leaders for guidance on data handling, evaluation criteria, use of computer techniques, etc. OSRD staff members frequently serve on advisory panels for data and information projects supported by other agencies.
3. Joint support of data work. In many instances, other agencies have transferred funds to NSRDS data projects to support some fraction of the work. Frequently, a specific data task is involved, and a specific product is provided. In several cases, OSRD contributes funds to a data project (usually at an academic location) which is also supported by another agency.
4. Project management by OSRD. Here another Federal agency contracts with OSRD to manage a program of substantial extent, involving several component projects, in order to develop a series of data compilations relevant to a major aspect of a problem-solving effort.

Illustrations of these relationships are given below.

OSRD Cohosts Meeting on Transport and Transformation of Pollutants on Land and in Water

Approximately two hundred scientists met at NBS on May 11-13, 1976, to discuss physical and chemical processes affecting pollutant behavior in water and on soil. The Symposium, entitled "Nonbiological Transport and Transformation of Pollutants on Land and in Water: Processes and Critical Data Required for Predictive Description," was cosponsored by NBS, EPA, ERDA, and NSF. It was chaired by L. H. Gevantman (OSRD) and R. G. Zepp (Environmental Research Laboratory, Athens). The 21 speakers dealt with the specifics of relating laboratory and field observations and the incorporation of these results into observational and conceptual models which could generalize the environmental behavior of pollutants.

It was the consensus that the meeting succeeded in highlighting the importance of the physical and chemical processes in the environment. Moreover, while it appeared possible to define and evaluate pollutant reaction paths in laboratory surroundings, it was far more difficult to relate these data to observation in the field. More data and more accurate data were considered vital to further progress in predicting pollutant behavior.

Radiation Chemistry Data Center Advisory Committee Meets

The Advisory Committee of the Radiation Chemistry Data Center (RCDC) met on April 30, 1976, at the University of Notre Dame for the purpose of

reviewing the past activities and future plans of the data center's operation. The day-long meeting included a presentation by L. H. Gevantman of the Office of Standard Reference Data on the new program structure of the Office and the impact of that program on the data center's activities. The representative from ERDA was also asked to comment on his agency's view of the data center. The RCDC is sponsored jointly by the OSRD and ERDA.

The Committee endorsed the data activities of the Center and offered valuable suggestions for improving the Center's image as a contributor to the broad field of physical science rather than its narrowly defined area of radiation chemistry. The Center was asked to increase its efforts toward improved communication with scientists outside the radiation chemistry area.

OSRD Coordinator in Compiling Energy Storage Data

The Lawrence Livermore Laboratory (LLL) has reached a contractual arrangement with the OSRD in which the Office acts for LLL in compiling and evaluating physical properties data on materials of importance for use in energy storage systems. Under this arrangement the LLL specifies the materials and properties for which data are required. These requirements are presented to OSRD, which arranges for the work to be carried out through its system of data centers or other centers of expertise as required. The final products, prepared with the guidance and oversight of the OSRD, are to be submitted to LLL for incorporation into an automated data storage and retrieval file residing at the Livermore Laboratory. The automated file, which is under the direction of Viktor Hampel and his associate, Terrence Quick, will be made accessible to ERDA contractors and others requiring the stored data. Where appropriate, the OSRD will also publish the data through its established outlet, namely the Journal of Physical and Chemical Reference Data and the NSRDS-NBS series.

A pilot study to test the efficacy of the arrangement has been initiated. It deals with selected properties data of molten salts, individually and as mixtures, which have potential use in storage batteries. The Molten Salts Data Center at Rensselaer Polytechnic Institute has been designated as a source of expertise for the effort. Funding of the effort has been accomplished by a transfer of funds from LLL to the OSRD.

B. Relationships with Private Users and Suppliers of Data

The ultimate value of reliable reference data lies in their application by users to the solution of real problems, ranging from the planning and interpretation of basic research to the design of engineering components, or the identification of a trace contaminant in water or air. OSRD regards its relationships to its users as the key factor in program management. These relationships call for good communication in both directions, a continuing educational program, and constant exploration by OSRD of additional channels for reaching and satisfying its customers. OSRD also recognizes its responsibility to work with private suppliers of data, to cooperate with them in avoiding duplication of effort, to supply data to them when appropriate, and to utilize fully their capabilities for disseminating data to specialized or general user groups.

A systematic effort to improve technical liaison with users is already in effect, as evidenced by the presence of a new staff position within OSRD. Other members of the OSRD technical staff continue as always to consult with users, to plan and manage cooperative data projects, and to associate their activities with those of private data suppliers.

Four categories of liaison and relationships are at present most important:

1. Cooperative data projects with private industrial users. The 1975 Status Report described the establishment of a project (with sponsorship by several industrial corporations) to develop a definitive set of thermophysical and related thermodynamic properties of ethylene. That project continues and has shown good progress. Further details are given in the relevant project description under "Industrial Process Data", Section IV.C. below. A second, and potentially much more far-reaching cooperative project is now in the early stages of exploration. It concerns the feasibility of a joint industry--government data base for use in chemical engineering process design calculations. The nucleus of the data base would consist of continuously upgraded data on the thermophysical and thermodynamic properties of 500 to 1000 ubiquitous chemicals which all industrial chemical manufacturers must deal with from time to time. While this new project is only in the early discussion stages, with no commitments of any kind, it indicates clearly the continuing role of OSRD as a partner of industrial data users.

2. Work with professional societies. OSRD has found repeatedly that it can obtain valuable leverage and increase the effectiveness of its communication with data users by working with professional and technical societies in cooperative planning and joint data projects. An example is the recent formation of an ad hoc panel on data for pollutant-soil reactions, convened at the annual meeting of the Clay Mineral Society in Corvallis, Oregon. The panel met on August 1, 1976. L. H. Gevantman of the Office of Standard Reference Data led the meeting. Representatives of the Environmental Research Laboratory, Athens, were also present.

Each of the participants reviewed briefly some of the aspects of the state of knowledge concerning pollutant-soil interactions. These presentations were followed by a discussion period which focussed on which data were suitable for compilation and evaluation. The consensus was that, despite the variety of reactions observed between soil and pollutants, a matrix of about 25 soil systems and a small selected group of typical organic and inorganic pollutants defined the area of primary interest, and that a critical review of the data relevant to these contributions would make a valuable contribution to the literature.

3. Work with specialized data groups. The establishment of data-oriented committees, panels, etc., for specialized scientific topics, is becoming a frequent occurrence. OSRD encourages such groups, sometimes sharing responsibility for bringing them into existence. The programs and outputs of these groups depend on the need in the field of concern. One common focus is on the quality of data being generated and reported in the primary literature. For example, a set of "Recommendations for the Presentation of Raman Spectral Data" has been formulated with approval of leading professional societies and with input from practitioners of Raman spectroscopy in the United States and Canada. The recommendations evolved out of discussions which began under the sponsorship of the Numerical Data Advisory Board of the National Academy of Sciences with the informal cosponsorship of the Joint Committee on Atomic and Molecular Physical Data (JCAMP). A. Lee Smith, of Dow Corning Corporation and Chairman of JCAMP, chaired the first session.

Gregory Rosasco, of the NBS Inorganic Materials Division, spearheaded the subsequent 6-month effort in which the recommendations were drafted, reviewed, and put into final form with the cooperation of JCAMP (representing 10 professional and technical societies) and the ASTM Special Committee on Molecular Spectroscopy. An appropriate channel for publication of the recommendations is now being considered. A similar set of recommendations for Mass Spectral Data is also being developed.

This particular phase of the NSRDS program goes back to the 1966 "Specifications for Evaluation of Infrared Spectral Data," prepared by the Coblenz Society Board of Managers, which has had substantial impact on the several reference catalogs of IR spectral data published throughout the world. Both the Raman and IR recommendations were prepared by groups of experts representing U.S. industry, government laboratories, and universities. NBS leadership in these efforts is recognized by the participants as a highly valuable catalyst for development of common ground.

4. Cooperation with publishers of handbooks and other data distributors. While OSRD tries to make its own publication efforts as effective as possible, there is clear recognition that many data-users have other channels for access to the data they need. Handbooks rank high among these channels. Accordingly, OSRD takes every opportunity to see that its data compilations get further distribution through other publishers and disseminators. For example, the 56th (1976) edition of the familiar Handbook of Chemistry and Physics contains 17 tables of data derived directly from NSRDS compilations. Another example has an international flavor. A professor at a Japanese university has recently taken a major initiative in helping to distribute NSRDS-NBS publications in Japan. Increased Japanese interest in these publications, particularly those produced with the cooperation of the Radiation Chemistry Data Center (RCDC) at the University of Notre Dame, has spurred the establishment of a unique arrangement between the Office of Standard Reference Data (OSRD) and the Japanese data distributor. Under this arrangement he collects orders for each document from scientists in Japan, and then sends an order for the required number to the OSRD. The first exchange, involving the sale of over 200 copies of four reports (NSRDS-NBS 43 and Supplement, NSRDS-NBS 46, and NSRDS-NBS 51) has been completed. The OSRD hopes that this new arrangement will lead to increased exposure and sales of its publications in Japan--not only those in the NSRDS series, but also the Journal of Physical and Chemical Reference Data.

C. International Cooperation

In the period since the establishment of NSRDS, data evaluation activities in other parts of the world have increased considerably. Formal governmental programs similar to NSRDS have been established in several countries. In the U.K., the Science Research Council administers a program which includes the support of a number of data centers in the physical sciences. In the Soviet Union, the Academy of Sciences supports several data evaluation projects, and the State Service for Standard Reference Data (GSSSD) has broad responsibility for scientific and technical data. The Federal Republic of Germany has recently (1975) established an overall organizational structure for an information system for physics data (including some physical chemistry aspects) to be operated by the Zentralstelle für Atomkernenergie-Dokumentation (ZAED). In France, the Bureau National pour l'Information Scientifique et Technique (BNIST) is developing a substantial information program with a strong data component. The Office of Standard Reference Data maintains liaison with these groups

with the aim of avoiding duplication in data compilation projects and promoting maximum compatibility of output. Proposals requesting support of projects in subject areas of mutual concern are exchanged for comments.

The establishment of the Committee on Data for Science and Technology (CODATA) in 1966 has provided a continuing formal framework for international cooperation. CODATA is a committee of the International Council of Scientific Unions (ICSU) and contains representation from twelve international unions and, at present, fifteen countries, plus two associated organizations. The Secretariat is located in Paris. The main purpose of CODATA is to encourage, on a world wide basis, the production and distribution of critically evaluated numerical data. One of its first tasks was to publish an International Compendium of Numerical Data Projects (Springer-Verlag), New York-Heidelberg-Berlin, 1969). This volume lists identifiable data compilation projects throughout the world, with information on their scope, mode of operation, and form of dissemination of output. A revision is in progress. A major feature of the CODATA program is a series of biennial conferences, which bring together leading compilers of data and sponsors of data programs throughout the world. The most recent of these conferences, held in Boulder, Colorado, in the summer of 1976, is described in Section III of this Report.

CODATA has established Task Groups in a number of special areas, including Chemical Kinetics, Presentation of Data in the Primary Literature, Accessibility and Dissemination of Data, Fundamental Constants, Key Values for Thermodynamics, Training in Data Handling, Computer Use, Transport Properties, Data for Industrial Needs, and Internationalization and Systematization of Thermodynamic Tables.

In other areas, CODATA task groups have received endorsement and sponsorship by Unesco on topics of common interest. The resources of CODATA are used by Unesco in constructing UNISIST, a developing world scientific and technical information system. Members of NSRDS data projects and staff members of OSRD have been active in all of the CODATA task groups.

While CODATA provides a major sponsorship for multinational attention to data needs, there are other international foci as well. For example, a subcommission of the International Union of Pure and Applied Chemistry (IUPAC) met recently to discuss the development of a specific data program. Subcommittee V.6.1. on Solubility Data of the International Union of Pure and Applied Chemistry (IUPAC) held its 3rd annual meeting at Virginia Polytechnic Institute (VPI) in Blacksburg, Virginia, on July 9-11, 1976. The meeting was chaired by A. S. Kertes of the Hebrew University and was attended by 13 other members and observers. L. H. Gevantman of the OSRD was invited to attend as an interested observer. The business of the subcommittee centered on the details of issuing a series of publications of data on the solubility of substances in three main categories, namely:

- a. The solubility of Gases in Liquids
- b. The solubility of Liquids with Liquids
- c. The solubility of Solids in Liquids

Discussions on technical guidelines for compiling and evaluating data, formats for reporting data, and assignment of responsibility to subcommittee members for identifying and persuading experts to carry out the actual work in the assigned areas took up the bulk of the allotted time. A course of action designed to deliver sufficient material to the publisher (Pergamon)

for issuance in 1978 was agreed upon. The next meeting of the Subcommittee was scheduled to take place in Warsaw, Poland.

OSRD relates to other long-established international data projects as well. The International Association for the Properties of Steam (IAPS) is the organization that provides the International Skeleton Tables for the Properties of Steam and the accompanying industrial and scientific formulations. The Skeleton Tables provide the thermodynamic and transport properties of steam used in the specification and design of power equipment the world over. At a 1976 meeting of IAPS, new formulations were proposed for viscosity and surface tension. These will be circulated for international ratification in the coming months. Work also proceeded toward the development of a new formulation for thermal conductivity, a new scientific formulation for the thermodynamic properties, and development of a data base for the chemical reactions of the minor components in the power cycle which can lead to expensive failures. NBS was represented at the meeting by J.M.H. Levelt-Sengers and Lester Haar of the Heat Division and by Howard J. White, Jr., of the Office of Standard Reference Data. White serves as the Executive Secretary of the International Association for the Properties of Steam.

Among the bilateral interactions in which OSRD participates, the most extensive is that with the USSR. Cooperation with data groups in the Soviet Union has taken place for a number of years under the auspices of international organizations such as CODATA and IUPAC. This interaction has been particularly strong in the area of thermodynamic data, where representatives from the NSRDS Thermochemical Data Center and the Institute for High Temperatures of the Soviet Academy of Sciences have worked together on the establishment of key values of thermodynamic properties. Following the US-USSR agreement on Cooperation in the Fields of Science and Technology, signed May 24, 1972, these interactions have been brought under the jurisdiction of the Joint Commission which supervises the bilateral exchange program. At the present time, Standard Reference Data is one of the items in the Cooperative Program in Metrology, and several exchanges of personnel have taken place. Much of the discussion during these exchanges is concerned with technical details of cooperative data projects. In addition, broader problems of data dissemination are considered. Translation and publication rights questions are a significant element of this bilateral relationship, and some protocols were drafted in 1976 to provide definitions for future formal action under the Agreement.

III. RECENT ACCOMPLISHMENTS

In the time since the 1975 Status Report appeared, a number of significant advances have occurred in the National Standard Reference Data System. They involve major new data evaluation projects, new cooperative undertakings, added service capabilities, and a variety of planning efforts. Some of these accomplishments have been described earlier in this report to illustrate specific aspects of relationships of OSRD with outside organizations. Others are listed below.

CODATA Holds Fifth Biennial Conference

The Committee on Data for Science and Technology (CODATA) held its Fifth International Conference in Boulder, Colorado, June 28 through July 1, 1976. More than 15 countries were represented among the 200-plus attendees, and the scientific program reflected their breadth of activities.

CODATA, a unit of the International Council of Scientific Unions (ICSU), was established in 1965 as an expression of worldwide concern for data, their compilation, critical evaluation, storage, and retrieval. Its scope includes quantitative data on the properties and behavior of matter, characteristics of biological and geological systems, and other experimental and observational data. CODATA covers all disciplines represented within the member Unions of ICSU, *i.e.*, the physical sciences, astronomy, the geosciences, and the life sciences, but CODATA's activities concentrate on problems which are common to the various disciplines.

CODATA conferences are held every second year. Previous conferences have taken place at Arnoldshain, Germany; St. Andrews, Scotland; LeCreusot, France; and Tsakhcadzor, Armenia, USSR. The Boulder Conference drew participants from Australia, Austria, Belgium, Canada, Costa Rica, Federal Republic of Germany, France, German People's Republic, India, Israel, Italy, Japan, Mexico, Poland, South Africa, United Kingdom, United States of America, and USSR. The United Nations UNESCO organization was also represented.

The program and conference chairman was David R. Lide, Jr., of the National Bureau of Standards, Office of Standard Reference Data. Other members of the program committee were Richard Donovan (USA), C.N.R. Rao (India), V. V. Sytchev (USSR), and G. A. Wilkins (UK). Attendees were housed in the Kittredge Residence Halls of the University of Colorado, and the scientific program was held on the same campus.

The program featured sessions on a wide variety of data problems in general and specific areas. Especially notable were discussions on Data for Technology, Data on Flavor and Aroma, Data Needs for Energy and Environmental Programs, Data in the Astro- and Geo-Sciences, and Biological Data. Other sessions covered General Problems of Data Evaluation and Analysis, Data Tagging, Computer Techniques in the Handling and Dissemination of Data, National and International Data Programs, Problems of Data Center Operation, Evaluation of Thermochemical Data, and Evaluation of Data in Solid State Properties.

Both preceding and during the conference, a number of task groups of CODATA held discussions and open meetings. These task groups are the means by which CODATA brings international expertise into close focus on specific data-related scientific problems.

National and international programs on data were described to the conferees, including those of USSR, Federal Republic of Germany, Japan, Unesco (UNISIST), European Economic Community (Euronet), and the World Federation of Engineering Organizations (WFEO).

Proceedings of the conference will be published by Pergamon Press and are scheduled for appearance early in 1977.

Committee to Study Needs for Reference Data

A one-year study of national needs for evaluated reference data has been initiated by the Assembly of Mathematical and Physical Sciences of the National Academy of Sciences-National Research Council. The study, which is being funded by the National Science Foundation, will assess current organized data evaluation activities in the United States and attempt to project future needs for data collections, particularly in support of national R & D programs in the areas of energy, materials, and the environment. A particular effort will be made to estimate the benefits from previous data evaluation activities.

The Steering Committee for the study, which is chaired by Professor Walter Stockmayer of Dartmouth College, held its first meeting in San Francisco on September 1 and 2, 1976. The Office of Standard Reference Data was represented by D. R. Lide. Representatives from ERDA and NSF also took part in the meeting.

OSRD Helps Revise Periodic Chart

Carrying on a cooperation which dates back over 50 years, the Office of Standard Reference Data has supplied to the Sargent-Welch Scientific Company needed data for a complete revision of the familiar "Periodic Chart of the Atoms." The first stage of the NBS/Sargent-Welch relationship occurred when Henry Hubbard, first secretary of NBS, designed a modernization of Mendeleev's periodic table, which was published by the W. M. Welch Manufacturing Company in 1924. Since then NBS has provided new data for each revision of the Chart; from 1940 through 1965 William F. Meggers was the active link, both before and after his retirement in 1958. Starting in 1967, the OSRD has worked with Sargent-Welch (successors to Welch Manufacturing) to revise and update the numerical information presented on the wall chart, which is well known to physics and chemistry students as a decoration of lecture halls, classrooms, and laboratories.

The latest revision is a sweeping one. All of the numerical and graphical data on the "Hubbard" chart have been updated by NSRDS Data Centers. OSRD has also suggested deletion of some outmoded visualizations of atomic structure. Sargent-Welch will also use the new data in revising a loose-leaf notebook-size tabular presentation. Both updates will appear early in 1977.

Accompanying the "Hubbard" chart is a booklet, "Key to the Periodic Chart of the Atoms." The booklet shares the history of the chart, with Hubbard as the original author, and revisions by Meggers. A complete rewriting of the booklet is being made by Martin Paul, retired Executive Secretary of the National Research Council Division of Chemistry and Chemical Technology. OSRD is assisting in the rewriting work. A number of NBS staff members shared in the updating.

Water Pollution Data

An ad hoc panel on Water Pollution Data was convened in Washington, D.C., August 14-15, 1975, under the auspices of the Numerical Data Advisory Board of the Academy of Sciences. The panel of experts chaired by J. Carrell Morris of Harvard University, consisted of representatives drawn from universities, government agencies, and national laboratories deeply concerned with the water pollution field. Their discussion focused on the evaluated data needs required to help establish a programmed approach to lowering the level of entry of pollutants into the water environment. The panel reviewed those pollutants identified by EPA to be of danger to the environment and listed in order of priority the specific types of numerical property data which would describe their behavior in aqueous media. They suggested that these prioritized needs could form the basis for data evaluation projects sponsored by the OSRD. It urged the issuance of data compilations for ready accessibility and use by modellers and other workers in the field.

National Center for Thermodynamic Data of Minerals Established in Cooperation with OSRD

The U.S. Geological Survey took steps in the Fall of 1976 to establish a National Center for Thermodynamic Data of Minerals in cooperation with the Office of Standard Reference Data as a component of the National Standard Reference Data System. The aim of the new Data Center is to acquire and provide, on a continuing basis, critically evaluated descriptions of the thermodynamic properties of minerals and other geologic materials over the ranges in temperature, pressure, and composition which are observed in the geological environment.

Primary emphasis will be placed upon coverage of numerical data needed to understand the geological environment and to utilize its resources. Specifically, the Data Center will develop critically evaluated thermodynamic data for all naturally occurring solid phases or the chemical end-members, as appropriate, and will cooperate with other Data Centers of the National Standard Reference Data System on the properties of gases and aqueous ions.

Both OSRD and USGS recognize the importance of assuring consistency of the output of the new Center with other thermodynamic tables. For that reason the methods of evaluation, including the auxiliary data on key substances used in analysis of the data on minerals, will be compatible with the practices of other centers in the National Standard Reference Data System.

The evaluated results will be disseminated to the scientific and industrial community through the Journal of Physical and Chemical Reference Data, the publications of the U.S. Geological Survey, by exchanges within the National Data Center community, and other outlets as appropriate to achieve the maximum distribution to interested users.

The Data Center will work to achieve thermodynamic consistency between its tables and related tables from other centers, will cooperate in the improvement of correlation methods, and will avoid duplication of effort. Vigorous attempts will be made to systematize the effort so that all groups can benefit from the sharing of common files and output, and the user can benefit from data referred to common bases.

Planning for Self-Consistent Thermochemical Data

A meeting of thermochemists and thermodynamicists interested in the compilation and evaluation of thermochemical data was held at NBS on January 20, 1975. The purpose of the meeting was to discuss ways in which data evaluators can cooperate to provide self-consistent tables of such data and most effectively make the results of their evaluations available to all. The meeting was sponsored by the Office of Standard Reference Data.

At the present time, self-consistent tables are compiled by small groups working closely together. This system is slow and the relationship of their results to other results, obtained independently, is uncertain. With the help of recently developed computer techniques, it should be possible to develop a network of compilers and evaluators who feed into a central system to produce larger, more comprehensive sets of self-consistent data.

The meeting on January 20 was an initial step toward the development of such a network. The meeting was attended by 15 thermodynamicists including representatives from Canada and the United Kingdom. Several others who could not attend sent comments in writing.

Phase Diagram Meeting

The Fourth CALPHAD (CALCulation of PHase Diagrams) Meeting was held at NBS August 18-22, 1975, under the sponsorship of the Metallurgy and Materials Science Division of the National Science Foundation and NBS. The Office of Standard Reference Data and the Alloy Data Center cooperated in arranging the meeting.

The meeting was a specialists' workshop on computer-based coupling of thermochemical and phase-diagram data and was attended by over 40 experts representing 7 countries. Computerized numerical data bases and systems for calculating thermodynamic data and phase diagrams from the data developed in France, the U.K., and the U.S.A. were discussed in detail and demonstrated in operation with the use of appropriate computer terminals and readout devices. Access to these computer-based data banks and computational systems is currently available by telephone connection in the U.K. and Western Europe, especially France and West Germany. A system to make similar services available in the U.S.A. is being started.

Sodium-Sulfur Battery Research

The Second Molten Salts Data Center Workshop was held on September 4-5, 1975, at Rensselaer Polytechnic Institute to review progress on the Sodium-Sulfur Battery Program. The workshop was organized by the Molten Salts Data Center, an NSRDS center directed by G. J. Janz of RPI. The research discussed at the workshop is partially supported by NSF-RANN and includes work at Rensselaer and the Ford Motor Company.

The discussions involved electrolyte kinetics, measurement standardization, electrode and cell material corrosion, and efforts to model cell behavior so as to understand the basic electrolytic reactions. A program for testing practical Na-S cells was described by M. Breiter of General Electric.

The workshop was attended by L. H. Gevantman of the Office of Standard Reference Data who presented a talk on the operation of the National Standard Reference Data System (NSRDS) and the management functions of the Office as they relate to physical properties data evaluation.

Engineering Information

A joint meeting of the Industrial Research Institute Task Group on Communication of Scientific and Technical Information and the Engineers Joint Council Commission on Engineering Information was held at NBS on October 2, 1975. The former group consists of industrial R&D managers and technical information specialists who are trying to promote more effective use of scientific and technical information in industry. The EJC group is concerned with general problems of transfer and use of engineering information.

NBS activities of interest to the two groups were presented in a half-day session. The programs described included the National Standard Reference Data System, Federal Information Processing Standards, Standard Reference Materials, Standards Information Services, and work of the WFEO Committee on Engineering Information. Considerable interest was shown in these NBS activities, and a useful interchange took place.

Third R.P.I. Molten Salts Data Center Workshop Conference

H. J. White, Jr., and L. H. Gevantman of the OSRD attended the 3rd Rensselaer Polytechnic Institute Molten Salts Data Center Workshop Conference on May 7, 1976. The conference, chaired by G. J. Janz, was held in Washington, D.C., and dealt with a review of the preliminary results achieved toward establishing KNO_3 and NaCl as standard calibrants for electrical conductance, viscosity, and surface tension measurements.

The Calibration Quality Data and Standards Program is an international effort, with participation from over eight countries, including France, England, Norway, Romania, Poland, and the German Democratic Republic. The scientists presented the results of their individual measurements and compared them with those of the others present. There followed a general discussion on what further efforts would be required to achieve the desired degree of agreement. The meeting was concluded with plans and recommendations for resolving the minor disparities which remain prior to adopting KNO_3 and NaCl as molten salt measurement standards.

Panel on Reference Nuclear Data Meets at Brookhaven National Laboratory

Representatives of national societies and organizations dealing with nuclear data assembled as a panel on October 19, 1976, to consider their needs for reference nuclear data and how these needs could best be met by the data centers now serving the nuclear science community. A number of observers representing the funding agencies, the data centers, and the publishers of nuclear data attended the meeting, which was convened by Brookhaven National Laboratory. L. H. Gevantman, as a representative of the NBS (OSRD), presented a short description of the National Standard Reference Data System and its role in promoting the publication of evaluated data in all scientific disciplines, including nuclear data.

The panel, chaired by James Cline of the Institute of Electrical and Electronic Engineers, listened to a number of talks describing the work going on at the various data centers which issue evaluated nuclear data. The panel then considered whether it should continue as an advisory group for the issuance of reference nuclear data particular to the needs of their societies. In a general discussion, the individual panel members studied the adequacy of current publications in meeting their needs. The panel concluded that it could serve a useful purpose in providing an interface between the data centers and national society members by disseminating information about ongoing data activities, and by acting as a channel for these societies in requesting from the data centers the issuance of specific nuclear data publications.

IV. ACTIVE DATA EVALUATION PROGRAMS

As mentioned earlier in this Report, OSRD has divided its overall data program into four problem-related technical areas: Energy and Environmental Data, Industrial Process Data, Materials Utilization Data, and Physical Science Data. The following pages provide a description of each of the areas; in the interest of greater specificity, the Energy Data and Environmental Data components are discussed separately. The descriptions indicate scope, general content, and special features of each area. Details of the individual data projects within each area are given in Appendix II.

ENERGY AND ENVIRONMENTAL DATA

The data activities associated with these two problem areas are closely interrelated. However, for ease of description they are presented separately. Consequently, the energy data program will be described first, followed by the environmental data program. In so doing, general reference will be made to data projects which, while pursued under other OSRD program areas, impact on the energy and environmental program area.

A. Energy Data Program

A rather substantial fraction of the NSRDS program has traditionally involved data projects related either directly or indirectly to energy and its applications. Past associations with the Atomic Energy Commission, as the predecessor of the Energy Research and Development Administration (ERDA), have led to cooperative activities in a number of selected areas which include radiation and radio-chemistry, basic nuclear physics, and thermochemistry. For example, the NSRDS has supported the compilation of data which are needed for nuclear reactor operation and safety. It has also been involved with data on the effects of radiation on chemical and biological systems. With the new ERDA responsibilities the NSRDS data activities have expanded to cover other aspects of the ERDA charter, such as data on fossil fuel systems, combustion kinetics, magnetohydrodynamics (MHD), energy conservation, energy storage, fusion, and material behavior. The OSRD has extended and strengthened its cooperation with ERDA so as to continue a useful input to the needs of a national energy program.

Program support in the nuclear data area continues primarily in the Photonuclear Data Center, where the issuance of evaluated photonuclear data should be of value in solving problems concerned with nuclear reactor safety and controlled thermonuclear research (CTR) materials. The updated version of NSRDS-NBS 29, "Photon Cross Sections, Attenuation Coefficients and Energy Absorption Coefficients from 10 KeV to 100 GeV," which will be completed in 1978, will also help improve reactor shielding technology and other radiation transport applications.

Other projects, such as the 7th edition of the Table of Isotopes, as well as an updated version of Nuclear Spins and Moments, should reach completion during FY 1977. The close relationships developed with ERDA and two newly-created nuclear data advisory panels will assure continued useful effort in these areas.

The energy program has also been expanded with the inclusion of the activities of the Atomic Energy Levels Data Center and the Transition Probabilities Data Center, whose data evaluations are used in the solution

of CTR problems. Recent publications on the energy levels of all 26 ionization states of iron, and the forthcoming issues on chromium, manganese, and the rare earths are examples of such useful data products. Similarly, transition probabilities for many stages of ionization of vanadium, chromium, manganese, and iron are being compiled and critically evaluated for publication in FY 1977. A critical compilation of electron collision cross section data for hydrogen and alkali metal atoms is being assembled by the Atomic Collision Cross Section Information Center to aid in modelling of MHD plasmas.

In the area of energy source utilization pertinent thermodynamic and physical properties data for a coal gasification handbook are being assembled. This project is described under the Industrial Process program. A new data center dealing with the thermodynamics of geological materials has just become affiliated with the NSRDS and should help to provide reliable data for R&D on geothermal energy. Some data outputs of the Aqueous Electrolyte Data Center should also be of use in this area. These, too, are more fully described under the Industrial Process program. The Chemical Kinetics Information Center has issued a bibliography entitled, "Chemical Kinetics of the Gas Phase Combustion of Fuels," and a project is now under way aimed at extrapolating kinetic rate data measured at room temperature to high temperatures where combustion reactions take place. Yet another project is evaluating rate data on reacting of electronically excited atomic and molecular species.

Finally, a sizable program has been launched in the area of energy conservation. The Lawrence Livermore Laboratory has requested the OSRD to use its data center resources for gathering evaluated data on materials designated for use in electrical, mechanical, and chemical storage devices. These evaluated data are to be entered into an automated data storage and retrieval file for use by scientists and engineers who are designing energy systems. To date, contracts have been let with the Molten Salts Data Center to evaluate selected molten salt systems proposed for use in storage batteries and fuel cells. The Plastics Technical Evaluation Center is examining mechanical properties data on composite materials for flywheels. Data on other energy storage systems, such as chemical storage of hydrogen, are under consideration.

OSRD program activities relevant to energy data should continue to expand as new technological breakthroughs occur in fields such as solar and fossil fuel utilization. Industrial emphasis on gaining increased efficiencies in energy use will be aided by more reliable data. These, in turn, must come from a harder evaluative look at the numerical data now extant in the literature.

B. Environmental Data Program

The capability previously established in the NSRDS in areas of gas kinetics and thermodynamics has permitted the OSRD to move expeditiously into data projects in aid of environmental research. For example, it was possible to select and apply evaluated thermodynamic data on waste materials to the design and operation of incinerators. Similarly, evaluated kinetic rate data on gas phase reactions of simple compounds could be selected and used to model their behavior as pollutants in the stratosphere. The task of compiling and evaluating data on pollutant behavior in the water environment is more difficult because of the size of the effort and the more complicated behavior of pollutants in water. A start has been made to identify data needs through close associations with the EPA and the Geological Survey.

Efforts by the Chemical Kinetics Information Center to furnish reliable kinetic rate data on reactions affecting the destruction of the stratospheric ozone layer continue. A series of evaluated data tables issued by the Center were used by the NAS-NRC Committee on Atmospheric Pollution in issuing its report recommending a plan for dealing with the ozone depletion problem. An important data compilation related to this problem and dealing with the rate constants of ClO reactions will appear in an early issue of the JPCRD. x

Projects to study the reaction kinetics of the combustion of fossil fuels have been initiated. While aimed primarily at an improvement in energy technology, such efforts also relate to modelling pollutant behavior in the atmosphere. Close liaison is maintained with data evaluation projects, both in the United States and in the United Kingdom, which are concerned with lower atmospheric pollution.

Several data projects dealing with problems related to water pollution have been established. An NAS ad hoc panel was convened to consider needs and priorities for water pollution data. A series of recommendations emerged dealing with both the inorganic and organic trace constituents now found in water. Specific requirements for the physical properties of many of the compounds were cited as needed for input to mathematical models used to describe the origins, reactions, and ultimate fate of these constituents in the water environment. High on the list of priorities was pollutant compound solubility. As a consequence, two projects on the solubilities and solubility products of inorganic materials in water are under way. A third, dealing with activity coefficients of inorganic compounds, is being pursued in the Aqueous Electrolyte Data Center. A report containing evaluated activity coefficient data for the alkaline earth halides is scheduled for publication in the JPCRD. All of the solubility efforts are being coordinated with the IUPAC Solubility Data Panel so that duplicative efforts are avoided.

A symposium on Pollutant Transport and Transformation in the Water and Soil Environment was sponsored jointly by the OSRD and the EPA Environmental Research Laboratory. The program was arranged to detail the state of knowledge concerning the various pollutants and their movement in soil and water. Included on the agenda were the results of an OSRD-sponsored data evaluation project which reviewed the hydrolysis rate constants of selected organic compounds in water under environmental conditions. The report is scheduled for publication in the JPCRD. A related data compilation produced by the Radiation Chemistry Data Center deals with the reaction rates of the hydroxyl radical with organic and inorganic compounds in water. Some symposium papers describing the use of mathematical models to follow pollutant behavior in the water and soil environment tended to confirm the lack of detailed information and data on these substances. It helped focus the attention of the participants on the need for additional pollutant physical properties data to improve the ability of models to predict pollutant behavior. A further lack of knowledge was cited regarding pollutant-soil interaction, both as soil aggregate and as particulates suspended in water. Copies of the program and extended abstracts are available from the National Technical Information Service (PB 257347).

As a follow-up to the symposium, an ad hoc panel on Pollutant/Soil Data Needs was convened to see where useful initiatives could be taken. While acknowledging that preliminary data activities could be pursued, the panel recommended a cautious approach to what they viewed as a complex problem. Discussions with knowledgeable scientists concerning useful data projects in this area are continuing.

The efforts described above have been possible because of existing data center activity in data projects related to the subject of energy and the environment. This storehouse of basic physical properties data and the associated scientific expertise represented in the data centers could be applied on short notice to newly identified problems. Continuation of such long-term data evaluation activities is planned to provide the versatility required for near-term data projects.

INDUSTRIAL PROCESS DATA

As is explained in more detail elsewhere in this report, the management of the National Standard Reference Data System has been reorganized to reflect major categories of utilization rather than the disciplinary categories used previously.

In formulating a program to provide Industrial Process Data, use was made of the results of an extended series of interviews with individuals in industrial organizations who are responsible for provision of reference data within their companies as well as with design engineers. It was clear that the most-used data are thermodynamic data and data on thermophysical and transport properties. The thermodynamic data include both the enthalpies and Gibbs energies of formation which are used to determine the equilibrium constants of chemical reactions and the PVT properties, enthalpies, and heat capacities of compounds which are needed to determine their physical behavior at different temperatures and pressures. The need for data on mixtures was particularly stressed, and the program in this area has been increased recently. Another area of need, particularly in the metallurgical field, is the area of phase diagrams. These can logically be considered thermodynamic data, but are often treated separately for emphasis as is the case here.

Data on enthalpies and Gibbs energies of formation are provided by the Chemical Thermodynamic Data Center at NBS, Gaithersburg, and by the Thermodynamics Research Center at Texas A&M University. Data on the PVT and related thermodynamic properties of fluids are provided by projects in the Cryogenics Division of NBS, Boulder, and the Heat Division of NBS, Gaithersburg, as well as at the University of Maryland. Mixture data are provided by the Aqueous Electrolyte Data Center at NBS, Gaithersburg, the Cryogenic Fluid Mixtures Data Center at NBS, Boulder, and the Thermodynamics Research Laboratory at Washington University in St. Louis. Transport properties are covered in the Cryogenics Division, NBS, Boulder, and CINDAS, Purdue University. For more detailed information on these and other projects in the Industrial Process Data Program, the reader is referred to the appendices of this report.

In keeping with increasing emphasis on Industrial Process Data, the Alloy Data Center has shifted its primary emphasis to phase diagrams of alloys and intends to become a major data activity in this field. This reprogramming starts to fill a serious gap in NSRDS coverage which has existed for several years. The activities of the Alloy Data Center will reinforce those of the project on Phase Diagrams for Ceramists which is supported by the American Ceramics Society.

The two groups, together with the Office of Standard Reference Data, combined to organize a Workshop on Applications of Phase Diagrams in Metallurgy and Ceramics which was held at NBS, January 10-12, 1977. This workshop was intended to initiate a more integrated program of data evaluation and measurement worldwide. It was well attended and enthusiastically received.

A new data center, the National Center for the Thermodynamic Data of Minerals, has been established as part of the NSRDS by the U.S. Geological Survey at Reston, Virginia. This center will provide thermodynamic data on minerals for the geochemical community, and these data will also be of industrial importance for a great many uses in metallurgy and the preparation and production of inorganic chemicals.

The utilization categories should not be thought of as rigid technical divisions. It is clear that the data produced by the thermodynamic centers will be of use in many ways in the solution of problems in other utilization areas, especially in the energy and pollution control areas. In addition to the general utility of the data produced, specific data compilations are being prepared by some of the thermodynamic centers in response to specific energy or pollution-control problems. Among these may be listed the project to compile thermodynamic data for industrial and municipal incinerator design in the Chemical Thermodynamic Data Center under the sponsorship of the ASME, the project to provide a compilation of thermophysical and thermodynamic properties of chemical compounds derivable from coal which is being carried out by the Thermodynamic Research Center under the sponsorship of the Institute of Gas Technology, the compilation of thermodynamic data on selected reactions that might occur in the stratosphere by the Chemical Thermodynamic Data Center under DOT sponsorship, and the compilation of thermochemical data on the reactions of selected substances containing heavy metal ions in aqueous systems being done by the Aqueous Electrolyte Data Center. The range and variety of these projects illustrate clearly how the combined resources of the various thermodynamic data centers make it possible for them to provide specific data compilations for many different, specific purposes as well as provide the wide-ranging basic data compilations that are their primary products and are useful for many users and purposes.

In a similar fashion, data centers in other utilization categories can, and are expected to, make important contributions to the Industrial Process Data field. The Chemical Kinetic Information Center, the Molten Salts Data Center, and the Ion Energetics Data Center can be mentioned in particular. The last, as the name would suggest, produces thermodynamic data on ionic species, although the data are not obtained by conventional thermodynamic methods.

The production of data compilations to aid in the solution of specific problems is discussed above. In addition to designing compilation projects to serve in the solution of individual problems, it often proves possible to use data compiled and evaluated for other purposes, often as part of the basic data compilation activities of one or several centers to produce a compilation tailored to the needs of a specific set of users. The data are repackaged to conform with usage in the field in question.

An example of a project of this genre is the project to prepare an LNG Handbook. This handbook will incorporate data on Liquefied Natural Gas, its components, and other substances, which have been measured, compiled, and evaluated for a number of purposes, into a useful engineering handbook.

MATERIALS UTILIZATION DATA

In developing a data program relevant to materials utilization interests, the OSRD has tried to take full advantage of the earlier planning for Mechanical Properties data, one of the seven categories which composed the original scope of the National Standard Reference Data System. At the same time, the program is shaped to a substantial degree by the capabilities of a number of on-going materials-related data projects which were formerly included in the Solid State Data portion of the NSRDS. These latter projects stressed crystallographic data, superconductive materials, certain aspects of metallurgy, and optical properties of solids relevant to laser research. The productivity of these existing projects has been well demonstrated, and a significant level of user expectation exists for NBS to continue to supply the data they need. Accordingly, the present Materials Utilization Data program and the plans for its possible expansion contain elements from both sources.

In 1964 an ad hoc NBS panel drafted a list of mechanical properties which seemed likely candidates for inclusion in the NSRDS Program. Financial limitations precluded the initiation of any systematic program in this area, and further formal planning was postponed for several years. In 1971, one of the OSRD advisory groups recommended (without ignoring budgetary restrictions) that "the office should give serious consideration to extending its activities to engineering areas, such as mechanical properties, electrical properties, environmental studies, and others."

In response, OSRD undertook a new planning effort which started with a review of the 1964 list and involved discussions with a number of materials research specialists to determine which properties were well enough defined to warrant consideration. This review yielded tentative lists of properties for metals, ceramics, glasses, polymers, and liquids (gases were included in the Thermodynamics and Transport Properties data area), which were then circulated to a larger group including users and producers.

The comments and suggestions which resulted were used in the formulation of a detailed program. Key guidelines included the following:

- Output should be useful to all who need and use mechanical properties data, including scientists, engineers, and designers;
- Material of transitory interest should be excluded;
- Information being produced by others should not be duplicated;
- Base or key values should be emphasized;
- A somewhat pragmatic interpretation of the NSRDS guideline, "well-defined properties," should be adopted in regard to mechanical behavior;
- Outside of the categories of single crystals and ordinary (low molecular weight) liquids, the major limitation on reproducibility of the values of most mechanical properties seems to be our ability to characterize the materials.

OSRD staff concluded that critical reviews would play a large part in the mechanical properties program. A number of comments suggested including papers designed primarily to describe the use of relatively new material properties (like plane strain fracture toughness). It appeared also that annotated lists of information sources would be useful, since present lists generally do not identify in a specific fashion the information available from each source.

As a result of this planning work, OSRD undertook support of three data initiatives in 1973-5:

- a) a series of reviews on elastic constant data for metals and alloys;
- b) a book on "Fracture Toughness Testing and Data with Reference to Meaning and Applications;"
- c) a series of critical surveys of data sources, covering selected materials and properties.

This three-part program was well under way, and already productive when OSRD restructured its management organization to achieve a better match with data needs of major national problem areas. One of the four new program areas was Materials Utilization Data, which as noted above, subsumed all of the Mechanical Properties efforts, plus several of the projects formerly within the area of Solid State Data.

Planning for the Materials Utilization Data program did not start from scratch. At hand were the results of several major outside studies sponsored by:

- a) the National Commission on Materials Policy,
- b) the National Academy of Sciences-National Academy of Engineering,
- c) the Committee on the Survey of Materials Science and Engineering,
- d) the Federation of Materials Societies, the Office of Technology Assessment, and other bodies.

These and other sources provide ample identification of specific needs for reliable materials properties data. A major data compilation and evaluation program can be developed on this basis if funds become available to support it. Anticipating that only partial funding will be available in the short term, closer scrutiny is required to set priorities, develop cooperative projects, define deficiencies in existing outside data programs, and estimate areas of greatest potential impact. Such a study is in process, and the results will be incorporated in the future plans for an enlarged program.

The study includes the following elements:

- a) Discussion with industrial users and suppliers of materials data;
- b) Discussions with managers of present major data projects operated by professional societies and cooperative industrial groups;
- c) Conversations with Deans and Professors of Engineering (especially mechanical and design engineering) at major universities and technological institutes;

- d) Participation with National Science Foundation in pilot studies of how engineers use data on the job;
- e) Convening of several small groups of scientists and engineers in special materials areas, to focus on details of present and future data needs--e.g., high-strength ceramics; synthetic polymers; composites, etc.

In terms of present status, the Materials Utilization Data program may be viewed as a rather scattered array of productive projects ranging across the whole spectrum of already-perceived user needs. The projects on crystallographic data serve the research community well, and are developing additional outputs to meet applied needs (analytical systems, compound identification via X-ray diffraction, etc.) as well. The series of four Critical Surveys of Data Sources has been completed, and users have expressed approval of the original concept as well as the results. The projects on diffusion in metals and on elastic constants of metals are concerned with key values of broad interest, where NBS competence can make a unique contribution. The project on fracture mechanics is a prototype effort--an early attempt to systematize the data aspects of a recently-developed field with broad relevance to both theoretical understanding and practical applications.

In summary, the present materials data program is a good starting place, a strong base on which to build.

PHYSICAL SCIENCE DATA

The previously-described portions of the NSRDS program are presented in terms relating to general or specific applications. While OSRD recognizes and emphasizes that many of its data outputs are very broadly useful in application to many different types of problems, it remains appropriate to place most of the projects in one particular category.

There are some projects, however, whose content is so universal, or so clearly focussed on frontier research, that assignment to a single problem-related area would be inappropriate. These projects comprise the final NSRDS program area, which has been given the rather vague title of Physical Science Data. By intent, the number of projects in this area remains small. Directly or indirectly, however, the data output of this area has a very large cumulative impact both on users and on the rest of the data program.

**FEDERAL COUNCIL FOR SCIENCE AND TECHNOLOGY
COMMITTEE ON SCIENTIFIC INFORMATION**

28 May 1963

Federal Policy on National Standard Reference Data System

There will be established a National Standard Reference Data System (NSRDS) to provide on a national basis critically evaluated data in the physical sciences. The NSRDS will consist of a National Standard Reference Data Center (NSRDC) at the National Bureau of Standards and such other Standard Reference Data Centers as may be required.

The National Bureau of Standards will be charged with the administration of the National Standard Reference Data System. This assignment will include the establishment of standards of quality, methodology including machine processing formats, and such other functions as are required to ensure the compatibility of all units of the NSRDS.

The National Bureau of Standards will be charged with funding and administering the National Standard Reference Data Center. This Center will be an identifiable part of the National Scientific and Technical Information System (NSTIS).

Standard Reference Data Centers covering certain specific areas of effort may be established by or be assigned to the various Departments and Agencies in accordance with their specific desires and capabilities. Such Centers will be financed and administered by the Department to which assigned but will meet the quality standards and other requirements of the NSRDS. Such Centers will be included as identifiable components of the NSTIS.

The NSRDS may also include Standard Reference Data Centers at universities, research institutes, and other appropriate non-Government activities. To be included in the NSRDS, such Centers will meet the quality standards and other requirements of the NSRDS and will be included as identifiable components of the NSTIS.

There will be an Advisory Board to review and recommend policy relative to the operation of the NSRDS. It will include among others, representation from the National Academy of Sciences, National Science Foundation, Federal Agencies engaged in research and development, and such other representatives of the scientific and technical community as the Director of the National Bureau of Standards may determine.

In establishing the NSRDS, the intent is to provide an articulated system of Centers and activities under such coordination and direction as to ensure an output meeting quality standards for national reference data in the physical sciences. The establishment of the System should not be construed as preventing the establishment of such Federal or Departmental Data Systems as are required for the collection of raw or evaluated data to serve engineering or operating needs of the Federal Government or various Federal agencies.



Public Law 90-396
90th Congress, H. R. 6279
July 11, 1968

An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

Standard Reference Data Act.

DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy.

82 STAT. 339
82 STAT. 340

DEFINITIONS

SEC. 2. For the purposes of this Act—

(a) The term "standard reference data" means quantitative information, related to a measurable physical or chemical property of a substance or system of substances of known composition and structure, which is critically evaluated as to its reliability under section 3 of this Act.

(b) The term "Secretary" means the Secretary of Commerce.

SEC. 3. The Secretary is authorized and directed to provide or arrange for the collection, compilation, critical evaluation, publication, and dissemination of standard reference data. In carrying out this program, the Secretary shall, to the maximum extent practicable, utilize the reference data services and facilities of other agencies and instrumentalities of the Federal Government and of State and local governments, persons, firms, institutions, and associations, with their consent and in such a manner as to avoid duplication of those services and facilities. All agencies and instrumentalities of the Federal Government are encouraged to exercise their duties and functions in such manner as will assist in carrying out the purpose of this Act. This section shall be deemed complementary to existing authority, and nothing herein is intended to repeal, supersede, or diminish existing authority or responsibility of any agency or instrumentality of the Federal Government.

Collection and publication of standard reference data.

SEC. 4. To provide for more effective integration and coordination of standard reference data activities, the Secretary, in consultation with other interested Federal agencies, shall prescribe and publish in the Federal Register such standards, criteria, and procedures for the preparation and publication of standard reference data as may be necessary to carry out the provisions of this Act.

Standards, etc. Publication in Federal Register.

SEC. 5. Standard reference data conforming to standards established by the Secretary may be made available and sold by the Secretary or by a person or agency designated by him. To the extent practicable and appropriate, the prices established for such data may reflect the cost of collection, compilation, evaluation, publication, and dissemination of the data, including administrative expenses; and the amounts received shall be subject to the Act of March 3, 1901, as amended (15 U.S.C. 271-278e).

Sale of reference data. Cost recovery.

SEC. 6. (a) Notwithstanding the limitations contained in section 8 of title 17 of the United States Code, the Secretary may secure copyright and renewal thereof on behalf of the United States as author or proprietor in all or any part of any standard reference data which

31 Stat. 1449; Ante, p. 34. U. S. copyright and renewal rights. 61 Stat. 655; 76 Stat. 446.

he prepares or makes available under this Act, and may authorize the reproduction and publication thereof by others.

(b) The publication or republication by the Government under this Act, either separately or in a public document, of any material in which copyright is subsisting shall not be taken to cause any abridgment or annulment of the copyright or to authorize any use or appropriation of such material without the consent of the copyright proprietor.

Appropriation.

SEC. 7. There are authorized to be appropriated to carry out this Act, \$1.86 million for the fiscal year ending June 30, 1969. Notwithstanding the provisions of any other law, no appropriations for any fiscal year may be made for the purpose of this Act after fiscal year 1969 unless previously authorized by legislation hereafter enacted by the Congress.

Short title.

SEC. 8. This Act may be cited as the "Standard Reference Data Act."

Approved July 11, 1968.

LEGISLATIVE HISTORY:

HOUSE REPORT No. 260 (Comm. on Science and Astronautics).

SENATE REPORT No. 1230 (Comm. on Commerce).

CONGRESSIONAL RECORD:

Vol. 113 (1967): Aug. 14, considered and passed House.

Vol. 114 (1968): June 13, considered and passed Senate,
amended.

June 27, House concurred in Senate
amendments.

APPENDIX II. LIST OF DATA CENTERS AND PROJECTS

Listed below are all of the continuing data centers and short-term projects which receive at least a part of their support from the Office of Standard Reference Data. Corresponding to the general analysis presented in Section IV of this Report, data activities in the Energy and Environmental Data program are subdivided into two portions. A supplementary list of continuing data centers in the United States which are recognized as part of NSRDS (even though they do not receive direct financial support from NBS) follows the project descriptions in each program area.

ENERGY DATA

1. Title: Atomic Energy Levels Data Center
Location: Optical Physics Division, NBS, Washington, D.C. 20234
Project Leader: W. C. Martin
Description: This data center issues bibliographies and critical data evaluations on atomic energy levels and spectra in support of programs involving plasma physics (MFE), laser development, and space astrophysics. The center is currently working on energy level evaluations for all spectra of the iron group elements.
2. Title: Transition Probabilities Data Center
Location: Optical Physics Division, NBS, Washington, D.C. 20234
Project Leader: W. L. Wiese
Description: The data center collects, compiles, and issues data evaluations and bibliographies on transition probabilities and atomic line shapes and shifts. These data are used in support of programs related to fusion power, plasma behavior, and astrophysics. The center's current activity is concentrated on producing tables of data on iron, vanadium, chromium, and manganese.
3. Title: Atomic Collision Cross Section Information Center
Location: Laboratory Astrophysics Division, NBS Boulder, Boulder, Colorado 80302
Project Leader: E. C. Beaty
Direct Inquiries To: J. R. Rumble
Description: The data center collects, compiles, and issues data evaluations on low energy collision cross sections for electrons and photons with atoms and molecules. Bibliographies on these subjects are also issued as required. A numerical data file is maintained. The data are used in support of programs dealing with laser and MHD technology. An evaluated data compilation on electron collision cross sections for the alkali metal atoms is currently being written and is planned for publication in 1978.
4. Title: Photonuclear Data Center
Location: Center for Radiation Research, NBS, Washington, D.C. 20234
Project Leader: E. G. Fuller
Description: This data center systematically abstracts, collects, and indexes data from the published literature; maintains a library of digitized cross section data; and serves as an information center for the field of photonuclear physics. A literature file from 1955 contains over 2000 journal papers; the data abstract files contain information on over 4800 separate measurements, and the digital library contains data for over 700 cross section curves. A comprehensive compilation of evaluated photonuclear reactions cross section data is being prepared.

5. Title: X-ray and Ionizing Radiation Data Center
Location: Center for Radiation Research, NBS, Washington, D.C. 20234
Project Leader: J. H. Hubbell
Description: The data center is concerned with standard reference data on the interactions of X-rays, gamma-rays, and charged particles with atoms and molecules and with bulk matter. The purpose is to provide information needed for the safe and efficient use of these radiations in nuclear energy technology, medicine, and national defense applications. While most of the center's work has been concentrated in the area of X-ray cross sections, added emphasis is now being given to the compilation of charged particle cross sections and of radiation transport data for engineering applications.
6. Title: Molten Salts Data Center
Location: Rensselaer Polytechnic Institute, Troy, New York 12181
Project Leader: G. J. Janz
Description: This center compiles and evaluates data on molten-salt systems. The properties covered are density, electrical conductivity, viscosity, surface tension, reversible electrode potentials, and to some extent vapor pressure. At the present time, the first four properties are being covered for binary-salt systems. Reports on halide mixtures, bromides, and iodides are in press.
7. Title: Kinetics of High Temperature Reactions
Location: 3130 Coronado, Santa Clara, California 95051
Project Leader: Robert Shaw
Description: This project attempts to develop a basis for extrapolating kinetic rate constant data to high temperatures where experimental data are lacking. A series of atom transfer reactions involving oxygen, hydrogen, and methane are being used as models for developing Arrhenius parameters for calculating the reaction rate constants.
8. Title: Reaction Rate Data for Electronically Excited Atoms and Molecules
Location: ChemData Research, 260 Loma Media, Santa Barbara, California 93103
Project Leader: K. Schofield
Description: This project compiles and evaluates reaction rate data on electronically excited atoms and molecules for application in chemical laser technology. A manuscript covering relaxation rates, radiative lifetimes, and reaction mechanisms for 13 excited species has been prepared for publication.
9. Title: Table of Isotopes
Location: Lawrence Radiation Laboratory, University of California, Berkeley, California 94720
Project Leader: C. Michael Lederer
Description: This project compiles and will publish in calendar 1977 the 7th edition of the "Table of Isotopes." The publication will furnish updated (1974) evaluated data on radioactive decay and nuclear structure properties for all nuclei as applied variously in medicine, chemical technology, and other areas. This effort will continue to furnish ERDA and the nuclear scientific community-at-large with updated evaluated data on the radioactive properties of the isotopes.

10. Title: Fundamental Vibration Frequencies of Molecules
Location: Department of Physical Chemistry, University of Tokyo, Tokyo, Japan
Project Leader: T. Shimanouchi
Description: This project provides continuing preparation and publication of tables of data of the fundamental vibration frequencies of molecules. Spectroscopic measurements reported in the open literature are collected, selected, analyzed, and evaluated to provide consistent and intercomparable data. Tables are published in sets (of about 50) bringing together data on molecules of similar structure and symmetry. The preparation of a second consolidated volume of tables, updating material from the last four sets of tables, has been completed and will be published in 1977.
11. Title: Index to High Resolution Spectral Data
Location: Optical Physics Division, NBS, Washington, D.C. 20234
Project Leader: Paul H. Krupenie
Description: This project provides for the compilation and dissemination of high resolution infrared spectral data for gases. The output of this project will be an index to high resolution measurements which will be useful for the application of lasers to many scientific fields of interest. Current effort is being directed to the indexing of diatomic and triatomic molecules.
12. Title: Molten Salts Data for Energy Storage Application
Location: Rensselaer Polytechnic Institute, Troy, New York 12181
Project Leader: G. J. Janz
Description: The Molten Salts Data Center is providing evaluated properties data on selected molten salt systems for use in energy storage systems. The data are to be delivered to Lawrence Livermore Laboratory for processing into a computerized file for automated retrieval. To date, three data sets have been delivered to Livermore. When complete, 26 salt systems and 15 properties will have been covered.
13. Title: Composite Materials Data for Energy Storage Application
Location: Plastics Technical Evaluation Center, Picatinny Arsenal, Dover, New Jersey 07801
Project Leader: H. E. Pebly
Description: The Plastics Technical Evaluation Center will compile and evaluate physical properties data on selected fiber and matrix materials for use in flywheel energy storage devices. Sixteen fibers, 19 matrix materials, and 27 properties are involved. The project is being pursued in two steps and will result in data sheets describing the properties of each material. These in turn will be delivered to Lawrence Livermore Laboratory (LLL) for insertion into a computerized file for automated retrieval.
14. Title: Solid Electrolyte Material Data for Energy Storage Application
Location: University of Utah, Salt Lake City, Utah 84112
Project Leader: Gerald Miller
Description: This project will compile and evaluate data on sodium β and β'' alumina which find use as solid electrolytes in battery systems. Nine physical properties will be documented. The data will be recorded on data sheets and transmitted to Lawrence Livermore Laboratory (LLL) for insertion into a computerized file for automated retrieval.

15. Title: Metal Properties Data for Energy Storage Application
Location: Cryogenics Division, NBS Boulder, Boulder, Colorado 80302
Project Leader: H. M. Ledbetter
Description: This project will compile and evaluate physical properties data on candidate metals for use in flywheel energy storage devices. Twenty-six materials and eleven properties are involved. The data will be delivered to Lawrence Livermore Laboratory (LLL) for insertion into a computerized file for automated retrieval.

The following data centers, not directly under NSRDS program management, also supply evaluated data relevant to this area of interest:

1. Title: Nuclear Data Project
Location: Oak Ridge National Laboratory, P.O. Box X, Oak Ridge, Tennessee 37830
Project Leader: B. Ewbank
Description: Data on the physics of nuclear structure and other nuclear properties. Emphasis is placed on evaluated energy level data for nuclides of $A > 40$.
2. Title: National Nuclear Data Center
Location: Brookhaven National Laboratory, Upton, New York 11973
Project Leader: S. Pearlstein
Description: Data on neutron- and charged-particle-induced nuclear reactions, structural data, and related parameters, consisting mainly of energy and angle dependent cross sections for use in reactor design, neutronics calculations and nuclear physics studies are compiled and disseminated.
3. Title: Physical Data Group
Location: Lawrence Radiation Laboratory, University of California, Livermore, California 94550
Project Leader: Robert F. Howerton
Description: Neutron and photon cross section data required for weapon effects, shielding and reactor calculations; static and dynamic parameters of critical assemblies and bulk experiments relating to neutron multiplication and transport are compiled.

ENVIRONMENTAL DATA

1. Title: Chemical Kinetics Information Center
Location: Physical Chemistry Division, NBS, Washington, D.C. 20234
Project Leader: R. F. Hampson, Jr.
Description: This data center abstracts and compiles chemical kinetic data from the literature. The center has recently prepared and issued tables of rate data for use in atmospheric modelling. It provides bibliographic services to the public, evaluates gas phase reaction rate and photochemical data, coordinates preparation of text on the chemistry of the stratosphere, and participates in international activities in the area of chemical kinetics.
2. Title: Radiation Chemistry Data Center
Location: Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana 46556
Project Leader: Alberta Ross
Description: The center's objectives are to compile, evaluate, and disseminate reviews of data from radiation chemistry. The project has developed an automated literature reference file pertinent to radiation chemistry. In addition to maintaining a searchable file (over 22,000 papers since 1966), and the issuance of a bi-weekly current-awareness publication and some bibliographies, the center prepares data compilations as input to critical reviews. A review entitled "Selected Specific Rates of Reactions of Transients from Water in Aqueous Solution. III. Hydroxyl Radical and Perhydroxyl Radical and Their Radical Ions" has just been published as NSRDS-NBS 59. (This center is funded under a joint agreement between NBS and the Energy Research and Development Administration.)
3. Title: Ion Energetics Data Center
Location: Physical Chemistry Division, NBS, Washington, D.C. 20234
Project Leader: H. M. Rosenstock
Description: This data center compiles, evaluates, and disseminates data on the energy of formation of all gaseous ions. The data are published in aid of developing analytical methods of measurement and modelling of atmospheric behavior. A comprehensive update of NSRDS-NBS 26, entitled "Energetics of Gaseous Ions," has just been published as a supplement in the Journal of Physical and Chemical Reference Data. Future efforts will be directed toward improving the data file as an automated system.
4. Title: Solubility Data of Inorganic Substances in Water, Part I
Location: Emory University, Atlanta, Georgia 30322
Project Leader: H. L. Clever
Description: This project will compile and evaluate the aqueous solubility data on selected metal salts and complexes, specifically Cu, Zn, Cd, Hg, Sn, Pb, and Sb. Solubility as a function of temperature will be evaluated where available. The results will be published in the Journal of Physical and Chemical Reference Data. This effort is closely coupled with Solubility Data, Part II, and follows the ongoing activities of the IUPAC Solubility Data Committee. (This collaboration between groups is designed to avoid duplicative effort.)

5. Title: Solubility Data of Inorganic Substances in Water, Part II
Location: Virginia Polytechnic Institute, Blacksburg, Virginia 24061
Project Leader: A. F. Clifford
Description: This project will compile and evaluate the aqueous solubility data on selected metal salts and complexes, including the alkali and alkaline earth metals and the transition metals. Where available, the data will also be evaluated as a function of temperature. The results will be published in the Journal of Physical and Chemical Reference Data. This project is closely coupled with the Solubility Data, Part I, and follows the ongoing efforts of the IUPAC Solubility Data Committee. (This collaboration between groups is designed to avoid duplicative effort.)
6. Title: Infrared Spectral Data for Environmental Applications
Location: The Coblenz Society
Project Leader: C. D. Craver
Direct Inquiries To: C. D. Craver, Chemir Laboratories, 761 West Kirkham, Glendale, Missouri 63122
Description: This project will collect, evaluate, and disseminate infrared spectra on materials encountered in the environment. Emphasis will be given to spectra on halogenated hydrocarbons, industrial plasticizers, and plastic additives and coatings. The data are required to improve the analyst's ability to detect and identify these substances. The product spectra will be added to a growing body of authoritative collections of spectra already issued through the Coblenz Society.
7. Title: Rate Constant Data on Hydrolysis of Organic Compounds
Location: Stanford Research Institute, Menlo Park, California 94025
Project Leaders: T. Mill and W. Mabey
Description: This project compiles and evaluates the hydrolysis rate constants of organic, pollutant-like compounds found in aqueous media. They include alkyl halides, esters, anhydrides, epoxides, amides, etc. The results will be published in the Journal of Physical and Chemical Reference Data.
8. Title: Ion-Molecule Reaction Rate Data
Location: Physical Chemistry Division, NBS, Washington, D.C. 20234
Project Leader: L. W. Sieck
Description: This project collects and evaluates ion-molecule reaction rate data used by modellers to describe effects in the normal and disturbed atmosphere. Attention is given to those reactions involving air pollutants. The results are published in the Journal of Physical and Chemical Reference Data. Work on Part II of a three-part series is in progress.
9. Title: NMR Data Compilation
Location: Department of Chemistry, Texas A&M University, College Station, Texas 77843
Project Leader: B. L. Shapiro
Description: This project is directed to the compilation, evaluation, and publication of data derived from high-resolution proton NMR spectroscopy (chemical shifts and coupling constants) on aromatic molecules in which the proton is attached directly to an aromatic carbon atom. The results are to be published in the Journal of Physical and Chemical Reference Data in 1977.

Addendum to Aqueous Electrolyte Data Center

A portion of the work of the Aqueous Electrolyte Data Center (see Appendix IIC, Item 12) is explicitly devoted to compilation of data for environmental problems. A review entitled "Evaluated Activity and Osmotic Coefficients for Aqueous Solutions: The Alkaline Earth Metal Halides," by R. N. Goldberg and R. L. Nuttall, will be published in the Journal of Physical and Chemical Reference Data.

The following data center, not directly under NSRDS program management, also supplies evaluated data relevant to this area of interest:

1. Title: AP144-TRC Selected Spectral Data

Location: Thermodynamics Research Center, Texas A&M University, College Station, Texas 77843

Project Leader: B. J. Zwolinski

Description: Infrared, ultraviolet, mass Raman, and nuclear magnetic resonance spectroscopic data on organic and inorganic compounds are compiled and disseminated.

INDUSTRIAL PROCESS DATA

1. Title: Chemical Thermodynamics Data Center
Location: Physical Chemistry Division, NBS, Washington, D.C. 20234
Project Leader: D. Wagman
Description: This center compiles data on the chemical thermodynamic properties of chemical substances on a continuing basis. These data are needed to calculate energy changes and product yields in chemical reactions in manufacturing, energy conservation, nuclear technology, environmental systems, and laboratory experiments.

Data on inorganic and selected organic substances are being evaluated to provide tables of enthalpies, and Gibbs energies of formation in their standard states at 298.15K; of the enthalpy, entropy, Gibbs energy and Cp at 298.15K; and of the enthalpy of formation at OK to the extent that the data will permit. These tables are published serially in the NBS Technical Note 270 Series.

The center's activities are highly automated. The center provides the inorganic section, the overall substance-property index, and the final copy for the Bulletin of Thermodynamics and Thermochemistry each year. New techniques for using computer solutions for large sets of equations are being developed to provide self-consistent sets of chemical thermodynamic data. These developments are being carried out jointly with workers in the United Kingdom. Other projects involving exchanges of computerized information are being carried out with workers in the USA and elsewhere.

In another cooperative program under the auspices of CODATA, key values for selected substances are being prepared jointly with a group at the Institute for High Temperatures in Moscow under the direction of an international advisory committee.

The center is currently nearly finished with the evaluation of the data for the actinide elements. This work has been carried out jointly with a group sponsored by the IAEA. The center has provided all data on non-actinide compounds needed by the IAEA group and will be involved with insuring the thermodynamic self-consistency of both sets of tables. Work on substances containing the alkali metals is well advanced.

2. Title: Thermodynamic Data for Industrial and Municipal Incinerator Processes
Location: Physical Chemistry Division, NBS, Washington, D.C. 20234
Project Leader: E. Domalski
Description: Tables developed in a previous project were incorporated in a book entitled Combustion Fundamentals for Waste Incineration, sponsored by the ASME Research Committee on Industrial and Municipal Wastes. This book provided thermodynamic information for incinerator designers and process engineers. In particular enthalpy of formation data were provided on materials identifiable by a single stoichiometric formula. However, there are other substances such as wood, newspapers, tires, etc., for which heat of combustion data may be available, and which often are processed through incinerators. This project is designed to extend the tables in the handbook to include data on such materials. The files of the Chemical Thermodynamics Data Center will be used for this project.

3. Title: Thermodynamic Data on Organic Compounds
Location: Texas A&M University, College Station, Texas 77843
Project Leader: B. J. Zwolinski
Description: This is a continuing project to provide reliable and complete data on important organic compounds to meet the needs of science in general, and the chemical and petrochemical industries in particular. The center provides current awareness services, loose-leaf data sheets, publications containing tables of reference data, and other data-related products.

The center has published tables of the ideal-gas properties of the halogenated hydrocarbons containing chlorine and/or fluorine. A cooperating group has prepared tables for the bromine- and iodine-containing compounds. It is currently developing a set of thermodynamically self-consistent tables of thermodynamic properties of a set of key oxygen-containing saturated organic compounds in the carbon range C1 to C4. These compounds are key compounds that will serve as a basis for extrapolation and estimation of data for higher molecular weight chemical substances. This center also prepares the organic sections of the substance-property index and the bibliography of the Bulletin of Thermodynamics and Thermochemistry.

4. Title: Properties of Coal-Derived Compounds
Location: Texas A&M University, College Station, Texas 77843
Project Leader: B. J. Zwolinski
Description: The utilization of coal as a raw material, either for the production of gaseous or liquid fuels, or for the production of chemicals, requires knowledge of the properties of those compounds most frequently produced as the large polymeric molecules that constitute coal start to break down. The Institute of Gas Technology is preparing an engineering handbook on coal gasification, and one part of this handbook will consist of data on the thermophysical and thermodynamic properties of such compounds. The Thermodynamic Research Center of Texas A&M University is compiling the data available in the literature on the chemicals derivable from coal that are liquids or solids at room temperature. These data will be provided in a format suitable for inclusion in the IGT Handbook.

5. Title: Thermodynamic Properties of Polar Fluids
Location: Heat Division, NBS, Washington, D.C. 20234
Project Leader: M. Klein
Direct Inquiries To: L. Haar
Description: This project is concerned with the description of the PVT surfaces and derived thermodynamic properties of one component polar fluids. A formulation of the properties of ammonia from the melting line to 750K and to pressures of 10,000 atmospheres has been completed and is in press. Work is nearing completion on the ideal-gas properties of water and the data for the gaseous and liquid phases are being analyzed as a first step in preparing a new formulation for water.

6. Title: Cryogenic Data Center

Location: Cryogenics Division, NBS, Boulder, Colorado 80302

Project Leader: N. A. Olien

Description: The Cryogenic Data Center maintains a thorough and systematic review of the current published report and patent literature of importance in the cryogenic field. It compiles, evaluates, correlates, and publishes evaluated reference data on physical and chemical properties of fluids and solids of cryogenic interest. Relevant papers are entered into an automated information system which permits speedy and flexible retrospective searching. The center provides a weekly cryogenic current-awareness service and quarterly reports covering liquefied natural gas and superconductivity. Users subscribing to the center's current-awareness services or requiring major literature searches number more than 1200 per year.

7. Title: LNG Materials and Fluids Data Book

Location: Cryogenics Division, NBS, Boulder, Colorado 80302

Project Leader: D. B. Mann

Description: This project is designed to provide a data book useful to engineers faced with the design and use of equipment for the handling and transporting of liquefied natural gas (LNG). It contains data on the thermodynamic and thermophysical properties of LNG, its major components, and binary mixtures of these components. Data are also given on the mechanical properties of various metals and alloys which can be expected to be used in the fabrication of equipment to handle LNG.

The project is also sponsored by the American Bureau of Shipping, the Maritime Administration, and the American Gas Association.

8. Title: PVT and Related Thermodynamic Properties of Ethylene
Location: See below
Project Leader: H. J. White, Jr., Office of Standard Reference Data,
NBS, Washington, D.C. 20234

Description: This project is supported jointly by industrial organizations and the government. The goal is a comprehensive, high-quality, self-consistent set of densities and related thermodynamic properties of ethylene. Since the data in the literature do not allow the preparation of such a set to the level of accuracy desired, the project involves selected measurements as well.

Measurements of the density as a function of temperature and pressure in the critical region and below have been carried out by the ERDA Energy Research Center in Bartlesville, Oklahoma, and in the Heat Division of NBS, Gaithersburg. These measurements overlap to some extent in the critical region and have been carried into the supercritical region to overlap with existing data sets there. The agreement between independent measurements is excellent and, as a result of these measurements, the behavior of ethylene in the immediate critical region and in the vapor phase for 50°C below the critical region is now well established. Measurements are currently being carried out by the ERDA Energy Research Center on the speed of sound in ethylene on either side of the two-phase line; by the Cryogenics Division at NBS, Boulder, on the density of the liquid; and by the Chemical Engineering Department of the University of Michigan on the heat capacity along the two-phase line. These experimental measurements should fill the major gaps in the experimental data in the literature and permit preparation of a definitive PVT surface over a wide range of temperatures and pressures.

Support for the project has been received from the Government and the following industrial organizations:

Celanese Chemical Company
Cities Service Oil Company
Continental Oil Company
Gulf Research and Development Company
Mobil Chemical Company
Monsanto Polymers & Petrochemicals Company
Phillips Chemical Company
Union Carbide Corporation

9. Title: Thermodynamic Properties of Fluids in the Critical Region

Location: Heat Division, NBS, Washington, D.C. 20234

Project Leader: M. Klein

Direct Inquiries To: J.M.H. Levelt Sengers

Description: Experimental measurements near the critical point are difficult; properties change abruptly and have unexpected values. Recent theoretical developments have provided superior methods for formulating properties in the critical region. This project has been concerned with the further development of these methods for evaluation of thermodynamic data in the critical region. Techniques have been developed to compare different sets of measurements of the same property and to compare measurements on different thermodynamic properties so that self-consistent formulations in the critical region can be developed.

Scaling-law techniques have been used to produce an equation of state in the critical region for ^3He , ^4He , O_2 , Xe , CO_2 , Ar , Kr , N_2 , H_2 , CH_4 , C_2H_4 , SF_6 and NH_3 . This work has been published recently. Further work on water has permitted preparation of a complete thermodynamically consistent set of state and thermodynamic properties in the critical region.

10. Title: Cryogenic Fluid Mixture Properties

Location: Cryogenics Division, NBS, Boulder, Colorado 80302

Project Leader: M. H. Hiza

Description: This project is devoted to the compilation and evaluation of data on fluid mixtures with emphasis on mixtures of cryogenic fluids. A comprehensive bibliography of data for low-temperature phase equilibria, densities, and calorimetric measurements has been published. A project for the compilation, evaluation, and correlation of the data on the liquid-vapor equilibrium and orthobaric densities of mixtures of methane and ethane is nearing completion. Work is underway on other mixtures containing methane.

11. Title: Excess Property Data for Binary Liquids

Location: Thermodynamic Research Laboratory, Washington University, St. Louis, Missouri 63130

Project Leader: D. Buford Smith

Description: The Thermodynamic Research Laboratory operates a data center on excess property data for sub-critical binary liquid systems. The center compiles and evaluates data on vapor-liquid equilibrium, enthalpy of mixing, and volume change of mixing. The systems currently being studied are systems containing C_3 hydrocarbons plus heavier hydrocarbons (through C_8), C_4 hydrocarbons plus heavier hydrocarbons (through C_8) and alcohols C_1 through C_4 plus hydrocarbons (C_3 through C_8). Future work is planned to include additional classes of compounds of industrial importance.

Data compiled from the literature are screened for the scatter of measurements, the extent to which the data extrapolate to accepted values for the single components and thermodynamic self-consistency via the Gibbs-Duhem Equation.

12. Title: Aqueous Electrolyte Data Center

Location: Physical Chemistry Division, NBS, Washington, D.C. 20234

Project Leader: B. R. Staples

Description: The thermodynamic properties of aqueous electrolytes are collected from the literature, organized and used to supply information services, reviewed and evaluated. These data are required in the analysis and solution of problems in water-quality control, geothermal energy production, corrosion, sewage treatment, desalination of water, industrial processes and in the interpretation of chemical, biochemical, and geochemical systems.

The osmotic and activity coefficients of electrolyte solutions are being evaluated. Reports have been published on the 1:1 electrolytes and are in press for calcium chloride and the other alkaline earth halides. Reports are in preparation on other 2:1 electrolytes, the 1:2 and 2:2 and higher valence electrolytes. Equilibrium constants for salts containing heavy metal ions of concern in pollution processes are also being evaluated.

The center cooperates with other projects in which solubility data are being compiled and evaluated, and with the Chemical Thermodynamic Data Center.

13. Title: High Pressure Data Center

Location: Brigham Young University, Provo, Utah 84601

Project Leader: H. Tracy Hall

Direct Inquiries To: Leo Merrill

Description: This center is concerned with the compilation and evaluation of data on properties of substances at high pressures. These data are useful in the discovery and production of useful high-pressure phases such as diamond and boron nitride, for pressure forming of metals, especially refractory and brittle metals, for geochemical purposes and for developing and defining a pressure scale.

The center has published papers on the high-pressure behavior of the elements and AB compounds. Work on the behavior of more complex compounds is underway. A bibliography on metal forming is also being completed. The center also publishes a current-awareness bulletin.

14. Title: Alloy Data Center

Location: Metallurgy Division, NBS, Washington, D.C. 20234

Project Leader: Gesina C. Carter

Description: The Alloy Data Center collects, indexes, evaluates, and disseminates evaluated reference data on phase diagrams of alloys. These data have wide utility in the metallurgical industry and are needed for solution of a variety of problems in materials utilization.

As a method of coordinating and organizing work on phase diagrams internationally, the center combined with the project on Phase Diagrams for Ceramists to run a workshop on Applications of Phase Diagrams in Metallurgy and Ceramics. A review of phase-diagram projects was also published which included an annotated listing of all published compilations of phase diagrams.

Current work involves following up on the opportunities for further coordination arising from the workshop and compilation and evaluation of phase diagrams of the alloys of hydrogen with metals such as Fe and Ti which may be useful as hydrogen storage systems.

15. Title: Phase Diagrams and Thermodynamic Data for Ternary Copper Aluminum Alloy Systems
Location: University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201
Project Leader: L. M. Schetky, International Copper Research Association, New York, New York 10022
Direct Inquiries To: Y. A. Chang, University of Wisconsin-Milwaukee
Description: This project is concerned with the compilation and evaluation of thermodynamic and phase diagram data on all ternary copper-aluminum alloys for which data are available. These data are needed for extractive metallurgy and in the industrial use of metals, for example, in devising techniques for brazing and welding, and for predictions of stability under severe or unusual environmental conditions.

The project is coordinated with a larger project covering all ternary copper alloy systems which is being sponsored by the International Copper Research Association. A paper on the copper-aluminum ternary alloys is in press.

16. Title: Fluid Transport Properties
Location: Cryogenics Division, NBS, Boulder, Colorado 80302
Project Leader: H.J.M. Hanley
Description: This project is concerned with the transport properties of fluids. Recent theoretical developments relating the transport and the equilibrium properties of fluids have been used to evaluate experimental data on transport properties and to provide methods for interpolating between and extrapolating limited data sets. These techniques allow development of formulations providing internally consistent sets of data on thermodynamic and transport properties from limited experimental results.

The simplest fluids have been covered in a series of recent publications. Papers containing evaluated data on the viscosity and thermal conductivity of gaseous and liquid methane and ethane are in press. Work is in progress on propane and nitrous oxide.

Work has been done on methods of extending the treatment of viscosity and thermal conductivity to binary systems. Techniques suitable to simple cryogenic systems have been developed and applied to LNG Papers on the techniques developed and their application to LNG are in press.

17. Title: Correlation of Thermophysical Property Data of Fluids

Location: University of Maryland, College Park, Maryland 20742

Project Leader: J. V. Sengers

Description: This project is concerned with the evaluation and correlation of data on the thermodynamic and transport properties of fluids in the neighborhood of the critical point and with the development of needed data-correlating techniques applicable in the critical region. These properties exhibit unique, and, in some cases, large changes as the critical point is approached and require special correlating techniques to reproduce the observed behavior and to develop consistent formulations covering more than one property. It is also necessary that any special techniques used in the critical region merge satisfactorily with classical formulations known to apply well away from the critical point.

Emphasis in the project has been put on the thermal conductivity, a property which changes strongly in the neighborhood of the critical point. A method has been devised for separating the thermal conductivity into a background portion which merges smoothly with the behavior well away from the critical point and an excess portion.

The methods developed have been applied to water. The density is a necessary factor in separating the two parts of the thermal conductivity and in developing an expression for the excess portion. The values used were taken from the set of self-consistent thermodynamic values developed in another project listed here. An equation expanding the excess portion of the thermal conductivity around the critical point by scaling-law techniques has been developed and applied to water with the result that there are now formulations for the thermodynamic properties and the thermal conductivity of water in the critical region which are consistent with one another. Application of the techniques to other fluids is being considered.

18. Title: Thermal Conductivity

Thermophysical Properties Research Center Purdue University,
Lafayette, Indiana 47906

Project Leader: Y. S. Touloukian

Description: This center compiles data on 8 thermodynamic and transport properties of materials, over the temperature range for which data are available, on a continuing basis. Another center in the same location compiles data on electrical and electronic properties. The purpose is to advance the precision of industrial process design, and extend the capability for optimum selection of engineering materials through the provision of critically evaluated data on the thermal and electrical conductivities and related transport properties of metals, alloys, and selected fluids.

The center has recently completed a paper on the thermal conductivity of 10 selected binary alloy systems, and another on the electrical resistivity of the 9 elements present in the binary alloys. A paper on the electrical resistivity of the same alloys is in preparation. Data on C_p , the viscosity and thermal conductivity of 73 fluids of industrial importance are also being compiled and evaluated.

The following data centers, not directly under NSRDS program management, also supply evaluated data relevant to this area of interest:

1. Title: National Center for the Thermodynamic Data of Minerals

Location: U.S. Geological Survey, Reston, VA 22092

Project Leader: J. L. Haas, Jr.

Description: The center will compile, index, and evaluate data on the thermodynamic and thermophysical properties of minerals, their synthetic analogs and geologic materials. These data are important for geochemical purposes and will be useful industrially in the fields of metallurgy and the synthesis and production of inorganic chemicals.

In particular, the center will develop critically evaluated thermodynamic data for naturally occurring solid phases or their chemical end-members. Properties under consideration are C_p , entropy, enthalpy, Gibbs energy, enthalpy and Gibbs energy of formation, molar volume, molar compressibility, molar expansivity, all as functions of temperature, and phase diagrams of systems containing mineral phases. The center cooperates closely with the Chemical Thermodynamic Data Center and the JANAF Thermochemical Tables Project.

2. Title: JANAF Thermochemical Tables

Location: Dow Thermal Research Laboratory, Midland, Michigan 48640

Project Leader: M. W. Chase

Description: Thermodynamic properties in the solid, liquid, and/or ideal gaseous state over the temperature range of 0-6000°K. Covered are the following elements: Al, B, Ba, Be, Br, C, Ca, Cl, Co, Cs, F, Fe, H, Hg, I, K, Li, Mg, Mo, N, Na, Nb, O, P, Pb, S, Si, Sr, Ta, W, Zr, and e^- and their simple compounds, principally those with the halogens, oxygen, and hydrogen. Properties given are heat capacity, entropy, Gibbs energy function, enthalpy (heat content), heat of formation, and Gibbs energy of formation for the ideal gas, liquid or solid state.

3. Title: International Copper Research Association

Location: International Copper Research Association, New York, New York 10022

Project Leader: M. L. Schetky

Description: The thermodynamic, thermophysical, and transport properties of copper and its alloys and compounds in the solid and liquid phases and in aqueous systems. The thermodynamic properties include phase diagrams as well as the thermodynamics of the individual phases. Transport properties include electronic transport as well as mass and heat transport.

4. Title: Thermochemistry of Metallurgy

Location: Department of Metallurgy, Massachusetts Institute of Technology, Cambridge, MA 02139

Project Leader: J. F. Elliott

Description: Selected elements and compounds involved in metallurgical chemistry and technology. The compounds include: carbides, nitrides, oxides, phosphides, silicides, and sulfides. Multicomponent alloys and solutions, complex oxide systems, and slags are also treated. The properties include: enthalpy (heat content) and temperature of phase changes; heat capacity; enthalpy, entropy and Gibbs energy function as appropriate.

5. Title: Contributions to the Data on Theoretical Metallurgy
Location: Thermodynamics Laboratory, Albany Metallurgy Research Center,
Albany, Oregon 97321
Project Leader: S. Hill; Project Director: A. D. Mah
Description: The elements and their inorganic compounds of interest in metallurgical and ceramic operations. Included are oxides, halides, carbides, carbonates, sulfides, sulfates, nitrates, nitrides, and some intermetallic and interoxide compounds. Properties given include Gibbs energy, entropy, enthalpy (heat content), high and low temperature heat capacity, heat and Gibbs energy of formation and phase change, and vapor pressure.

MATERIALS UTILIZATION DATA

- Title: Superconductive Materials Data Center
Location: General Electric Company, Schenectady, New York 12301
Project Leader: B. W. Roberts
Description: The Superconductive Materials Data Center collects and disseminates the publicly known data on the basic physical properties of superconductive materials. The data include superconductive critical temperatures, critical magnetic field, material state, crystallographic description, etc. In 1976 a comprehensive "Survey of Superconductive Materials and Critical Evaluation of Selected Properties" was published in Volume 5, No. 3, of the Journal of Physical and Chemical Reference Data. This publication comprehends the substance of earlier output from the center. In the immediate future, the center will develop a mechanized central data file on superconductive materials, deriving from present internal holdings plus additional material being collected.
- Title: Crystal Data Center
Location: Inorganic Materials Division, NBS, Washington, D.C. 20234
Project Leader: Helen M. Ondik
Description: The Crystal Data Center compiles and evaluates inorganic crystallographic data from the literature for dissemination to the scientific and technical community. With the third edition of "Crystal Data Determinative Tables" in print, the effort is aimed at preparing and publishing a series of supplements containing data from 1967 to date. Data for the first supplement are being compiled, and publication is planned for late 1977. The center has used the existing automated files for the preparation of "Crystal Data Space-Group Tables," by Alan Mighell of the center and Bettijoyce Molino of the OSRD Data Systems Design Group. The Space Group Tables permit the user to find crystals of a specified symmetry, locate isostructural molecules, etc.
- Title: Cambridge Crystallographic Data Centre
Location: Cambridge University, Cambridge, England
Project Leader: Olga Kennard
Description: The Cambridge Data Centre searches, extracts, compiles, and stores crystal data from the world literature on organic compounds. In addition, the Centre extracts information from the literature on inorganic compounds, intermetallics, and minerals which it sends to the Crystal Data Center at NBS. The data on organic compounds are stored in a computerized file and include unit cell constants, densities, and space group designations. These parameters serve as a basis for the identification and analytical determination of such diverse material as petrochemicals, insecticides, drugs, biological compounds, and others. This data file in selected form was automated to produce the Organic Compound volume of the third edition of "Crystal Data - Determinative Tables," and is being used in the preparation of the first Organic Supplement which will appear in 1977.

4. Title: Mossbauer Effect Data Center
Location: University of North Carolina, Asheville, NC 28804
Project Leader: John G. Stevens
Description: The literature involving Mossbauer effect measurements has grown steadily in recent years; it has application in such diverse areas as solid state physics, analytical chemistry, biophysics, etc. Annual publication of the Mossbauer Effect Data Index (MEDI) was initiated to provide workers with a single source of data and bibliographic reference thereby avoiding duplication of effort spent in searching the literature. The data include radioactive source, absorber employed, temperature, degree of shift, quadruple splitting, etc. The MEDI has been published annually starting with 1970. The 1975 Index was published in 1976 by IFI/Plenum Data Company.

5. Title: Diffusion in Metals Data Center
Location: Metallurgy Division, NBS, Washington, D.C. 20234
Project Leader: J. R. Manning
Description: The project objective is the publication of standard reference data monographs which provide a review and critically evaluated data on diffusion in metals and their alloys. Papers from the technical literature are systematically collected and classified according to the alloy systems on which they report diffusion data. More than 4000 papers are examined each year, of which about 2000 are entered into the files of the center. Monographs for alloy systems important in technology are being produced, starting with diffusion in copper and copper alloys. The fourth compilation of evaluated data prepared under this project, "Diffusion in Copper and Copper Alloys, Part IV, Diffusion in Systems involving Elements of Group VIII," was published in 1976 in Vol. 5, No. 1 of the Journal of Physical and Chemical Reference Data. Current efforts of the center focus on additional monographs in the copper series, involving a) N, P, As, Sb, Bi, and b) O, S, Se, Te.

6. Title: Elastic Constant Data for Metals and Alloys
Location: Cryogenics Division, NBS, Boulder, Colorado 80302
Project Leader: R. P. Reed
Direct Inquiries To: H. Ledbetter
Description: Elastic properties data for materials that are of scientific or technological interest because of their relationship to the interatomic potential in solids and, consequently, to a wide variety of solid-state phenomena. Technologically, elastic constants are essential design parameters in any mechanically stressed component-pressure vessels, ship hulls, rotating machinery, etc.

The first review in this series covered Iron, Nickel, and Iron-Nickel Alloys (J. Phys. Chem. Ref. Data, 2 (1974), 531-618).

A paper on the elastic properties of copper was published (J. Phys. Chem. Ref. Data, 3 (1974, 397-935). Also a note on the elastic constants of polycrystals was published (Phys. Status Solidi, 2, 26 (1974), K67-70). A manuscript on the elastic properties of zinc has been completed and will be published in 1977.

Reviews on copper-zinc alloys and on aluminum are at present in preparation.

7. Title: Optical Properties of Materials
Location: Center for Information and Numerical Data Analysis and Synthesis (CINDAS), Purdue University, West Lafayette, Indiana 47907
Project Leader: H. H. Li
Description: This project has been established to produce compilations of critically evaluated refractive index data and related information pertinent to laser, holographic, and electro-optic systems. The work includes informal collaboration among NBS, the Research Materials Information Center (RMIC) at Oak Ridge National Laboratory, and the Center for Information and Numerical Data Analysis and Synthesis at Purdue University. A substantial compilation of carefully evaluated data for 20 alkali halides was prepared by H. H. Li of CINDAS and published in 1976 in Volume 5, No. 2, of the Journal of Physical and Chemical Reference Data. Current efforts under the project include compilation of data for the alkaline earth halides as well as specific coverage of silver halides.
8. Title: Fracture Mechanics Data Handbook
Location: Metallurgy Division, NBS, Washington, D.C. 20234 and Department of Mechanical Engineering, University of Maryland
Project Leader: R. deWit, National Bureau of Standards, Washington, D.C. 20234
Description: The objective is to advance the application of fracture mechanics analysis methodologies to materials engineering and design and to materials selection processes through the provision of compilations of reliable data on fracture, a survey of fracture toughness testing procedures, and a critical review of the applications of advanced materials properties. To date, four papers (prototype sections of the eventual handbook) have been prepared on various aspects of fracture mechanics and dynamic fracture testing.
9. Title: Vibrational Force Field Constants for Polyethylene
Location: Polymers Division, NBS, Washington, D.C. 20234
Project Leader: D. H. Reneker
Description: Review of the previous efforts to describe the force field of polyethylene revealed inadequacy in the manner in which those force fields were formulated. Also, a large body of new data, principally in the low frequency Raman region, has been published since the last comprehensive review. Molecular vibrational data from the literature and from measurements made at NBS have been collected and used to obtain the best fit to theoretical dispersion curves of polyethylene crystals. A draft report has been completed for presentation of the results in the Journal of Physical and Chemical Reference Data in 1977.

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51. High Temperature Properties and Decomposition of Inorganic Salts, Part 4. Oxy-Salts of the Halogens, *Kurt H. Stern*, Vol. 3, No. 2, pp. 481-526 (1974) \$4.50
52. Diffusion in Copper and Copper Alloys, Part II. Copper-Silver and Copper-Gold Systems, *Daniel B. Butrymowicz, John R. Manning, and Michael E. Read*, Vol. 3, No. 2, pp. 527-602 (1974) \$5.50
53. Microwave Spectral Tables, I. Diatomic Molecules, *Frank J. Lovas and Eberhard Tiemann*, Vol. 3, No. 3, pp. 609-770 (1974) \$8.50
54. Ground Levels and Ionization Potentials for Lanthanide and Actinide Atoms and Ions, *W. C. Martin, Lucy Hagan, Joseph Reader, and Jack Sugar*, Vol. 3, No. 3, pp. 771-780 (1974) \$3.00
55. Behavior of the Elements at High Pressures, *John Francis Cannon*, Vol. 3, No. 3, pp. 781-824 (1974) \$4.50
56. Reference Wavelengths from Atomic Spectra in the Range 15 Å to 25000 Å, *Victor Kaufman and Bengt Edlén*, Vol. 3, No. 4, pp. 825-895 (1974) \$5.50
57. Elastic Properties of Metals and Alloys, II. Copper, *H. M. Ledbetter and E. R. Naimon*, Vol. 3, No. 4, pp. 897-935 (1974) \$4.50
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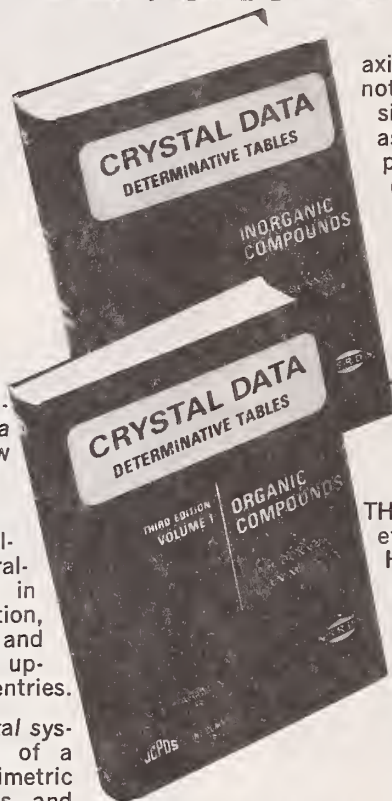
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