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Critical Evaluation of Data in the Physical Sciences —

A Status Report on the National Standard Reference Data System

June 1972

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NATIONAL BUREAU OF STANDARDS

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Office of Standard Reference Data—Office of Technical Information and Publications—Library—Office of International Relations.

¹ Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

² Part of the Center for Radiation Research.

³ Located at Boulder, Colorado 80302.

⁴ Part of the Center for Building Technology.

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Critical Evaluation of Data in the Physical Sciences –

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National Standard Reference Data System June 1972

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Washington, D.C. 20234

NBS Technical Notes are designed to supplement the Bureau's regular publications program. They provide a means for making available scientific data that are of transient or limited interest. Technical Notes may be listed or referred to in the open literature.



U.S. DEPARTMENT OF COMMERCE, Peter G. Peterson, *Secretary*
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P R E F A C E

The previous report on the status of the National Standard Reference Data System appeared two years ago. Since that time, the programs of the system have been operating with substantially a constant budget. The limitations of steady-state funding mean that few new projects are started each year and that few on-going projects can be staffed or supported at a level commensurate with their assigned task. Change, therefore, is slow. However, since the last Status Report appeared (NBS Technical Note 553, June, 1970) a number of large undertakings have reached full productivity, a new channel has been established for the primary distribution of the output of the system, and explorations are underway for a modest data program in the area of mechanical properties. These developments are described in some detail in the present report.

Communication and collaboration have continued with other programs sharing the goals of NSRDS. While government-wide constrictions on research and development funding have reduced some data-evaluation efforts of Federal agencies, the challenge of emerging national problems (air and water quality, alternate energy sources, etc.) offer major opportunities for joint technical undertakings, in which reliable reference data can be vitally important. The Office of Standard Reference Data is aware of the need for a flexible but soundly-based program which can respond to these challenges.

Until the appearance of the new Journal of Physical and Chemical Reference Data, the NSRDS-NBS Series was the principal outlet for the primary products of this program. There are now 50 titles in this series; in addition, approximately 70 other data compilations, bibliographies and translations have appeared. Over 100,000 copies of NSRDS-NBS Series documents have been distributed since this program began, and this total is augmented by wide-spread secondary distribution of data in various handbooks. The distribution of the core of the NSRDS output through the new journal is expected to improve the accessibility of reliable reference data to the scientific and technical community.

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 June 1972. Recent activities of the Office of Standard Reference Data are summarized and future plans are indicated. A complete list of data evaluation projects supported by the Office of Standard Reference Data during Fiscal Year 1972 is included; this list also includes projects which received financial support during an earlier fiscal year, and which are still actively involved in some aspect of data compilation and evaluation, or which are still preparing a product for publication. Progress in data processing and in information services is reviewed. The appendix includes a listing of continuing data centers in the United States and a list of publications resulting from the standard reference data program.

Key words: Atomic and molecular data; chemical kinetics; colloid and surface properties; data systems design; information services; mechanical properties; nuclear data; standard reference data; solid state data; thermodynamic and transport properties.

CRITICAL EVALUATION OF DATA IN THE PHYSICAL SCIENCES

A STATUS REPORT ON THE NATIONAL STANDARD REFERENCE DATA SYSTEM

June 1972

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 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 is restricted to well-defined physical and chemical properties of substances and systems which are well-characterized. While this definition leaves some borderline cases, the intent is to concentrate the effort on intrinsic properties which are clearly defined in terms of accepted physical theory. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. Likewise, materials of uncertain or variable composition are not included. Biological properties and data relating to large natural systems (e.g. the atmosphere, the oceans) also fall outside the program.

One major aim of the program is to provide critically evaluated numerical data, in a convenient and accessible form, to the scientific and technical community. Certain secondary outputs, such as annotated bibliographies and procedures for computerized handling of data, are also made available. A second equally important aim is to provide feedback into experimental work 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 encourage 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 obvious 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.

A list of continuing data centers in the United States appears in Appendix II. Those data centers which currently receive financial support from OSRD are listed by title only, with reference made to their full description in Chapter II. Projects which are supported primarily from other sources are described in somewhat more detail. It is significant that many other Federal agencies and private groups (in addition to OSRD) find good reasons to support data centers.

C. 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 I.

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. Special services provided to individuals or groups are to be largely reimbursable, while charges for data compilations of general interest are expected to defray primarily the cost of their publication and distribution.

D. Journal of Physical and Chemical Reference Data

In 1971, OSRD began exploration of alternate publication procedures which would make use of the new authority mentioned above and be responsive to the intentions of Congress in granting it. A simultaneous objective was better (i.e. wider, prompter, and more user-oriented) dissemination of Standard Reference Data. As a result of these considerations, a journal format was selected, to be produced with the active collaboration of the American Chemical Society and the American Institute of Physics. The first issue of the quarterly Journal of Physical and Chemical Reference Data appeared in March 1972.

It is anticipated that the major compilations of physical and chemical property data produced under the NSRDS program will be published in this Journal. In addition, the Journal will be open to contributions of acceptable quality from other sources. The Editorial Board contains representation from the American Institute of Physics, the American Chemical Society, and the National Bureau of Standards. The participation of these societies, with a combined membership of over 150,000, is a recognition of the key role that individual scientists must play in providing reliable reference data.

The Journal of Physical and Chemical Reference Data will initially appear as a quarterly publication, with about 1200 pages planned for Volume I (1972). Compilations of evaluated data and critical reviews of moderate length will be published in the Journal. Longer data compilations which would overcrowd the regular issues will appear as Supplements to the Journal. In addition, copies of individual compilations appearing in the Journal will be available for separate purchase. Information on subscriptions may be obtained from the American Chemical Society, 1155 Sixteenth Street, N. W., Washington, D. C. 20036.

E. Advisory Mechanism

For good management of the NSRDS program it is essential to have reliable feedback from the scientific and technical community. At the time the program was established, the services of the National Academy of Sciences-National Research Council were enlisted for this purpose. The Executive Committee of the Office of Critical Tables of the NAS-NRC provided the focal point for advisory services to the Office of Standard Reference Data. That Office arranged for meetings of advisory panels in the various technical areas, which made recommendations on priorities to OSRD.

As a result of reorganization within the NAS-NAE-NRC, the Office of Critical Tables was replaced in 1969 by 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 a following section of this report.

The NDAB also 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 cosponsor with OSRD of symposia and conferences on special topics when a broader level of professional interaction appears appropriate to a special subject. An example of this latter type of advisory mechanism is the symposium held in June, 1972, on industrial needs for critically evaluated P-V-T data on ethylene and other gases.

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

F. 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 Office of Scientific and Technical Information (OSTI) 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 in the physical sciences, and the State Service for Standard and Reference Data (GSSSD) has broad responsibility for scientific and technical data. 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 major concern to two or more countries are circulated to those countries for comment.

In November, 1971, a symposium on data compilation was held in Tokyo under the auspices of the U.S. - Japan Treaty on Scientific Cooperation. Representatives from OSRD and from several NSRDS Data Centers participated in this symposium. A base was established for future cooperation on data programs in the two countries.

The establishment of the Committee on Data for Science and Technology (CODATA) in 1966 has provided a formal framework for international cooperation. CODATA is a committee of the International Council of Scientific Unions (ICSU) and contains representation from ten international unions and, at present, thirteen countries. The central office is located

in Frankfurt, Germany. 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.

CODATA has established task groups in a number of special areas, including computer handling of numerical data, key values of thermodynamic properties, chemical kinetics, and fundamental constants. Scientists associated with NSRDS data projects are active in all of these task groups. Probably the most significant accomplishment of any of these bodies is the adoption of standard values for thermodynamic properties of certain key substances. This will reduce inconsistencies and uncertainties resulting from the use of data from different thermodynamic tables and is hopefully the first step toward creation of an internationally accepted set of tables of thermodynamic properties. The staff of the Chemical Thermodynamics Data Center at NBS has played a major role in this effort.

Other task groups are now being organized in such areas as transport properties, presentation of data in the primary literature, and data accessibility.

A prominent example of international cooperation on a working level is provided by the Thermodynamics Tables project of the International Union of Pure and Applied Chemistry. The aim of this project is to generate standard tables of thermodynamic properties of industrially important gases. It is directed by Dr. Selby Angus of Imperial College, London. Several data projects in the United States supported by the Office of Standard Reference Data form key parts of this program.

A part of the NSRDS program derives from bilateral cooperative efforts under the auspices of Special Foreign Currency Programs authorized by Public Law 480 and other legislation. Certain funds allocated to NBS are used to support projects which result either in data compilations or in data-oriented products, such as theoretical calculations, bibliographies, or translations, which are helpful to NSRDS data centers and to users of reference data. The projects which receive grants for this work (primarily in India and Israel) are monitored by NBS data center scientists and OSRD staff. Special Foreign Currency projects associated with NSRDS are included with appropriate identification in Section II of this report.

G. Highlights of Recent Accomplishments

The ultimate justification of the NSRDS program must rest on the usefulness of its output to scientists and engineers who require physical property data for the solution of their problems. During the last two years the Office of Standard Reference Data has placed increased emphasis on identifying the needs for reliable data in various areas, particularly those related to important national problems that have a strong technological component. Not surprisingly, it is often found that the data needed to attack a particular problem must come from a variety of disciplines. The coherent structure of the National Standard Reference Data System is a strong asset in focussing the resources of many specialized, discipline-oriented centers on a specific problem or mission. The collections of evaluated data maintained by these centers can be used to provide prompt responses to new data demands.

Examples of NSRDS efforts at providing data pertinent to important national problems are given below. These include completed projects as well as those in progress or in the planning stage.

Improvements in Incinerator Design

In 1970 the Research Committee on Industrial Wastes of the American Society of Mechanical Engineers wished to prepare a monograph on industrial incinerator design to upgrade existing design practices and produce more efficient, less polluting incinerators. They realized that thermodynamic data on the combustion process were needed. The Chemical Thermodynamics Data Center, with its expertise and extensive files of data on thermodynamic processes, was in an ideal position to collect such data quickly and inexpensively. With support from the Society a compilation of heats of combustion of about 1000 substances commonly burned in industrial incinerators has been prepared. This compilation combined with information on how to use it for incinerator design will provide a basic handbook for engineers in the field. This handbook is expected to make an important contribution to the design of more efficient and reliable industrial incinerators.

Metering of Gases Transferred in Pipelines

The rapid increase in the production of ethylene and related gases, as well as the introduction of new methods of storage and transfer, has presented a difficult measurement problem. Flow through pipelines is most easily measured in terms of volume, which must be converted to units of weight for accurate records of material balance in transfers from one place (or owner) to another. This conversion requires an accurate equation of state (PVT surface) for the fluid in question, and under current practices the data must cover a wide range of temperature and pressure. In the case of ethylene, our knowledge of the PVT surface is inadequate to meet present needs, and similar problems are expected to arise in the near future with gases such as propylene and butadiene. The Office of Standard Reference Data organized a three-day meeting on this subject in June 1972, which was attended by representatives of a number of industrial concerns. The nature of the problem was outlined and priorities established; efforts are now being made to set up suitable data evaluation projects. The objective will be to produce definitive tables and formulations that will be accepted by all parties concerned and that will remove the confusion currently existing in custody transfer of ethylene.

Surfactant Data

The publication of NSRDS-NBS-36, Critical Micelle Concentrations of Aqueous Surfactants, has provided chemists, biochemists, agricultural scientists, and sanitary engineers with a definitive collection of data for characterizing the surface activity of 720 compounds used in detergency and washing, the dispersion of dyes and pigments, the beneficiation of ores and other industrial applications. The publication brings together in a single comprehensive volume all of the pertinent reference information on a particular category of chemically active materials and provides a highly important data resource for a number of fields of great national importance.

Air Pollution

The present concern with understanding the chemistry of polluted atmospheres has revealed many gaps in our knowledge of reaction rate

constants and other properties of the most common air pollutants. Modelling calculations intended to predict the consequences of introducing a pollutant into the atmosphere under a particular set of circumstances often give a very uncertain result because of poorly known input data. NSRDS is now collecting the best data for this purpose, including estimates made by experts when no experimental measurements are available. The Chemical Kinetics Data Center has taken the lead in this effort, drawing on their extensive files and experience in compiling rate data. Preliminary reports on data relevant to stratospheric pollution have been prepared, and a more definitive collection of reaction rates, photochemical data, other pertinent properties is in progress.

Aqueous Electrolytes

A new data center has been established on the thermodynamic properties of aqueous electrolytes in order to meet data needs in such diverse fields as battery development, steam turbine design, biochemistry, sanitary engineering, and oceanography. The Center will compile data on salt solutions that are important in all of the above areas. The output will consist of broad compilations of critically evaluated electrolyte data plus detailed treatments of specific important systems.

Other Plans

Several systematic studies are being carried out with the aim of identifying the needs for physical property data in major R & D programs. A panel of the Numerical Data Advisory Board is considering data requirements for the development of practical methods of coal gasification. A similar study is being considered on innovative techniques in electrical power transmission. The need for data on the mechanical properties of metals and alloys is being studied in some detail, as pointed out elsewhere in this report. Studies such as these will be of value in setting priorities on the allocation of resources in the NSRDS program.

II. PROGRESS OF THE DATA EVALUATION PROGRAM

The original (1963-64) planning of the NSRDS program envisioned a two-year period of moderate funding, followed by fairly rapid expansion to a level which would have permitted a comprehensive attack on all subject-areas of high priority. Under such a schedule, data evaluation activities would have processed a major portion of the scientific literature since about 1950, and would then have moved to a steady-state handling of the current material as it appeared. The actual expansion has been far more modest than anticipated; in fact, the operating budget of the Office of Standard Reference Data has changed very little during Fiscal Years 1967-1972. Many of the initial goals, therefore, have not yet been reached. However, a good start has been made in at least two technical areas, and much experience has been gained in modes of operation of data centers. Of equal importance is the insight achieved into users' interests on the basis of feedback involving a now-substantial volume of data compilations and critical reviews.

The scope of the standard reference data program has been divided into seven technical areas for operational convenience: (1) Thermodynamics and Transport Properties, (2) Atomic and Molecular Data, (3) Chemical Kinetics, (4) Solid State Data, (5) Nuclear Data, (6) Colloid and Surface Properties, and (7) Mechanical Properties. This chapter is devoted to progress reports for these technical areas. A general discussion is given of important developments in each area, followed by individual progress reports for each data evaluation project supported (fully or partially) by the Office of Standard Reference Data during Fiscal Year 1972, plus those projects supported during previous years which remain active. Descriptions of the individual projects and their output are essentially technical in nature, and are addressed to potential users who have their own needs clearly in mind. For this reason, the report avoids generalized indications of applications of the data.

The area of Mechanical Properties was not discussed in any detail in the previous (1970) NSRDS Status Report. Since then, a study has been initiated of the subject content and users' needs in this area, to provide the basis for establishing a data evaluation program. An interim report on that study is included.

The progress reports include both individual, short-term projects and continuing data centers which receive at least a part of their support from the Office of Standard Reference Data. 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) is given in Appendix II.

A full list of publications which have appeared under the auspices of the NSRDS program may be found in Appendix III.

A. THERMODYNAMIC AND TRANSPORT PROPERTIES

The two years since the last status report have seen two developments which have added to and have caused changes in the on-going basic program. These are the further evolution of international programs and the increase of activities focussed on specific problems of a practical engineering nature.

Considering the latter of these first, it might be pointed out that data needed for the solution of a specific engineering problem often do not differ in kind or in accuracy from those needed for solving any other type of problem. Focussing on the specific problem leads to identification of specific data needs and hence makes possible packaging together of the needed data in the form most useful to those involved in solving the problem.

An example of such an activity is the project concerned with assembling enthalpy data needed in the design of industrial incinerators, a project of the Office of Standard Reference Data sponsored by the American Society of Mechanical Engineers and carried out by the NBS Physical Chemistry Division using the extensive files of the Thermochemical Data Group. Further details are given in the descriptions of individual projects. In a similar, although less formal way, contributions have been made to a planned handbook which lists selected properties of a set of chemical species of importance in air pollution.

Another example - which is an entirely different activity - is a conference held at Airlie House, Warrenton, Va., June 13-16, 1972, on data needs for custody transfer and design calculations for ethylene and related substances. The conference was sponsored by the Numerical Data Advisory Board of the National Academy of Sciences-National Research Council at the request of the Office of Standard Reference Data. The conference was held to determine what ranges and reliabilities of data were needed for custody transfer calculations and for equipment design and what further steps, if any, should be taken to provide them.

Finally, mention can be made of some steps taken with respect to the Bulletin of Thermodynamics and Thermochemistry. The Bulletin provides bibliographic information on thermochemical data, indexed according to substance and property, on an annual basis. To make this reference source more valuable, it is being prepared in a searchable magnetic tape form.

Turning to international activities, an important development has been the CODATA Task Group on Key Values for Thermodynamics. This Task Group has prepared a set of values of standard enthalpies of formation, standard entropies, and standard enthalpy increments referred to 298.15K for 32 chemical species of particular importance in thermochemical calculations. The set of values was widely circulated for comment and has recently been published by CODATA as an internationally accepted set. The Task Group is currently preparing an additional provisional set of values for another group of 15 important compounds. The Thermochemical Data Group at NBS and a counterpart Russian group played the primary roles in preparing the initial provisional sets. A further, closely related, development is a proposed US-USSR project for preparation of jointly acceptable thermochemical tables. This project is still in the planning stages.

The IUPAC Commission on Thermodynamics and Thermochemistry sponsors a Thermodynamic Tables Project under Dr. Selby Angus of Imperial College, London. The purpose of the project is the development of internationally agreed upon tables of the P-V-T properties of industrially important gases. The Project relies on the cooperation of data evaluators throughout the

world, who prepare tables for individual gases, and a series of panels of experts who compare tables and, if necessary, resolve differences between them. There are evaluation projects leading to the preparation of tables for six gases which are supported wholly or in part by the Office of Standard Reference Data. In addition seven of eleven U. S. panel members receive support from the Office of Standard Reference Data as does the Cryogenic Data Center which serves as the primary source of bibliographic information for all evaluations sponsored by the Project.

Another IUPAC Commission with a long-term interest in data is the Commission on Equilibrium Properties of the Analytical Chemistry Division, which is interested in complex stability constants. A project on liquid-liquid distribution reactions is being sponsored by the Office of Standard Reference Data in cooperation with the Commission's overall program.

Finally, mention should again be made of the Bulletin of Thermodynamics and Thermochemistry which is sponsored by the IUPAC Commission on Thermodynamics and Thermochemistry and has an international editorial board and list of contributors.

The productivity of the program on thermodynamic and transport properties has remained high. There have been two monographs published in the NSRDS-NBS Series (32, 37) three Technical Notes (270-5, 270-6 and 384), and one bibliography (NBS-OSRDB-70-1). Publication details will be found elsewhere in this report. One paper in the first issue of the Journal of Physical and Chemical Reference Data, namely that of Marrero and Mason, resulted from the program on thermodynamics and transport properties, and five additional papers and two major monographs, each of which will constitute a Supplement to the Journal, have been scheduled for early publication.

Eight products of the U.S.S.R. standard reference data program, which have been translated at the request of the National Bureau of Standards, should also be mentioned since, for the most part, they cover subjects in the thermodynamics and transport properties area. These are listed in detail elsewhere in this report.

Active Projects:

1. Title: Chemical Thermodynamic Data Group

Principal Investigators: D. D. Wagman, W. H. Evans

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

Date Initiated: 1963 (Data Center started in 1940)

Objective: The compilation and evaluation of the heats, entropies and free energies of formation of all inorganic substances in the standard state and of selected thermodynamic properties of selected organic materials.

Current Status: The systematic review and evaluation of the thermodynamic properties of compounds of a group of 61 elements (the first 61 in the "Standard Order" of arrangement) and of the six alkaline earth metals, have been completed and published. Work on the rare earths is well advanced and work on the alkali metals has been started.

The group has played a major role in the activities of the CODATA Task Group on Key Values for Thermodynamics. The Task Group has prepared two sets of values of standard enthalpies of formation, standard entropies and standard enthalpy increments, all referred to 298.15K, of chemical species of particular

importance in thermochemical calculations. One set covering 32 chemical species has been widely circulated for comment and then published by CODATA as an internationally accepted set. A second set covering 15 chemical species has been published in provisional form for comment.

A compilation of the heats of formation and combustion of selected organic compounds has appeared in the Journal of Physical and Chemical Reference Data (see Appendix III, NSRDS Publications List).

Automated techniques for data and text handling have been developed further. All new data and related bibliographic information are stored on magnetic tape and printed on data cards for easy and rapid access. The latest issue of the Bulletin of Thermodynamics and Thermochemistry has been printed from magnetic tape and a tape containing the indexing and bibliographic information in a standard transferable form has been prepared. Most computer centers should be able to work with this tape and prepare search programs to utilize the information on it.

Future Plans: The systematic coverage of the standard enthalpies, Gibbs energies and entropies of compounds will be completed and the documentation of the evaluation process will be carried out. The activities involving the Bulletin of Thermodynamics and Thermochemistry and the international activities mentioned will be continued.

2. Title: Extraction of Thermodynamic Information From Papers in Russian and Other Eastern European Languages

Principal Investigator: Y. Levi

Location: Israel Program for Scientific Translations, Israel

Date Initiated: 1968 (Special Foreign Currency Program fund)

Objective: The extraction of pertinent thermodynamic information from articles written in Russian or other Eastern European languages.

Current Status: This project extracts information as directed from articles supplied by the project on Chemical Thermodynamic Properties.

Future Plans: Continuation along current lines.

3. Title: Thermodynamics of Incinerator Processes

Principal Investigator: Eugene S. Domalski

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

Date Initiated: 1970 (Project supported by ASME)

Objective: The preparation of a compendium of heats of formation of selected materials for use by engineers concerned with the design of industrial incinerators for waste disposal.

Current Status: Data on the heats of formation of about 1000 organic compounds, 40 polymers and about 300 inorganic oxides have been compiled. The materials have been selected as important in industrial incineration processes. The data have been arranged in tabular form and are accompanied by a discussion and aids for use of the tables and an annotated list of other sources of data.

Future Plans: It is anticipated that the material just mentioned along with an additional explanatory text, to be prepared elsewhere, will be published by the American Society of Mechanical Engineers as a contribution toward pollution abatement. The project has been completed.

4. Title: Thermodynamic Data on Organic Compounds

Principal Investigator: B. J. Zwolinski

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

Date Initiated: 1964 (Center also receives funds from other sources,
notably the American Petroleum Institute)

Objective: Compilation and evaluation of data on selected
thermodynamic and thermophysical properties of organic compounds.

Current Status: A monograph on the thermodynamic and physical
properties of the aliphatic alcohols is being published as a
supplementary volume of the JPCRD; a full reference is given
elsewhere in this report. Properties evaluated include
refractive index, density, vapor pressure, phase transitions, heat
capacity, properties of the saturated real gas and the ideal gas,
properties of standard states at 25°C and critical properties.

Work has been started on the compilation and evaluation of
the thermodynamic properties of key saturated organic oxygen-
containing compounds in the carbon range C₁ to C₄. The thermal
functions (Gibbs energy, enthalpy, entropy and heat capacities as
functions of temperature) are being evaluated and tabulated.

The section on single organic compounds in the Bulletin of
Thermodynamics and Thermochemistry is prepared by this center.
Automated methods are used in connection with the preparation of
this section and steps are being taken to automate the center's
bibliographic and data files further.

Future Plans: Comprehensive reports on the halogenated hydrocarbons
and organic oxygen-containing compounds will be completed. The
work on the Bulletin of Thermodynamics and Thermochemistry and
work leading to further automation of the center's files will be
continued.

5. Title: Physical and Thermodynamic Properties of Chemical
Substances

Principal Investigator: A. P. Kudchadker

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1970 (Special Foreign Currency Program fund)

Objective: The critical analyses of data on the thermodynamic and some
physical properties of selected organic compounds.

Current Status: The materials currently being studied are haloalkanes,
in particular the bromo and iodo methanes and the
chlorofluoroethanes. Properties evaluated include refractive
index, density, vapor pressure, phase transitions, heat capacity,
properties of the saturated real gas and the ideal gas, properties
of standard states at 25°C and critical properties.

The work of this center is closely coordinated with that of
the Thermodynamics Research Center at Texas A&M.

Future Plans: The compilation and evaluation of properties of selected
haloalkanes will be completed.

6. Title: Polar Gas Properties

Principal Investigator: Lester Haar

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

Date Initiated: 1966

Objective: The preparation of comprehensive compendia of critically
evaluated data on the thermodynamic properties of the
technologically important polar gases.

Current Status: The gas under consideration at the present time is ammonia. A formulation of the PVT properties of ammonia which is thermodynamically consistent and which covers the liquid phase and the dense and ideal gas has nearly been completed.
Future Plans: A definitive report on the PVT properties of ammonia will be prepared.

7. Title: Thermodynamic Properties of Nitrogen

Principal Investigator: R. B. Stewart

Location: University of Idaho, Moscow, Idaho

Date Initiated: 1969 (Center also receives support from NASA)

Objective: Critical evaluation of thermodynamic data for nitrogen and compilation of tables of thermodynamic properties for the solid, liquid and gas phases over the temperature range 10K to 3000K with pressures up to 10,000 atm.

Current Status: An equation of state has been developed which covers the ranges cited above. Deviations from the selected experimental data on which the formulation is based may be as much as one or two percent for the vapor at very low temperatures and in the vicinity of the critical point. For all other regions the fit is considerably better. The results have also been compared with calorimetric heat capacities, enthalpies, and latent heats and with speed of sound data.

Future Plans: A final monograph on the PVT properties of nitrogen is being prepared.

8. Title: Thermodynamic Properties of Propane

Principal Investigator: J. E. Powers

Location: University of Michigan, Ann Arbor, Michigan

Date Initiated: 1971

Objective: Critical evaluation of the data for the thermodynamic properties of propane and compilation of tables covering these properties.

Current Status: This project is in its early stages. Emphasis is being placed initially on the vapor-liquid saturation region from the triple point to the critical point, the low pressure gas and the compressed liquid. State data, calorimetric data and speed-of-sound are being covered.

Future Plans: Completion of current work and coverage of the solid and dense fluid regions as well.

9. Title: Cryogenic Data Center

Principal Investigator: N. A. Olien

Location: Cryogenics Division, NBS, Boulder Laboratories, Boulder, Colorado

Date Initiated: 1959 (OSRD Support 1970) (Center also receives support from other sources, notably NASA)

Objective: Identification, compilation and indexing of the thermodynamic properties of fluids of cryogenic interest.

Current Status: Files of bibliographic information on the thermodynamic properties of fluids of cryogenic interest are maintained current. Custom bibliographies are prepared as needed and a current awareness service is published weekly.

Future Plans: Continuation along current lines.

10. Title: Cryogenic Fluid Mixture Properties

Principal Investigator: M. J. Hiza

Location: Cryogenics Division, NBS Boulder Laboratories,
Boulder, Colorado

Date Initiated: 1971

Objective: The compilation and critical evaluation of phase equilibrium and thermodynamic property data for fluid mixtures of cryogenic interest.

Current Status: This project is in its early stages. A bibliography of important equilibrium properties for fluid mixtures of cryogenic interest is being compiled.

Future Plans: Phase equilibrium and thermodynamic data will be extracted from the literature and evaluated.

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

Principal Investigator: J. M. H. Sengers

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

Date Initiated: 1970

Objective: A description of the thermodynamic properties of fluids in the vicinity of the critical point.

Current Status: Fluids currently under examination are carbon dioxide and water. Experimental data in the critical region have been compiled and critically evaluated. Scaling law techniques are being used to attempt to describe the available data within their accuracy in the range of about $\pm 20^\circ\text{C}$ from T_c and $\pm 40\%$ from p_c . Two model equations are being fitted to $\mu - \rho - T$ data.

Future Plans: Calculations will be made to determine C_p data and other thermodynamic properties. On the basis of these calculations the better equation will be selected and best formulations for the critical regions of water and carbon dioxide will be developed.

12. Title: Critical Evaluation of Vapor-Liquid Equilibrium Data

Principal Investigators: L. N. Canjar and L. S. Kowalczyk

Location: Detroit University, Detroit, Michigan

Date Initiated: 1967

Objective: The compilation and evaluation of data on vapor-liquid equilibria for binary systems at low temperatures (below 300°C) and low pressures (below 2 atm.).

Current Status: A report on the vapor-liquid equilibria of selected pure substances below 2 atmospheres pressure and below 300°C is in preparation.

Future Plans: The project is being terminated.

13. Title: Excess Thermodynamic Properties for Liquid Mixtures of Hydrocarbons

Principal Investigator: B. D. Smith

Location: Washington University, St. Louis, Missouri

Date Initiated: 1967 (Center also receives support from a group of industrial organizations)

Objective: The compilation and critical evaluation of data on the excess free energy, excess enthalpy and excess volume of mixing for selected binary systems.

Current Status: A comprehensive report has been prepared covering the data for liquid mixtures of hydrocarbons containing 5 to 8 carbon

atoms. Emphasis has been placed on the internal thermodynamic consistency of the data.

Future Plans: A start is being made to a critical review of the excess properties of the methanol-water system.

14. Title: Review of Data Near the Critical Points of Binary Liquid Mixtures and Magnets

Principal Investigator: M. S. Green, G. F. Allan, F. J. Cook, A. Stein

Location: Temple University, Philadelphia, Pennsylvania

Date Initiated: 1969

Objective: Examination of the data in the vicinity of the critical points at which immiscible binary liquids become miscible and ferromagnetic materials become diamagnetic with respect to quality of measurement and conformity with appropriate scaling-law equations of states.

Current Status: The similarities between the various types of critical points have suggested a common nature and a basic underlying unity. The use of scaling laws has provided a means of expressing behavior near the critical point with an accuracy and economy of adjustable parameters previously unobtainable. This, in turn, makes possible interpolation between data points, correlation of independent sets of data points and conversion of data from one type to another for correlation.

Two reports have been prepared. One covers the experimental data for the coexistence curves for the nine binary liquid mixtures for which extensive data are available. The other gives a detailed analysis of the specific heat data for magnetic solids in the critical region. Scaling law techniques were used to analyze and correlate the data.

Future Plans: With the completion of the reports mentioned, the project will have been completed.

15. Title: Physical and Thermodynamic Properties of Molten Salts

Principal Investigator: G. J. Janz

Location: Molten Salts Data Center, Rensselaer

Polytechnic Institute, Troy, New York

Date Initiated: 1965 (Center also supported by U. S. Air Force)

Objective: The compilation and evaluation of data on thermodynamic, electrochemical and physical properties of molten salts and their mixtures.

Current Status: The Center compiles and evaluates data on the conductivity, density, surface tension and viscosity of fused salts and on the thermodynamics of some electrode processes. A report on the properties of binary systems of nitrites, nitrates and their mixtures has been submitted for publication and is identified more fully in Appendix III, NSRDS Publications List. The Center is compiling and evaluating data on the above properties for binary halide systems. The files of the Center have been automated and its monthly listings are used to assist in the preparation of an awareness service put out by Sandia Corporation.

Future Plans: A report will be prepared on the binary halide mixtures and the data for other binary systems will be compiled and evaluated. The files for single-salt melts will be kept up-to-date.

16. Title: Electrolyte Thermodynamic Data

Principal Investigator: R. L. Nuttall

Location: Aqueous Electrolyte Data Center, Physical Chemistry
Division, NBS, Washington, D. C.

Date Initiated: 1971

Objective: The compilation and critical evaluation of thermodynamic data on aqueous electrolyte systems.

Current Status: The Center has been organized only recently and is currently in the process of developing the scope of its operations. One known task will be to cooperate with the Chemical Thermodynamic Data Group in the evaluation of the standard enthalpies and entropies of aqueous electrolyte systems. A publication on the activities of 1:1 electrolyte solutions resulting from the activities of a previous project in this field is listed elsewhere in this report.

Future Plans: These will be determined in large measure by a current planning effort.

17. Title: Complex Stability Constants

Principal Investigator: Y. Marcus and S. A. Kertes

Location: Hebrew University, Jerusalem, Israel

Date Initiated: 1968 (Special Foreign Currency Program fund)

Objective: The compilation and critical evaluation of data on the equilibrium constants for the formation of complexes in homogeneous and heterogeneous liquid systems.

Current Status: This project is a cooperative project with Commission V6, the Commission on Equilibrium Data, of the Division of Analytical Chemistry of the International Union of Pure and Applied Chemistry. A paper on the equilibrium constants of liquid-liquid distribution reactions for organophosphorus extractants (alkylphosphoric acids; alkylphosphonates and phosphinates, and alkylphosphine oxide) has been prepared and will be printed by IUPAC.

Future Plans: Work is proceeding on the compilation and evaluation of data for other classes of organic extractants.

18. Title: Constitution of Binary Alloys

Principal Investigator: R. P. Elliott

Location: Binary Metal and Metalloid Constitution Data
Center, ITT Research Institute, Chicago, Illinois

Date Initiated: 1967 (Center also supported by AEC
and U. S. Air Force)

Objective: Compilation and critical evaluation of data on phase equilibria and constitution of binary metallic systems.

Current Status: A comprehensive report on the phase diagrams for binary alloys, one component of which starts with the letter "a", is being completed. An extensive automated bibliographic file has also been developed.

Future Plans: It has become necessary to terminate this project.

19. Title: High Pressure Data

Principal Investigators: H. T. Hall and L. Merrill

Location: High Pressure Data Center, Brigham Young
University, Provo, Utah

Date Initiated: 1965

Objective: The compilation and evaluation of data on the high pressure properties of solids.

Current Status: The center has completed a critical review on the measurement of high pressures which should serve as a source book for the development of an international pressure scale. Two indexed bibliographies covering the world's literature in high pressure research have also been completed. Formal listings of these three products can be found elsewhere in this report. The center also produces a current awareness service covering the world's literature.

Future Plans: A preliminary report on the properties of high pressure phases has already been prepared and a comprehensive critical evaluation is in process. The Current Awareness Service will also be continued.

20. Title: Thermal Conductivity of Selected Materials

Principal Investigator: Y. S. Touloukian

Location: Thermophysical Properties Research Center,
Purdue University, West Lafayette, Indiana

Date Initiated: 1964 (Center receives funds from many sources, notably U. S. Air Force)

Objective: Compilation and evaluation of data on the thermal conductivity of the elements and selected solid materials.

Current Status: A comprehensive critical evaluation of the data on the thermal conductivities of the elements has been completed. All elements and all phases are included over the temperature range for which data are available. A condensed version of the evaluation is being published in the Journal of Physical and Chemical Reference Data; the comprehensive evaluation will be published as a supplementary volume of the Journal. A formal reference is given elsewhere in this report.

Future Plans: Work has been started on the thermal conductivity of alloys. Data on electrical conductivity as well as thermal conductivity will be compiled and evaluated. Data on the viscosities and heat capacities of a set of industrially important fluids have also been compiled and may be evaluated. The files on the thermal conductivity of the elements will be kept up-to-date.

21. Title: Transport Properties of Fluids

Principal Investigator: H. J. M. Hanley

Location: Cryogenics Division, NBS, Boulder, Colorado

Date Initiated: 1968

Objective: Critical evaluation of data on the transport properties of fluids of cryogenic interest.

Current Status: Techniques for interrelating the transport properties of a fluid, i.e., the viscosity, thermal conductivity, diffusivity and thermal diffusivity, with one another and with equilibrium thermodynamic properties have been developed and refined. The development of tables of critically evaluated data on a set of fluids has been started. Tables for fluorine have been completed.

Future Plans: A set of tables for Ar, Kr, Xe, O₂ and N₂ will be completed in addition to the table for F₂ just mentioned.

22. Title: Transport Properties of Fluids in the Critical Region

Principal Investigator: J. V. Sengers

Location: Institute of Molecular Physics, University
of Maryland, College Park, Maryland

Date Initiated: 1972 (Center also receives funds
from U. S. Air Force)

Objective: A critical evaluation of data for the transport properties
of fluids in the critical region.

Current Status: This project is in its early stages. New developments
based on scaling law theory are being applied to existing
experimental data in the critical region to assist in the
comparison of data from different experimenters and to interpolate
between sets of measurements. The critical region is of
particular importance, both for equilibrium properties and for
transport properties. Many properties change character
drastically in the vicinity of the critical region and these
changes are of both theoretical and technological importance, the
more so as more technological processes approach or span the
critical region. Since critical properties are difficult to
measure, are markedly different from the same properties away from
the critical region, and are used as base points for a variety of
extrapolation and estimation procedures, a critical analysis of
the data on these properties is badly needed.

Future Plans: A critical assessment of thermal conductivity data in
the critical region will be completed.

B. ATOMIC AND MOLECULAR DATA

The NSRDS program for Atomic and Molecular Data places major emphasis on two elements. The first element is timely completion of data compilations on atomic and molecular spectroscopy, collision and ionization processes and related subjects. NBS staff scientists are deeply involved in many of these projects. The second element is cooperative development and application of data standards, evaluation criteria, and compilation planning for several of the specific fields of molecular spectroscopy. Panels of outside advisors, including representatives of appropriate professional societies, are features of these latter efforts, which seek more to coordinate and assist actual data compilation activities than to operate them.

In its support of both elements, OSRD follows the priority list which evolved during two meetings (in 1965 and 1967) of the Advisory Panel on Atomic and Molecular Properties. While the Advisory Panel as a whole has not met for five years, OSRD has had much valuable counsel from ad hoc subpanels on a number of special subjects. The two most recently-formed of these subpanels are concerned with interatomic distances and microwave spectral data. Other panels focus on infrared and laser Raman spectral data and data derived from NMR spectroscopy.

The Joint Committee on Atomic and Molecular Physical Data, which was originally formed (with the encouragement of OSRD) to provide a focus for the participation of professional societies and trade associations in the compilation of infrared spectra, has expanded its goals to include other spectral areas. This Joint Committee, in fact, has become an important channel for the cooperative efforts mentioned above. It provides a valuable augmentation of the efforts of OSRD through the volunteer services of many dedicated scientists in government laboratories, private industry and universities. The Joint Committee has set up subcommittees on each of the major areas of applied molecular spectroscopy - IR, NMR, Laser-Raman, Mass and Microwave Spectra, which parallel the NDAB ad hoc Advisory Panels in interest (and which include many of the same experts). With modest support from OSRD for travel and similar expenses, these subcommittees have taken a leading role in the development of criteria for the production of reliable analytical spectra, and in promoting international acceptance of these criteria through the Commission on Molecular Structure and Spectroscopy of the International Union of Pure and Applied Chemistry. A set of "Recommendations for the Presentation of Raman Spectra for Cataloging and Documentation in Permanent Data Collections" was approved by IUPAC in July, 1971. Tentative approval has been achieved for parallel documents on Infrared and NMR Spectra.

The data evaluation projects in this area continue to emphasize atomic and molecular spectra, collision cross-sections and certain other molecular properties. In the two-year period since the last status report, publications have been issued which deal with atomic data derived from optical spectra, ionization of atoms by electron impact, ultraviolet photo-absorption cross-sections, the absorption spectrum of carbon monoxide, molecular vibrational frequencies, and the spectrum of molecular oxygen. While funding limitations have prohibited the start of any major new projects, small efforts have begun on a revision of the fundamental constants and an exploration of the value of high quality infrared molecular spectral data. Planning has been completed for a project on interatomic distances, and compilation work has started at an informal level.

The charter of the standard reference data program recognizes the appropriateness of support of experimental determination of data to which a particularly high importance is attached. Such "benchmark" data can include

measurements aimed at either (a) clearing up major discrepancies in key physical properties; or (b) providing a reliable value of a quantity to which a large number of relative measurements can be tied. A project of this type has been underway for some time on the measurement of the absolute cross section for excitation of helium by electron impact. This experiment has been designed to provide a definitive value of the cross section, with a reliable estimate of the limits of systematic error; in addition, it is expected to lead to criteria for making cross section measurements of other types. This experiment will be completed in the coming fiscal year.

Active Projects:

1. Title: Precision Measurement and Fundamental Constants

Principal Investigator: Barry N. Taylor

Location: Electricity Division, NBS, Washington, D. C.

Date Initiated: 1971

Objective: To provide continuing review and appropriate analysis and updating of the values for the fundamental physical constants and their precise measurement. These measurements are ultimately related to the basic standards maintained by NBS.

Current Status: The status of the fundamental constants is being reviewed, and a new least-squares adjusted set of recommended values is being developed for international adoption.

Future Plans: The set of recommended values will be submitted to CODATA; its official adoption and recommendation for international use is expected during the next year. A manuscript detailing the evaluation procedures will be prepared.

2. Title: Atomic Energy Levels Data Center

Principal Investigators: W. C. Martin

Location: Optical Physics Division, NBS, Washington, D. C.

Date Initiated: 1966

Objective: The objective is to compile, evaluate and disseminate data on atomic energy levels and spectra. A literature file is maintained.

Current Status: An automated system involving punched paper tape and transfer to magnetic tape for storage is in operation for bibliographic information. The tape can be reformatted, sorted by authors for an author index, and can be converted to Linotron tape for publication. A new bibliography entitled, "Bibliography on Atomic Energy Levels and Spectra, July 1968 through June 1971," NBS Spec. Pub. 363 appeared in June 1972. Additional sections of NSRDS-NBS 3 "Selected Tables of Atomic Spectra" have been published by C. M. Sitterly for C I - C VI and N IV - N VII; in preparation is N I - N III. The tables for H I, D I, and T I will appear soon.

Future Plans: Work on a compilation of the energy levels of the lanthanide atoms and ions is underway. Another planned publication is a similar volume covering the actinide elements. Revised compilations of energy levels for the elements covered in Vols. 1-3 of Atomic Energy Levels are also planned. Such a revised compilation for the iron spectra Fe I - XXVI is nearing completion. Also planned are additional sections of NSRDS-NBS 3 for helium, lithium, beryllium, boron and oxygen.

3. Title: Spectroscopy of Two-Electron Atoms

Principal Investigator: C. L. Pekeris

Location: Weizmann Institute of Science, Rehovoth, Israel

Date Initiated: 1968 (Supported by Special Foreign
Currency Program)

Objective: The objective is to provide very accurate solutions of the Schrodinger wave equation to give the transition parameters and term values for two-electron atoms. This will involve the evaluation of f values for transitions between singlet and triplet S states and singlet and triplet P states. The results will be compared with existing values. This work is directly useful to the compilation activities of the NBS Atomic Energy Levels Data Center.

Current Status: Two papers have already been published resulting from this project. They are:

- 1) "Fine-Structure of the 2^3p , 3^3p , and 4^3p States of Li^+ ", B. Schiff, Y. Accad and C. L. Pekeris, Phys. Rev. A1 1837 (1970).
- 2) "Low-Energy Photionization for the 1^1S and 2^1S States of Helium", Verne Jacobs, Phys. Rev. A1 289 (1971).

Two further papers are under preparation on the calculation of energy levels, f -values, and other properties of selected states in the heliumisoelectronic sequence up to $Z=10$.

4. Title: Calculations of Atomic Spectra of the Transition Groups and Rare Earth Elements

Principal Investigators: Y. Shadmi and Z. B. Goldschmidt

Location: Hebrew University, Jerusalem, Israel

Date Initiated: 1968 (Supported by Special Foreign Currency
Program)

Objective: The objective is to calculate spectral energy levels for the transition groups and rare earth elements and theoretically predict their spectra. Results are directly useful to both data compilation and experimental programs at NBS concerning atomic spectra and energy levels.

Current Status: Theoretical interpretation of many rare-earth spectra has been developed to the point where it is possible to make detailed predictions about their structure even in cases where the experimental material is very poor.

Special results include:

- a) extensive analysis of odd and even configurations of Ce I, with results to be published shortly;
- b) theoretical interpretation of several configurations of Eu I and Gd II (results published);
- c) similar results ready for publication on Yb I and Ce II;
- d) systematic analysis of magnetic interactions and inclusion of these interactions in energy level calculations.
- e) progress in the development and application of algebraic formulas for the matrix elements for theoretical interpretation of complex spectra.

Future Plans: Extension of the theoretical interpretation of Ce I spectra, and completion of the work on Gd I, Yb I, Eu I, La II, Ce II, Gd II, Yb II, Hf II, Pr III, Er IV.

5. Title: Description and Analysis of the Spectra of Neutral and Singly Ionized Erbium and Holmium

Principal Investigator: N. Spector

Location: Soreq Nuclear Research Center, Yavne, Israel

Date Initiated: 1967 (Supported by Special Foreign Currency)

Objective: The objective of the project is to measure, describe, classify and compile the line spectra of neutral and singly ionized erbium and holmium. The results will be employed in an interpretation of atomic energy levels.

Current Status: The full description of the erbium spectrum in the photographic region in air has been completed. Two separate lists, one of Er I and the other of Er II, are available. The wavelength range covered is 2100A to 12300A. The accuracy of the measurements is compatible with the requirements for term analysis, which is still needed in both spectra, and which is now in progress.

Active work is in progress on the coverage of the holmium spectra in the photographic infrared. A line list will be compiled of Ho I and Ho II from 7300A to 1200A, fully separated into I and II.

Associated work on other lanthanides is also being performed, including calculations on singly ionized samarium and gadolinium and neutral terbium.

Future Plans: Completion of the description of the holmium spectra and their subsequent analysis (both to be done in collaboration with the NBS spectral data project) are first priority.

6. Title: Atomic Transition Probabilities Data Center

Principal Investigator: W. L. Wiese

Location: Optical Physics Division, NBS, Washington, D. C.

Date Initiated: 1960

Objective: This center compiles, evaluates and disseminates data on radiative transition probabilities of atoms and atomic ions in the gas phase. All elements are covered. The literature relevant to the subject is covered comprehensively, and bibliographies are issued as the content of the literature file warrants.

Current Status: Two critical compilations of atomic transition probabilities covering the first twenty elements of the periodic table have been published as NSRDS-NBS 4 and NSRDS-NBS 22. A critical compilation on Ba I and II was published as NBS Technical Note 474. A compilation of forbidden transitions of the iron group is being prepared for publication in the Journal of Physical and Chemical Reference Data. Two bibliographies on transition probabilities have appeared.

Future Plans: Analysis of the literature on transition probabilities will proceed, and additional tables will be issued, covering elements of higher atomic number. Additional bibliographies will be prepared.

7. Title: Data Center on Atomic Line Shapes and Shifts

Principal Investigator: W. L. Wiese

Location: Optical Physics Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1972

Objective: This center compiles, evaluates, and disseminates data on atomic spectral line shapes and shifts. All elements are covered.

The literature relevant to the subject is monitored comprehensively, and bibliographies are issued as the content of the literature file warrants. Critical reviews and evaluations of the numerical material are made and are published under the NSRDS system.

Current Status: The file on the line broadening literature has been recently completed and contains now more than 1400 articles. A comprehensive bibliography on atomic line shapes and shifts covering the literature through March 1972 is in the process of publication (NBS Special Publication 366).

Future Plans: The literature on atomic line shapes and shifts will be monitored, and additional bibliographies will be prepared when sufficient new material is compiled. A critical review on the present status of hydrogen Stark broadening data is in the planning stage.

8. Title: Atomic Collision Cross Section Information Center

Principal Investigator: L. J. Kieffer

Location: Joint Institute for Laboratory Astrophysics,
University of Colorado, Boulder, Colorado

Date Initiated: 1963

Objective: To compile, evaluate and disseminate low energy atomic collision cross section data needed for modeling low pressure ionized gases.

Current Status: Annotated bibliographies of papers containing data on measurements or calculations of low energy electron collision cross sections, photo-absorption and photo-ionization cross sections, electron swarm data, and rate coefficients are maintained on a current basis. A data bank of such data which are needed for the critical review and data compilation projects being carried out in the Information Center is kept up to date. Storage, retrieval and manipulation of these bibliographies and data files are carried out using computers.

Future Plans: Preparation of a series of critical compilations of low energy electron impact cross sections and electron swarm coefficients for all molecular species relevant to aeronomy and modeling of gas discharges and gas lasers; a critical compilation of photo-absorption and photo-ionization cross sections for molecular oxygen; publication of an up-dated version of the "Bibliography of Low Energy Electron Collision Cross Section Data."

9. Title: Atomic and Molecular Processes Information Center

Principal Investigator: C. F. Barnett

Location: Oak Ridge National Laboratory, Oak Ridge,
Tennessee

Date Initiated: 1965 (Joint AEC and NBS support)

Objective: The objective is to collect and maintain a literature file on atomic and molecular collision processes. The abstracted data, with emphasis on heavy particle-heavy particle collision cross sections, are compiled, evaluated, and disseminated in the form of critical reviews.

Current Status: One monograph, entitled "Ion-Molecule Reactions," by McDaniel, Ferguson, Cermak, Friedman and Dalgarno, was published by John Wiley & Sons, Inc., in 1970. Two monographs, "Theory of Charge Exchange," by R. A. Mapleton, and "Excitation in Heavy Particle Collisions," by E. W. Thomas, were published as part of the same series in 1972. Three other volumes are in various stages

of preparation and publication.

Future Plans: Formal support for this Center from the National Standard Reference Data System ceased in June, 1972. The Center will continue to maintain its literature file, and the principal investigator will serve as editor of the monographs which are now being written.

10. Title: Effect of Excitation Upon Atomic Collision Cross Sections

Principal Investigator: J. W. McGowan

Location: University of Western Ontario, London, Ontario, Canada

Date Initiated: 1967 (Advanced Research Projects Agency support)

Objective: This project is intended to provide a review of the quantitative data on the excitation cross sections for collisions of energetic particles (electrons, protons, etc.) with atoms and molecules. Emphasis is given to data describing the production and destruction of long-lived and metastable excited species.

Current Status: The book is being completed following the compilation and evaluation of the data. Five chapters have been drafted and a final report has been submitted to the Office of Standard Reference Data covering the chapters written by the principal investigator.

Future Plans: The monograph will be completed (several co-authors are still preparing their contributions) and published.

11. Title: Compilation and Verification of X-ray Wavelengths

Principal Investigator: J. A. Bearden

Location: Johns Hopkins University, Baltimore, Maryland

Date Initiated: 1966 (NSF support for experimental aspects)

Objective: The objective of this project is to remeasure the wavelength ratios between the W K α x-ray standard and four important secondary standard lines and to place these wavelengths on a more accurate absolute basis through a ruled grating measurement of the Al K α doublet.

Current Status: Tabulations of selected x-ray wavelengths and a reevaluation of x-ray energy levels have been published. The remeasurements have also been completed. A critical monograph entitled "High Precision X-ray Spectroscopy" containing the state-of-the-art in the field and a compilation of x-ray wavelengths and atomic energy levels has been written and submitted to the Office of Standard Reference Data.

Future Plans: The text of the report will be published as a chapter of the forthcoming book "X-Ray Spectroscopy," edited by Leonard Azaroff.

12. Title: X-Ray Attenuation Coefficient Information Center

Principal Investigator: J. H. Hubbell

Location: Center for Radiation Research, NBS, Washington, D. C.

Date Initiated: 1964

Objective: The objective is to compile and evaluate data on attenuation coefficients for high energy photon (1 keV-100 GeV x-rays and gamma rays) interaction with matter including Compton and Rayleigh scattering, atomic photo-effect and electron-positron pair production. A literature reference file on these data, now encompassing the energy range 10 eV to 13.5 GeV, is maintained.

Current Status: A critical monograph, entitled "Photon Cross Sections, Attenuation Coefficients and Energy Absorption Coefficients from 10 keV to 100 GeV," has been published as NSRDS-NBS 29. Ten additional contributions by the principal investigator, all dealing with data aspects of photon interactions, have been published elsewhere. Four other related publications by other authors have appeared with acknowledgement of NSRDS support for their contents via this center.

Future Plans: The basic objectives of the Center will be pursued. The data now covering 23 elements and 13 other substances will be extended to cover 100 elements. The energy range will be extended below 1 keV.

13. Title: Diatomic Molecule Spectral Data Center

Principal Investigator: P. H. Krupenie

Location: Optical Physics Division, NBS, Washington, D. C.

Date Initiated: 1967

Objective: To compile tables and evaluate data, e.g., bandheads, spectral frequencies, molecular energy levels and parameters, and dissociation energies. All pertinent regions of the electromagnetic spectrum are covered.

Current Status: Critical reviews have been published on CO (NSRDS-NBS-5) and O₂ (in the Journal of Physical and Chemical Reference Data, Vol. 1, No. 2).

Future Plans: A similar review on N₂ will be completed.

14. Title: Microwave Spectral Data Center

Principal Investigator: F. J. Lovas

Location: Optical Physics Division, NBS, Washington, D. C.

Date Initiated: 1970

Objective: The objective of this project is to provide a continuing data center for the collection, critical evaluation and dissemination of microwave spectral data for gases. A literature file dating from 1960 is maintained.

Current Status: The spectra of 50 compounds consisting of more than 3000 reported transitions have been evaluated and transferred to punched cards for subsequent storage in the computer.

Very thorough reviews (including some remeasurements and recalculations) have been completed for four of the molecules discovered in recent radiotelescope observations of the interstellar medium. These reviews, on formaldehyde, formamide, methanol and thioformaldehyde, have been circulated in preprint form and are currently in press.

Future Plans: The evaluation, computer storage and computer-controlled printing process will be tested on a small number of molecules exhibiting all anticipated complications in spectral splittings, spectral assignments; and molecular parameters. Evaluation of spectral data will be continued, first for diatomic and triatomic molecules and later for larger molecules, leading to publication of tables of microwave spectra in a format similar to NBS Monograph 70.

15. Title: Criteria for and Issuance of Evaluated Infrared Spectra

Principal Investigator: Coblenz Society Inc.,

R. P. Bauman, President

Location: 761 Main Ave., Norwalk, Connecticut

Date Initiated: 1965

Objective: The Board of Management advises the Office of Standard Reference Data on criteria for the production of high quality infrared spectra. Once the criteria are established, it is to aid in the publication of evaluated infrared spectra.

Current Status: Criteria have been established and published by the Coblenz Society Board of Management and accepted by the Office of Standard Reference Data. These criteria have also been accepted and endorsed in a slightly modified form by IUPAC. With the completion of this phase of the work, the Coblenz Society has undertaken to apply these criteria in the preparation and publication of its own infrared spectral data collection. Four sets, totalling 4000 spectra of Class II and Class III quality, have been published. This work is done without financial support from OSRD.

Future Plans: This project has been formally terminated, although the selection and publication of spectra continues.

16. Title: Specifications for Evaluation of Spectroscopic Data

Principal Investigator: Joint Committee on Atomic and Molecular Physical Data, A. Lee Smith, Chairman

Location: Spectroscopy Laboratory, Dow Corning Corp., Midland, Michigan

Date Initiated: 1971

Objective: To provide a coordinated and cooperative approach to the development of evaluation of various types of atomic and molecular spectroscopic data.

Current Status: Criteria and specifications have been defined and accepted for infrared, NMR and Raman spectral data. Tentative criteria have been prepared for microwave spectral data.

Future Plans: Efforts will be made to further the general adoption and application of criteria already prepared. Final approval will be sought for criteria for microwave spectral data. Studies will be made of needs for criteria for mass spectral data and ultraviolet and visible spectral data.

17. Title: Infrared Bibliography

Principal Investigator: C. N. R. Rao

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1969 (Special Foreign Currency Program fund)

Objective: The objective of this project is to prepare bibliographies on infrared spectroscopy. Using the NRC-NBS Spectral Data File as a base, the effort will search and compile references from 1960 to the present. The material will be indexed by compound including the empirical formula.

Current Status: The text of the completed bibliography is being typed for publication.

Future Plans: The current phase of this undertaking will be completed when the bibliography is published. Future phases will be considered at that time.

18. Title: Data Center for Atomic and Molecular Ionization Processes

Principal Investigator: H. M. Rosenstock

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

Date Initiated: 1966

Objective: The objective is to collect and maintain a literature file from which data on ionization and appearance potentials can be compiled, evaluated, and disseminated.

Current Status: A critical monograph, entitled "Ionization Potentials, Appearance Potentials and Heats of Formation of Gaseous Positive Ions," NSRDS-NBS 26, has been issued. Since that publication, the Center has accumulated an archive of more than 2000 documents concerning approximately 5000 different ions. This material is being used in the preparation of a revision of NSRDS-NBS 26, planned for completion toward the end of 1972. The new compilation will be two to three times the size of the original.

Future Plans: When the revised compilation is completed, the Center will continue its coverage of the literature, with modifications of output and services to be determined by needs of the technical user community.

C. CHEMICAL KINETICS

The program in Chemical Kinetics continues to emphasize critical reviews of rate constant data on gas phase reactions. The continued need for rate data on atmospheric reactions, important to the solution of air pollution problems, was endorsed at an ad hoc meeting of the NAS-NRC Kinetics Panel in Los Angeles in 1971. Subsequent review of the program by the OSRD Evaluation Panel of the National Academy of Sciences has emphasized the similar importance of chemical kinetics data to other NBS program areas, such as fire research and water pollution studies. Current development of the OSRD kinetics program is influenced by expressions of need for data in these areas.

In the past two years, the two Kinetics Data Centers at NBS and the University of Notre Dame have continued to improve their data handling capabilities, and to move toward greater compatibility and sharing of data resources. They now exchange computer tapes containing bibliographic references which they enter in their files. They have issued computer generated bibliographies on selected topics. The Radiation Chemistry Center now publishes a semi-annual index to its weekly current awareness bulletin. Manuscripts of critical reviews in radiation chemistry are also being produced on computer tape for direct phototypesetting and printing. Finally, two projects dealing with solution kinetics have been initiated. The Chemical Kinetics Information Center has issued two reports on evaluated rate constants of air pollution reactions and will soon issue evaluated data sheets on the molecules found to be important in studies of air pollution. Other critical reviews are nearing completion and will be published. A proposed review on Dissociation-Recombination Reaction Rate Constants of H_2 , N_2 , NO, HNO and NO_2 will not be published since the data which were to have been examined in this review have recently appeared in evaluative reviews by Baulch and others.

The program has also increased its role internationally. Representatives of the OSRD and the Chemical Kinetics Information Center are active participants in a CODATA Task Group on Chemical Kinetics which meets regularly. Recent meetings have been held in Paris (May, 1971) and Le Creusot (June, 1972), and a report has been prepared for CODATA by Dr. David Garvin of the NBS Chemical Kinetics Information Center on "Compilation and Data Evaluation Activities in Chemical Kinetics, Photo Chemistry and Radiation Chemistry." The OSRD cooperates actively in exchange of information with its counterparts in the U.K. (OSTI) and the U.S.S.R. A Russian compilation on "Rate Constants of Gas Phase Reactions," by V.N. Kondratiev, has been translated and distributed through the National Technical Information Service.

Active Projects:

1. Title: Chemical Kinetics Information Center

Principal Investigator: David Garvin

Location: Physical Chemistry Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1964 (This project is partially supported by Navy Material Command and the Department of Transportation)

Objective: The objective of this project is to collect and maintain an automated literature reference file on kinetic rate data for

reactions in the gas, liquid, and solid phases. Rate data for selected reactions are compiled, evaluated and published.

Current Status: The number of papers indexed and on file at the Center has reached approximately 24,000. Two bibliographies on the reaction kinetics of sulfur atoms and compounds with H, O, O₂, O₃ and the nitrogen oxides have been issued. In addition, nine short bibliographies on specialized topics (e.g., the combination of radicals in gas phase) have also been issued. A world-wide survey of compilation and evaluation activities in kinetics was prepared for publication in the CODATA Bulletin.

Future Plans: The activity of the Center will continue in accordance with its stated objective.

2. Title: Radiation Chemistry Data Center

Principal Investigator: Alberta Ross

Location: Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana

Date Initiated: 1966 (Cosponsored by AEC)

Objective: The project will develop an automated literature reference file pertinent to radiation chemistry. The Center will compile, evaluate and disseminate reviews on selected topics dealing with radiation chemical data.

Current Status: In addition to a searchable file of over 4,000 papers, the issuance of the weekly bulletin and some bibliographies, the Center has helped prepare five data compilations as input to critical reviews. Three of these are in final stage of publication and have been prepared using computer tape for direct phototypesetting.

Future Plans: Three critical reviews dealing with the radiation chemistry of gaseous ammonia, the solvated electron in alcohols and the hydrated electron will be published in the NSRDS-NBS series. The other activities of the Center will also continue.

3. Title: Reactions of the Hydroxyl Radical in Water

Principal Investigators: L. M. Dorfman and G. E. Adams

Location: Ohio State University, Columbus, Ohio

Date Initiated: 1969

Objective: A monograph is to be written giving a critical evaluation of absolute and relative reaction rate constants for OH radical interactions with various compounds in water. The reactions will cover organic addition, hydrogen abstraction, electron transfer, radical-radical reactions and, for comparison, selected O₂ reactions. Optical absorption, acid dissociation constants, and other properties will also be discussed.

Current Status: A final manuscript has been submitted by the authors and is undergoing review.

Future Plans: The manuscript will be published in the NSRDS-NBS series.

4. Title: Evaluation of Selected Dissociation and Recombination Reaction Rate Constants in Gas Phase

Principal Investigator: K. Schofield

Location: Delco Electronic Laboratories, Goleta, California

Date Initiated: 1970

Objective: The study calls for an evaluation of available gas phase reaction rate data of important dissociation-recombination

reactions which pertain to the lower atmosphere. They include reactions involving the molecules CO, SO₂, SO₃, H₂S, NH₃, CH₄, C₂H₆, NO, NO₂, N₂O, N₂O₄ and the atoms and radicals H, O, SO⁴, HS, NH₂, CH₃ and C₂H₅.

Current Status: A manuscript has been reviewed and is now in its final stages of revision prior to publication.

Future Plans: The revised manuscript will be published in the Journal of Physical and Chemical Reference Data.

5. Title: Solvent Effects in Solution Kinetics

Principal Investigator: R. Parlin

Location: University of Maryland, College Park, Maryland

Date Initiated: 1971

Objective: An annotated bibliography is to be prepared on solvent effects on reaction rates in solution.

Current Status: This project was originally undertaken by Dr. G. Akerlof (deceased) who planned a critical monograph on the subject. The work was halted by his death. The present author plans to use some of the material compiled by Dr. Akerlof. A format has been evolved and the annotation is in preparation.

Future Plans: The final publication will be delayed due to the author's illness.

6. Title: Atom and Radical Abstraction Reactions With Organic Substrates in Liquid Phase

Principal Investigators: Dale G. Hendry and T. Mill

Location: Stanford Research Institute, Menlo Park, California

Date Initiated: 1972

Objective: Selected atom and radical abstraction reactions with organic substrates in liquid phase will be compiled. The data will be evaluated for inclusion in a critical review.

Current Status: The reactions to be compiled and reviewed will include Cl, alkyl (C₁ - C₇), alkoxy and alkylperoxy radicals. Best values for the rate constants will be selected wherever possible. The project has just been initiated.

Future Plans: The review material on Cl atom reactions will be compiled from the literature and the data evaluated.

Title: Air Pollution Data Handbook

Principal Investigators: R. F. Hampson and D. Garvin

Location: Physical Chemistry Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1971

Objective: Data sheets on the basic physical and chemical properties of a number of gaseous air pollutants are to be prepared. The evaluated data are required in the solution of air pollution problems.

Current Status: A number of consultants primarily within NBS have collected and evaluated thermochemical, spectroscopic and kinetic rate data for seven molecules found important in air pollution. They are O, O₃, C₂H₄, CO, CO₂, NO₂ and SO₂. In addition, two NBS reports reviewing the chemical kinetic rate data of 27 reactions of interest in the stratosphere have been released.

Future Plans: The data sheets for the seven species mentioned above will be published. The data for other species will be evaluated and published.

D. SOLID STATE

The Solid State program has grown slowly over the past two years with continued emphasis on the issuance of "Crystal Data Determinative Tables." This latter effort is now in its final stage of completion. Arrangements with the NBS and Cambridge Crystal Data Centers have been finalized for continuing the cooperative production of an updated single crystal data file. The contents of the file would be published at suitable intervals.

Activities in other solid state areas have produced a number of publications. Following the advice of the Ad Hoc Panel on Mossbauer Effect the OSRD has supported the publication of the 1970 Mossbauer Effect Data Index (MEDI). Two new bibliographies describing the computerized file of the Alloy Data Center have been published. The Center is also completing two evaluated data reviews on Knight Shift and Soft X-Ray Spectroscopy. The Superconductivity Center has updated its compilation of data on superconductive materials and these will soon be published. A critical review of diffusion data in copper and copper alloys is now being written by the Diffusion in Metals Data Center. A bibliography on the Properties of Defect Centers on Alkali Halides and a critical review of Phase Transformation Properties in Alkali Halides have also been published. An evaluative effort on the elastic constants of iron-nickel alloys is in progress. The review on energy gaps has been superseded by a recent compilation of band gap data on binary compounds carried out by Dr. W. H. Strehlow of the Minnesota Mining and Manufacturing Co. His compilation will be published by the OSRD.

An Ad Hoc Panel on Electrical Properties of Solids was convened to review the state of the field and provide advice on the needs for data evaluation and compilation on electrical properties. The panel recommended critical reviews on refractive index, dielectric constants and energy band structure of the important materials. The panel noted that it was important to relate OSRD compilation priorities to the growth rate of certain fields, e.g., superconductivity, and to stimulate data efforts on the part of other organizations wherever and whenever possible. The OSRD has responded to these directives by exchanging information on data gathering activities with such organizations as Electronic Properties Information Center (EPIC) in California and the Research Materials Information Center at Oak Ridge. This cooperation led to the identification of an independent compilation effort by the 3M Company on the energy band gaps of binary compounds. This document is now scheduled for publication by the OSRD. Similar cooperative efforts are being sought.

Active Projects:

1. Title: Single Crystal Data Center

Principal Investigator: H. M. Ondik

Location: Inorganic Materials Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1964

Objective: To compile, evaluate and publish selected crystallographic properties of single crystals. An information file to the data is also maintained.

Current Status: The first volume (Organic) of the 3rd edition of Crystal Data has been delivered to the publisher for printing. The second volume (Inorganic) is being completed. A cooperative arrangement between the Center and the Cambridge University

Crystallographic Data Centre has been concluded for handling future data compilation and evaluation of single crystals.
Future Plans: The 3rd edition of "Crystal Data" will be published. The Data Center will continue to compile and evaluate single crystal data in the new mode.

2. Title: Cambridge Crystallographic Data Centre

Principal Investigator: O. Kennard

Location: University of Cambridge, Cambridge, England

Date Initiated: 1964

Objective: Compiling and evaluating single crystal data for organic compounds. An active data file of the selected properties will be maintained. The Centre will cooperate actively with the NBS Single Crystal Data Center in the publication of evaluated single crystal data.

Current Status: The literature has been searched and papers on inorganic and intermetallic compounds and minerals have been sent to the NBS Single Crystal Data Center. About 1,600 organic compound data abstracts have been prepared and entered into an automated file.

Future Plans: The Centre will continue its present activities. A feasibility study is being initiated in the use of an optical character reader device for bibliographic data input.

3. Title: Alloy Data Center

Principal Investigator: G. C. Carter

Location: Metallurgy Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1966

Objective: The primary objective is to maintain an automated file of literature on the properties of alloys, with particular emphasis on Knight shifts and soft X-ray data. Critical evaluations are carried out in these two areas.

Current Status: The automated literature reference file has been improved and continually updated. Two bibliographies listing the file holdings, both by material and by author, have been issued. Two critical reviews on "Metallic Shifts in NMR" and "Soft X-ray Emission Spectroscopy" are in varying stages of completion.

Future Plans: A bibliography on hyperfine fields in metals and alloys is planned. The activities of the data center will continue. The two critical evaluations will be published.

4. Title: Diffusion in Metals Data Center

Principal Investigator: J. R. Manning

Location: Metallurgy Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1964

Objective: The objective is to collect and maintain a literature reference file on diffusion data in metals and alloys. The data are to be compiled, evaluated, and issued as a series of monographs covering pure metals and binary alloys.

Current Status: This activity has been accelerated and boasts a reference file of 8,600 papers on diffusion data in metals and alloys. A monograph of critically evaluated diffusion data for copper and copper alloys is now being written.

Future Plans: The monograph on the copper will be completed and published. Desirability of automating the bibliographic file is being evaluated.

5. Title: Superconductive Materials Data Center

Principal Investigator: B. W. Roberts

Location: General Electric Research and Development Center,
Schenectady, New York

Date Initiated: 1965

Objective: The objective is to maintain a data set on superconductive materials which is evaluated and arranged for dissemination. Data include transition temperatures, critical field strengths, and crystal structure.

Current Status: A third manuscript of superconductive properties data is now in publication. It will be published as NBS Technical Note 724.

Future Plans: A critical evaluation of all the data will be initiated. The compilation and publication of new data will continue.

6. Title: Compilation of Thermal Expansion Data

Principal Investigator: R. K. Kirby

Location: Inorganic Materials Division, National Bureau of
Standards, Washington, D. C.

Date Initiated: 1970

Objective: The objective of this project is to compile and analyze the data on the thermal expansion of the elements in the solid state. The principal investigator will cooperate with the Thermophysical Properties Research Center (TPRC) at Purdue University, which will furnish bibliographic assistance and other data information, so that a selection of recommended values of linear expansion and expansivity can be made.

Current Status: The desired format for exchanging information between groups has been achieved. The analysis of data for five elements is in progress.

Future Plans: Tabulation and evaluation of thermal expansion data will continue.

7. Title: Compilation of Static Dielectric Constants

Principal Investigator: K. F. Young

Location: Inorganic Materials Division, National Bureau of
Standards, Washington, D. C.

Date Initiated: 1970

Objective: The objective of this project is to provide enlarged and improved on the static dielectric constants of selected inorganic materials. The information listed, when available, will include the effect of temperature, pressure, and frequency on the constant. Data on ϵ'' or $\tan \delta$ (losses) will be included.

Current Status: Data for over a hundred dielectric materials have been tabulated and evaluated. A critical review is now being written.

Future Plans: The review will be completed and published, probably in the American Institute of Physics Handbook of Physics.

8. Title: Compilation on Defect Properties of Non-Metallic Crystals

Principal Investigator: S. C. Jain

Location: Originally at the Indian Institute of Technology, now at Solidstate Physics Laboratory, New Delhi, India

Date Initiated: 1967 (Supported by the Special Foreign Currency Program)

Objective: The objective of this project is to compile and evaluate the properties of defects in non-metallic crystals. The properties to be covered are the optical properties and energy levels of ions and molecules in crystals; energies of formation, migration, solution, and association of point defects in crystals; colloidal and surface properties in crystals.

Current Status: A bibliography on impurity center properties in alkali halides has been published as OSRDB 71-1. A critical review of the optical properties of defects in alkali halides is being written.

Future Plans: The critical review will be published.

9. Title: Compilation of Data on Phase Transformations in Solids

Principal Investigator: C. N. R. Rao

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1967 (Supported by the Special Currency Program)

Objective: This project will survey the literature on phase transformation in solids with a view toward preparing bibliographies and compilations of evaluated data. In addition to transition temperatures, other important and related thermodynamic and kinetic parameters will be given. The reviews will be limited to simple inorganic compounds such as chlorides, cyanides, sulfates, nitrates, chlorates, phosphates and oxides.

Current Status: A critical review of data on phase transformations in binary halides has been completed and will be issued as NSRDS-NBS 41. Another review on the metal oxides is being written.

Future Plans: The review on the metal oxides will be completed and published. Other reviews will be initiated.

10. Title: Compilation of Elastic Constant Data for Metals and Alloys

Principal Investigator: H. M. Ledbetter

Location: Cryogenics Division, National Bureau of Standards, Boulder, Colorado

Date Initiated: 1971

Objective: The elastic constant data for metals and alloys of technological importance will be compiled and evaluated. All variables for both single crystal and "bulk" constants will be examined.

Current Status: The constants of iron-nickel alloys have been chosen for review. The data have been compiled and evaluated and the manuscript is now in draft stage.

Future Plans: Elastic constant data for other materials will be reviewed.

E. NUCLEAR DATA

The U. S. Atomic Energy Commission has recently established a U. S. Nuclear Data Committee (USNDC) to serve as an informal advisory group to its Physical Research Division. The charter for the USNDC calls upon it to provide advice and recommendations on data compilation activities to the Office of Standard Reference Data, as well as to the Atomic Energy Commission. The Chief of the Office of Standard Reference Data attends relevant meetings of the USNDC and a physicist from the NBS Center for Radiation Research serves as a member of the committee.

Joint sponsorship of nuclear data projects by the OSRD with the AEC now includes the Table of Isotopes Group in Berkeley, California. This group is cooperating actively with the Nuclear Data Group at Oak Ridge National Laboratory in compiling, updating and indexing nuclear property data. The final aim is a computerized file which can be used as a basis for publishing an updated version of the "Table of Isotopes." International cooperation with groups in Russia (Leningrad) and with the International Atomic Energy Agency in Vienna is also taking place.

Several ongoing projects continue their progress. The Center has issued four publications. The Photonuclear Data Center is initiating an evaluative effort, and work on the updating of "Tables of Nuclear Spins and Moments" is nearing completion. Similarly, a compilation of data on "Lifetime of Nuclear States" is nearing completion.

Active Projects:

1. Title: Photonuclear Data Center

Principal Investigator: E. G. Fuller

Location: Linac Radiation Division, National Bureau of Standards, Washington, D. C.

Date Initiated: 1963

Objective: To maintain files of references and data on the interactions of high energy electromagnetic radiation with nuclei; to compile and evaluate cross sections and other data on selected nuclei.

Current Status: New techniques for improving the computerized data file have been introduced. The files have been expanded to include data in over 350 graphical displays. A third supplement to the photonuclear data index is being produced.

Future Plans: The third supplement to the photonuclear data index will be completed. An effort to evaluate and publish photonuclear cross section data has been initiated.

2. Title: Fundamental Particle Data Center

Principal Investigator: A. H. Rosenfeld

Location: Lawrence Radiation Laboratory, University of California, Berkeley, California

Date Initiated: 1969 (Particle Data Group has been in operation since 1958) (Cosponsorship by AEC)

Objective: To compile and evaluate data on particle properties and cross sections for particle reactions.

Current Status: In addition to issuing the annual data reports on particle properties, a compilation of cross sections and angular

distributions is in progress. The Center plans to issue current lists of experiments being conducted at accelerator sites. Tapes of Data on Stable Two Body (S2) and Quasi Two Body (Q2) interactions have been acquired. A compilation of Inclusive Reactions is nearly complete. A compilation of NN and ND Reactions has been issued.

Future Plans: The Center will complete and publish the various compilations now in progress.

3. Title: Table of Isotopes Project

Principal Investigator: J. H. Mollander

Location: Lawrence Radiation Laboratory, University of California, Berkeley, California

Date Initiated: 1970 (Sponsored by AEC and OSRD)

Objective: The "Table of Isotopes" data will be revised and updated as required. The data will be entered into a computerized data file for easy handling and for use in the production of subsidiary data compilations.

Current Status: The project is proceeding with data compilation and evaluation. Approximately 25 mass numbers have been reviewed. A cooperative literature searching technique has been achieved with Oak Ridge.

Future Plans: The group will establish a computerized file of the data. It will evaluate an additional body of mass numbers.

4. Title: Nuclear Spins and Moments Project

Principal Investigator: G. Fuller

Location: 9016 Moneybee Lane, Bethesda, Maryland

Date Initiated: 1970

Objective: The tables on nuclear spins and moments which appeared in Nuclear Data Tables A5 Nos. 5-6 (1969) are to be updated.

Current Status: The updating and revision of several tabular sections have been completed. A draft of the final manuscript is being written.

Future Plans: The tables will be completed and published.

5. Title: Lifetimes of Nuclear States Project

Principal Investigator: G. N. Rao

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1970 (Supported by the Special Foreign Currency Program)

Objective: This project will compile and evaluate hyperfine fields and the magnetic properties of nuclear states and lifetimes. It will also examine related angular correlation data of species resulting from a variety of nuclear reactions.

Current Status: The compilation on nuclear lifetime data has been reviewed as a final draft. A manuscript on hyperfine field data is in preparation.

Future Plans: Both manuscripts will be completed and published.

F. COLLOID AND SURFACE PROPERTIES

Three publications have resulted from projects in this area in the period since the last status report: NSRDS-NBS 36 on critical micelle concentrations, and two papers on critical supersaturation and evaporation coefficients in Vol. 1, No. 1, of the Journal of Physical and Chemical Reference Data. In addition a monograph on surface tensions has been scheduled for early publication in the Journal and two additional critical reviews are themselves in the review process. Because of budget limitations it has not been possible to initiate new data compilation projects. However, OSRD continues active planning and consultation with advisors in this important technical area.

Active Projects:

1. Title: Properties of Importance in Phase Transformation Kinetics

Principal Investigator: G. M. Pound

Location: Stanford University, Palo Alto, California

Date Initiated: 1967

Objective: The critical review of several properties of importance in the study of phase transformation kinetics including coefficients of evaporation and condensation of liquids and solids, critical supersaturation for homogeneous and heterogeneous nucleation, and slopes of liquidus lines on phase diagrams.

Current Status: Two papers, one on critical supersaturation for nucleation of liquids and one on evaporation and condensation coefficients have been published and formal references are present elsewhere in this report. Two other reports are in the review process.

Future Plans: Studies on critical supersaturations for nucleation on a substrate and for equilibrium distribution coefficients in alloys are in their latter stages. Work is also proceeding on evaluation of specific surface free energies for solid surfaces. With the completion of these topics the project will come to a close.

2. Title: Electrochemical Properties of Interfaces

Principal Investigator: J. Lyklema

Location: Agricultural University, Wageningen, The Netherlands

Date Initiated: 1965

Objective: The compilation and evaluation of data on such properties as double layer charge and capacity, electrocapillary curves, electrokinetics, surface conduction and points of zero charge.

Current Status: A comprehensive compilation of the data from the literature on the properties listed above has been completed. The critical evaluation of this is well along and a final report is being prepared.

Future Plans: With the submission of the final report this project will be completed.

G. MECHANICAL PROPERTIES

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 have precluded the initiation of any systematic program in this area, and further formal planning was postponed for several years. Although funds for a major effort are still not available, it is believed that a start on a modest program can be made within the next year or two, and work to develop a detailed plan for this area is again underway.

The planning effort started with a review of the 1964 list, involving 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 are included in the Thermodynamics and Transport Properties area), which were then circulated to a larger group including users and producers.

The comments and suggestions of this larger group, about eighty individuals, have been received, and the formulation of a detailed program which tries to meet the varied needs expressed has been started, beginning with metals. We mention here only a few points on which there is a general consensus, and a few others on which there is some disagreement.

We should develop a program whose output will be useful to all who need and use mechanical properties data--including scientists, engineers, and designers. But we should not include material of only transitory interest, nor duplicate without some very good reason the information being produced by others. We should try to emphasize base or key values, but in some cases it is not yet clear which properties and materials are implied by this requirement.

There is little disagreement that we must adopt a somewhat pragmatic approach in interpreting "well defined properties" which express many kinds of mechanical behavior. In many cases the properties used to express important aspects of mechanical behavior are valid only within certain limits on the type or rate of deformation, the sample size, or other aspects of the test involved.

Often the most important information about the mechanical behavior of a material is given by quantities like a glass transition temperature, or an activation energy, or by structural information like the slip, twinning, and fracture systems for a given material. Such information should be included with the direct mechanical properties as appropriate for various materials.

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. This is true even when we include, as we must at present, details of sample history (thermal and mechanical) in addition to composition and the structural parameters we can now define, measure and use.

It is clear that critical reviews will play a large part in the mechanical properties program. A number of the comments suggested including also papers designed primarily to describe the use of relatively new material properties (like plane strain fracture toughness). We believe that the NSRDS Program should continue to emphasize data, with whatever textual material is needed to explain its significance and limitations, but stopping short of papers primarily of a tutorial nature.

A number of objections were made to our initial suggestion that the materials covered be limited to relatively simple systems. Most (though not all) of those interested in metals, for example, maintain that commercial alloys should be included, despite the inherent variability of such materials due to the range in composition and details of production accepted in practice. Typical values and ranges for many properties of such alloys are given in various handbooks, publications by ASTM and other societies, and data sheets or handbooks compiled by producers. Also, several organizations can provide additional information in response to specific requests and prepare special compilations from time to time. The needs expressed seem to reflect in varying degrees the difficulty of finding desired information scattered through many diverse sources and an uncertainty about the reliability of the values quoted.

We are exploring the question of whether, and if so how, the NSRDS Program should complement the varied activities and the existing references mentioned above. It may be that an annotated list of information sources would be useful, since present lists generally do not identify in a specific fashion the information available from each source.

The properties which give rise to the questions noted above are primarily those describing nonlinear, plastic, or ultimate (strength, fracture, etc.) behavior. A number of other, well defined, material properties have been identified, including elastic constants and moduli, and the activation energies, transition temperatures, etc. mentioned earlier. There is reasonable agreement on which properties of this type should be included for metals, ceramics, and simple liquids; for polymers the replies indicate a substantial question about the reliability of available data, and the timeliness of any extensive program coverage of these materials is not yet clear.

III. DATA SYSTEMS DESIGN ACTIVITIES

The Data Systems Design Group is engaged in computer programming, systems design, and application. The present activities include the design and application of a number of general-purpose computer programs for: storage and retrieval, for file manipulation, and for computer-assisted text preparation, editing and printing. In the latter area, the Group is working in close collaboration with the Electronic Printing Section of the NBS Office of Technical Information and Publications in devising a variety of computer-based systems for more effective use of the Electronic Composing System at the Government Printing Office.

The work in this area includes four main activities:

- (a) Development of general-purpose computer programs required for the generation and updating of data files and the preparation of publications therefrom.
- (b) The design of computer-based data files and the retrieval systems to make them accessible to as wide a segment of the technical community as is economically possible.
- (c) Consultation and advisory services to the data centers adhering to the NSRDS System.
- (d) Source automation of technical manuscripts.

The specific projects described below each involve one or more of these main activities. Among the projects in which the Data Systems Design Group is engaged or is promoting are the following:

(1) Computer-Assisted Text Editing and File Manipulation.

The writing of general-purpose programs is continuing with the purpose of developing a system of compatible programs which will exploit the capabilities of the newest computer configurations. The programs and the subroutines they require are being written in ANSI Standard FORTRAN IV. The use of a standard FORTRAN and other self-imposed restraints will make it easier to use the programs on a variety of machines.

The first two releases: NBS Tech. Note 444^{1/} and Tech. Note 470^{2/}, containing the programs SUBSTITUTE and REFORM, have proven to be the "work horses" in a number of larger typesetting programs in daily production. The basic concepts in these two programs have been used with various modifications in two other programs, COMBO and SETAB, which are described in detail below.

^{1/}McClenon, R. C., and Hilsenrath, J., REFORM: A General-Purpose Program for Manipulating Formatted Data Files, NBS Tech Note 444 (Aug. 1968). Available from the National Technical Information Service (NTIS), Department of Commerce, 5285 Port Royal Road, Springfield, Virginia 22151, Price \$3.00.

^{2/}Messina, C. G., and Hilsenrath, J., EDPAC: Utility Programs for Computer-Assisted Editing, Copy Production, and Data Retrieval, NBS Tech Note 470 (Jan 1969). Available from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402, Price 75 cents.

The third release in this series is called COMBO and is described in NBS Tech. Note 700^{3/}. It consists of a main program and modified versions of REFORM, SEARCH, and multiple table SUBSTITUTE. The need for search and retrieval of information in the bibliographic file of the Molten Salts Data Center at Rensselaer Polytechnic Institute motivated the writing of this program. The file consists of cards or card images on magnetic tape. An entry consists of a property card, a journal card, an author card and one or more compound cards. The program can be instructed to search for various terms using a different list of terms for each type of card. When an item is retrieved the lines can be reformatted to produce a more meaningful printout. Although the molten salts file provided the impetus for writing this program, it has been used on other files of similar structure.

(2) Automatic Typesetting and Composition of Data Tables.

Valuable experience has been gained in writing computer programs to convert existing tapes for automatic typesetting of NSRDS publications. An important consideration in this work is to design the programs in so far as possible for general rather than specific applications. While complete generality has not been achieved, the programs produced thus far have wider applicability than to the documents on which they were used.

The experience gained in turning out about a half-dozen publications - more-or-less automatically - is encouraging enough for us to be optimistic that the conversion techniques will soon be simple enough so that each data center will be able to handle the file conversions themselves. This is in sharp contrast to the experience in the recent past when each book of tables required the services for a period of one or more months of a programmer experienced in both computing and typesetting.

The phrase, "more-or-less," is used in the above paragraph because experience has shown that the most expeditious means for producing a finished product is to combine hand operations with computer-aided generations. One reason for our quick success in producing a number of data tables of complex structure is a decision to have the table captions and column headings set by hand and placed on a transparent film. The film is laid over each table, in turn, as the negatives are made.

SETLST and KWIND were the first programs released in this series. These are ANSI FORTRAN IV programs which accept a card deck or FORTRAN record on magnetic tape and insert the appropriate flags and shift symbols required by many of the "standard" typesetting programs associated with phototypesetting devices. KWIND is a program for formatting data entries for KWIC (Key Word In Context) lists. These lists have a space running down the middle of each page, with entries split to straddle the "gutter" and ordered so that successive descriptors to the right of it are in alphabetical order. SETLST is a program for automatically preparing computer listings for automated photocomposition. These programs and their

^{3/}McClenon, R. C., and Hilsenrath, J., COMBO: A General-Purpose Program for Searching, Annotating, Encoding-Decoding and Reformatting Data Files, NBS Tech Note 700. In press.

characteristics are described in NBS Tech. Note 500^{4/}. The SETLST, KWIND, REFORM and EDPAC programs have been put on tape and are being distributed by the NTIS^{5/}.

The second release in this series is called SETAB, an edit-insertion program used mostly for typesetting spectroscopic tables. SETAB is a FORTRAN program that accepts fixed field records on cards or FORTRAN records on magnetic tape and inserts typesetting flags or strings to produce a magnetic tape for input to typography programs such as those used by the Government Printing Office. An example of the typographic complexity that this program can handle is shown in Figure 1. Here the information in the classifications column is handled quite differently depending on whether the character in position 44 is numeric or alphabetic. The program and its characteristics are described in NBS Tech Note 740^{6/}.

(3) Applications of the General Purpose Scientific Document Code System.

A text-handling system based on the General Purpose Scientific Document Code (GPSDC)^{7/} is used by a number of the data centers at NBS. This system was designed and programmed primarily by B. C. Duncan and D. Garvin. W. Evans of the Chemical Thermodynamics Data Center and members of the Data Systems Design Group have added special programs. GPSDC contains a set of 188 characters including upper and lower case Roman and Greek. These can be printed on the line, above the line (as superscripts), and below the line (as subscripts). Characters may be overprinted to form composite characters. The character set has been chosen to be a proper extension of the ASCII^{8/} set. The basic system provides: for input from a variety recording typewriters, for editing and reformatting, for search and retrieval and for output to a line printer and a photocomposition machine. To provide GPSDC printout, a special print train was purchased which contains the 188 GPSDC print characters. This train is used with an IBM 1403 line printer that has 16 half lines per inch line spacing^{9/}.

^{4/}Messina, C. G., and Hilsenrath, J., Edit-Insertion Programs for Automatic Typesetting of Computer Printout, NBS Tech Note 500 (April 1970). Available from Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402, Price 60 cents.

^{5/}NBS Magnetic Tape 2, Fortran Programs for Text Editing, File Manipulating and Automatic Typesetting. Available from the National Technical Information Service (NTIS), Department of Commerce, 5285 Port Royal Road, Springfield, Virginia 22151, Price \$250.

^{6/}Thompson, R. C., and Hilsenrath, J. "SETAB: An Edit Insertion Program for Automatic Typesetting of Spectroscopic and other Computerized Tables". (To appear as NBS Tech Note 740).

^{7/}"The Document Image Code" NBS Tech News Bull. 52 No. 4, 86 (April 1968).

^{8/}"Proposed Revised American Standard for Information Interchange" Communications of the ACM, 8 207 (1965).

^{9/}"Prototype General Purpose Scientific Document Writer Installed" NBS Tech News Bull. 54 No. 2, 35, (Feb. 1970).

Phototypeset output is available via a special program written by Carla Messina that takes the GPSDC information, both textual and tabular, and prepares a magnetic tape which drives the Linotron 1010 phototypesetter at the Government Printing Office.

Use of GPSDC by NSRDS Data Centers is illustrated by the following examples:

The NBS Chemical Kinetics Data Center maintains an automated literature reference file in GPSDC. The information is keyboarded on a Dura (Itel) paper tape typewriter or on a Model 37 teletype. In addition, Linofilm keyboarding has been converted using special programs written by David Garvin. Several NSRDS monographs on kinetics were keyboarded by the U. S. Government Printing Office as part of the normal publication process. The machine-records were converted to GPSDC to add the contents of these publications to the kinetics data file without rekeyboarding. The search and retrieval programs are used to extract bibliographies and data on specific reactions from the data file.

The NBS Chemical Thermodynamics Data Center is using the GPSDC system to print 5x8 cards for their card file. Annotated bibliographic information is keyboarded on a Dura (Itel) paper tape typewriter for input to GPSDC. Special programs written by W. Evans are used to format author and substance-property cards which are then printed on the GPSDC printer. A portion of this input combined with some additional keyboarding is used to construct the inorganic section of the Bulletin of Thermodynamics and Thermochemistry. Programs written by W. H. Evans interpret the chemical formulae and reactions to generate index and sort keys. These keys are used to sort the information and generate an index by chemical formulae. The bibliographic and index sections are printed on the GPSDC printer for use as camera copy.

The Thermodynamics Research Center at Texas A&M University also use GPSDC for their contribution to the Bulletin of Thermodynamics and Thermochemistry. They keyboard the material for the organic section on a Frieden Flexowriter according to instructions from the NBS Chemical Thermodynamics Data Center. All editing, sorting, arranging, and final copy preparation are performed in the GPSDC system in the same manner as the inorganic section.

The NBS Crystal Data Center keyboarded the material for the book "Crystal Data" on a Linofilm keyboard. Later a decision was made to phototypeset the book on the Linotron machine because less errors would be introduced and a better publication schedule could be obtained. The Linofilm records were converted to GPSDC, proof copies were made on the GPSDC printer, and the corrected copy processed to drive the Linotron.

The NBS Alloy Data Center has issued two publications^{10/ 11/} that have passed through GPSDC on their way to publication. The program SETLST was used to convert the information into the desired format for input to GPSDC. Then a Linotron driver tape was produced which was used to prepare the printed copy.

^{10/} Carter, G. C., et al, The NBS Alloy Data Center: Permuted Materials Index, NBS Special Publication 324. Available from the Superintendent of Documents, U. S. Government Printing Office, Washington, D. C. 20402, Price \$7.00.

^{11/} Carter, G. C., et al, The NBS Alloy Data Center: Author Index. NBS-OSRDB-70-2 (COM-71-00722). Available from National Technical Information Service, Springfield, Va. 22151, Price \$10.00.

The NBS Atomic Energy Levels Data Center has keyboarded a bibliography on a Dura (Itel) paper tape typewriter. This bibliography has now been converted to GPSDC. An authors index was generated in GPSDC. The bibliography and index were phototypeset on the Linotron from a driver tape written at NBS via the programs SETDIC and ALGRID.

The NBS Mass Spectroscopy Data Center is preparing a revision of NBS-NSRDS 26. The tables and text are being keyboarded on a Model 37 teletype. The teletype tape is converted to GPSDC. Printout from the GPSDC printer is used for proofreading. After correction the report will be printed by generating a Linotron Driver tape. This is another example of source automation of NSRDS publications.

The Radiation Chemistry Data Center at Notre Dame University is keyboarding reports on a Dura paper tape typewriter. The paper tape is converted to magnetic tape, which is sent to NBS for conversion to GPSDC. Printout from the GPSDC printer is returned for proofreading. Corrections in the GPSDC system are keyboarded on the Dura and converted to magnetic tape which is sent to the Data Systems Design Group for tape updating. After one or more editing cycles the material is processed by Carla Messina's SETDIC and ALGRID programs to produce a magnetic tape to drive the Linotron 1010. This example of source automation is interesting because it was done at some distance rather than close at hand at NBS.

The Analytical Chemistry Division has used SETLST to convert their annotated Activation Analysis bibliography file from all upper case to GPSDC with upper and lower case. They are using the GPSDC system to generate indexes which will be published with the bibliography.

The Fundamental Vibration Frequencies of Molecules project at the University of Tokyo, Japan is keyboarding tables on punched cards using a coding scheme developed by NBS for input to GPSDC. A duplicate deck of cards is sent to NBS to be converted to GPSDC. Printout from the GPSDC printer is returned to Tokyo for proofreading. Editing and corrections of the cards is performed at Tokyo. When the cards for the tables in a report have been punched and corrected, a duplicate set will be sent to NBS to be converted to GPSDC. Then the material will be processed by the SETDIC and ALGRID programs to produce a magnetic tape to drive the Linotron 1010 phototypesetter. The original cards will be retained at Tokyo for updating and to produce a combined publication after several papers have been published. This example of source automation is interesting because it is done in a foreign country.

(4) Automated Citation and Abstract Retrieval.

The various abstracting and alerting services have began supplying their service to customers on magnetic tape. These tapes can be leased and used to supply SDI services and retrospective searches. A number of commercial and nonprofit organizations are presently selling these services. At the present time, they provide hard copy output on cards or paper but they supply no machine readable output. If computer printout is acceptable to the user, these organizations provide the most economical source of such services.

It has been suggested that a machine readable form would be more usable by the data centers associated with NSRDS. To determine the validity of this concept, the Data Systems Design Group has obtained sample SPIN and INSPEC tapes covering the current physics research literature. Computer programs have been written to search these tapes and to reformat the output. Sample searches have been performed for four data centers. Results of these experiments served to convince us that the determination of the utility of computerized abstracts in data center operations required experiments on the

regular releases rather than a sample tape. Accordingly, OSRD has subscribed to the SPIN tapes produced by the American Institute of Physics.

Programs are being written to convert the output of the search to GPSDC so the results can be printed on the GPSDC printer using an extended character set.

(5) Source Automation of Technical Manuscripts. In addition to automating the book production of the National Standard Reference Data System, the staff of the Data Systems Design Group has undertaken the development of on-line keyboarding techniques for the NBS publications. The objectives of the work is to devise techniques that are so simple and cost-effective as to enable the computerization of technical manuscripts literally at the authors desk. The system which has already produced two major publications in the Applied Mathematics Series 12/13 has the following characteristics:

- (a) Keyboarding on a "scripting" typewriter provided upper and lower case Latin and Greek alphabets, in three positions and in two colors.
- (b) On-line keyboarding and text editing at only \$3.00 per hour connect time.
- (c) Conversion via magnetic tape from IBM Archival format provides an additional opportunity for formatting and corrections on the UNIVAC 1108.
- (d) Processing on the 1108 via SETDIC and ALGRID programs produces driver tapes for the Linotron 1010.

When undertaking the development of keyboarding techniques that would be attractive enough for authors and their typists to assume responsibility for supplying machine readable version of their manuscripts, we deemed it essential to change as little as possible, the normal "good practice" employed by typists experienced in the preparation of manuscripts for publication.

The experienced typist is usually careful to align columns of numbers and to center numerators over denominators in displayed mathematical expressions. Our programs rely on these spatial relationships between characters normally found in well typed manuscripts to achieve the corresponding distribution on the typeset page. Excerpts from NBS publications phototypeset from machine readable media produced at the source are shown in Figures 4, 5, and 6.

^{12/}John, et al., Cyclic Designs, NBS Applied Mathematics Series 62, April 1972.

^{13/}Clatworthy, et al., Tables of Two-Associate-Class Partially Balanced Designs, NBS Applied Mathematics Series 63. In press.

(6) Other Activities.

The success of the NBS computerized typesetting operations has attracted attention in a number of government agencies. Prominent among these are the publications office of the Navy Department, the Department of Commerce and the Government Printing Office.

The Office of Publications of the Navy Department has made extensive use of the Robert Thompson's multiple table SETLST program for producing a variety of publications ranging from spare parts lists to Navy training manuals. That program has been rewritten for the IBM 360. It now operates on the computer at the Government Printing Office. At the request of the late Public Printer N. Spence, Carla Messina's program ALGRID was rewritten to operate on the IBM 360/50 at the G.P.O. The use of the ALGRID program reduces to a trivial number the grid changes that are required to typeset scientific material on the Linotron 1010. The use of the ALGRID program reduces the time required to typeset a typical page of complicated scientific text on the Linotron 1010 from a minute to a few seconds. Without this facility it would not be practical to phototypeset the U. S. Patent publications.

TABLE 3. Observed and classified lines of W 1

Wavelength Å	Intensity		Wavenumber (cm ⁻¹)		Classification
	Arc	Spark	Observed	o - c	
2746.734	40		36396.11	+0.02	15 ₃ - 518 ₄
2747.005	50	2	36392.52	+0.06	³ P ₁ - 496 ₂
2747.155	15	3	36390.54		
2747.826	40	2	36381.65	-0.21	⁵ D ₄ - 426 ₃
				+0.16	⁵ D ₂ - 397 ₂
2746.734	40		36396.11	+0.02	153 - 51840
2747.005	50	2	36392.52	+0.06	3P1 - 49620
2747.155	15	3	36390.54		
2747.826	40	2	36381.65	-0.21	5D4 - 42630
				+0.16	5D2 - 39720
2748.312	20	155	36375.21	-0.04	3G4 - 528 ₃
2748.577	30	3	36371.71	+0.02	18 ₃ - 553 ₄
2748.767	5		36369.20	-0.10	20 ₂ - 573 ₃
2748.844	80	20	36368.17	+0.03	⁵ D ₃ - 411 ₄
2748.997	25	2	36366.15	+0.15	19 ₂ - 556 ₂
2749.538	1	2	36359.01		
					³ G ₃ - 496 ₂
					826 ₅ - 561 ₄
					19 ₂ - 561 ₄

Figure 1. A portion of a spectroscopic table set from information supplied on ordinary punched cards. Note how differently the lines containing pure numerics are treated from those that contain mixtures of letters and numbers. This specialized treatment was handled by a general-purpose program called SETAB.

146. Ehmann, W. D., Huizenga, J. R.
Bismuth, thallium and mercury in stone meteorites by activation analysis.
Geochim. Cosmochim. Acta, 17, 125-135 (1959).
(ENGLISH). ARGONNE NATIONAL LAB., LEMONT, ILLINOIS.
147. Eichholz, G. G.
Activation assaying for tantalum ores.
Nucleonics, 10, No. 12, 58-61 (1952).
(ENGLISH). RADIOACTIVITY DIVISION, DEPT. OF MINES AND TECHNICAL SURVEYS, OTTAWA, CANADA.
151. Facchini, U., Orsoni, L.
A method for the determination of uranium content in minerals by using the fission of U-235.
Nuovo Cimento, 6, 241-254 (1949).
(ITALIAN) (ENGLISH SUMMARY). CENTRO INFORMAZIONI STUDI ESPERIENZE (C.I.S.E), MILANO, ITALY.

Figure 2. A portion of a test run of a bibliography produced on the Linotron 1010 at the GPO direct from a tape generated at NBS using the program SETLST. Here the source consisted of fixed field records in all caps. While the need for so much typographic variation is doubtful the exercise illustrates the flexibility of the general-purpose programs employed here.

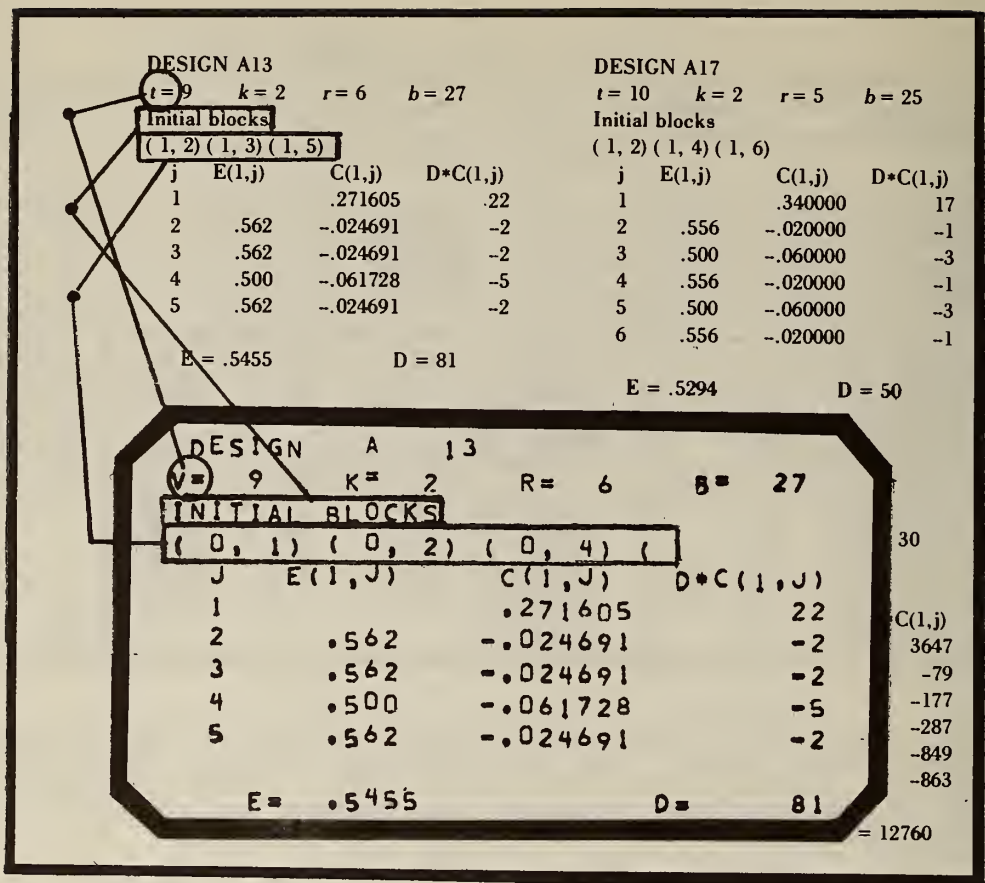


Figure 3. The design tables in AMS 62 were typeset from information on magnetic tape which required three types of transformations shown here. These transformations were handled via a general purpose substitution program instructed by a short substitution table.

References

- Bock, R.D. (1958). Remarks on the test of significance for the method paired comparisons. Psychometrika 23, 323-334.
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- Bock, R.D. (1958). Remarks on the test of significance for the method paired comparisons. Psychometrika 23, 323-334.
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Bose, R.C. and
problem
objects.

10. References

- Bock, R.D. (1958). Remarks on the test of significance for the method of paired comparisons. Psychometrika 23, 323-334.
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- Bose, R.C. and Cameron, J.M. (1967). Calibration designs based on solutions to the tournament problem. J. Res. Nat. Bur. Stand. 71B, 149-169.

tournament
ing pairs of
-332.

Figure 4. A portion of the reference list in AMS 62 shown: as keyboarded on the Model 37 Teletype; as produced on the line-printer after passing through the justification program; and as it appeared on the printed page. Note that the author is able to see, from the computer listing, line for line how the final material will appear when typeset.

	DATA							
	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8
α_1	-25.0	-14.0		-25.0				
α_2		3.1	-8.0		-8.0			
α_3			-22.0	-22.0		-33.0		
α_4				-50.7	-51.7		-59.8	
α_{11}							-66.1	
α_{12}		8.2						-13.0
α_{13}	-3.5		-3.8					
Totals	125.6	15.7	64.9	138.9	104.8	148.0	199.9	155.2

	DATA													Totals
	β_1	β_2	β_3	β_4	β_5	β_6	β_7	β_8	β_9	β_{10}	β_{11}	β_{12}	β_{13}	
α_1	-25.0	-14.0		-25.0						-32.0				-96.0
α_2		3.1	-8.0		-8.0						-16.9			-29.8
α_3			-22.0	-22.0		-33.0						-38.0		-115.0
α_4				-50.7	-51.7		-59.8						-62.9	-225.1
α_5	-40.0				-40.1	-51.0		-50.0						-181.1
α_6		-13.0				-35.9	-34.0		-31.0					-113.9
α_7			-31.1				-40.0	-41.0		-38.0				-150.1
α_8				-41.2				-51.2	-48.0		-50.0			-190.4
α_9					-5.0				-11.0	-11.8		-20.3		-48.1
α_{10}						-28.1				-23.2	-25.2		-28.0	-104.5
α_{11}	-57.1						-66.1				-65.7	-73.1		-262.0
α_{12}		8.2						-13.0				-19.0	-14.3	-38.1
α_{13}	-3.5		-3.8						-10.1				-15.0	-32.4
Totals	125.6	15.7	64.9	138.9	104.8	148.0	199.9	155.2	100.1	105.0	157.8	150.4	120.2	-1586.5

Figure 5. A table from "Cyclic Designs" (AMS 62) as keyboarded on a Model 37 Teletype and as typeset on the Linotron 1010 at the G.P.O. Note that except for the hats that are typed in red to designate bold face, the normal typewritten layout serves to produce a properly aligned photocomposed table.

$$\hat{M}^{-1} = \omega \hat{I} - (1/k)(\omega - \omega') \hat{J}$$

The quantities ω and ω' which enter into the above equations are not known and have to be estimated from the observations themselves. This can be done by forming an auxiliary analysis of variance table (Table 2).

We estimate σ^2 and σ_p^2 by equating b_{ss} and E_{ss} to their expectations. This gives estimates of ω and ω' .

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$$\hat{\omega} = \frac{bk-b-t+1}{E_{ss}}$$

$$\hat{\omega}' = \frac{t(r-1)}{kB_{ss} - \frac{(t-k)E_{ss}}{bk-b+t+1}}$$

$$\hat{\omega} = \frac{bk-b-t+1}{E_{ss}}$$

$$\hat{\omega}' = \frac{t(r-1)}{kB_{ss} - \frac{(t-k)E_{ss}}{bk-b+t+1}}$$

Figure 6. A portion of the text from a book on Cyclic Designs (NBS Applied Mathematics Series 62) as it was keyboarded on a Model 37 Teletype and as it appears in the printed work. The phototypesetter - the Linotron 1010 at the U. S. Government Printing Office - was driven directly from a magnetic tape generated from the original keyboarding by a suite of programs developed under the aegis of the Office of Standard Reference Data. It is an important feature of the system employed here, that it accepts typescript in a form nearly identical to the standard good practice in preparing scientific text for publication on an ordinary typewriter.

IV. INFORMATION SERVICES

Four major activities comprise the Information Services: the maintenance of a data file; editorial liaison assistance between groups producing the data compilations and the publishers; answering inquiries; and analyzing present and future requirements for reference data.

Data File. The mission of the Data File is to acquire selectively world-wide reference data compilations and ancillary publications within the scope of the NSRDS and to organize the collection systematically. A listing, including abstracts of the reference data collection, was published in September 1970 as NBS Technical Note 554, Annotated Accession List of Data Compilations of the NBS Office of Standard Reference Data. It contained almost 1300 items. The Data File has an additional collection of about 600 related documents. As of June 1, 1972, the Data File housed more than 1600 reference data and ancillary publications and more than 1000 related documents. Data File personnel are also in the process of developing an index for NSRDS publications.

Editorial Liaison Services. This activity serves as the editorial intermediary between the data centers of the NSRDS and other individuals and groups producing data compilations and reviews, on the one hand, and publishers on the other hand. A new publisher since early 1972 is a consortium of the American Chemical Society and American Institute of Physics which publishes the Journal of Physical and Chemical Reference Data. Other publishers include the U.S. Government Printing Office, commercial publishers, and the National Technical Information Service. One of the functions of the Editorial Liaison Services is to produce the monthly newsletter, NSRDS NEWS, which has a mailing list of almost 6000. The newsletter contains general information on data evaluation, news of specific projects and announcements of new publications.

The program has produced thus far three quarterly issues of the Journal of Physical and Chemical Reference Data; 53 publications in the NSRDS series of critically evaluated data compilations; 16 other compilations of data; 29 nondata publications from NSRDS-related projects, as well as 33 publications under the aegis of various of its associated data centers.

Inquiry Services. This activity responds to inquiries received by the Office of Standard Reference Data. 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 receives about 1200 requests and inquiries during a calendar year. Negative replies sent during 1971 because of a complete lack of information or inability to refer the correspondent to a likely source of information totalled only eleven.

Analysis and User Relations. The mission of this activity is to provide the Office understanding of requirements, both present and future, of NSRDS's actual and potential users. Among its recent efforts have been two surveys, which are described in the two following paragraphs.

Because technical librarians often serve as intermediaries between National Standard Reference Data System publications and their users, the Office of Standard Reference Data in 1970 surveyed by mail 2,700 selected members of the Special Libraries Association to check their knowledge and use of NSRDS publications as well as to learn the problems they encounter in providing the publications or their data to their users. On the basis of a 22% response, the survey results showed that almost 88% of the responders

have heard of the NSRDS and that about 59% have indicated that their libraries acquire NSRDS publications, but less than 44% of the responders have used an NSRDS publication; however, 94% of this latter percentage (the users) indicated that they have found NSRDS publications very, or to some extent, useful. The survey revealed that distribution and dissemination procedures of NSRDS publications need improvement and that better ways need to be found to acquaint both librarians and users with the data and information contained in NSRDS publications.

In 1971, OSRD surveyed purchasers of NSRDS publications to assess what benefits the publications provided its users as well as to obtain feedback on user experience, requirements, and problems of use. Returns provided evidence that the publications were meeting the two goals of the NSRDS programs: (1) making available reliable physical and chemical reference data; and (2) helping improve the quality and productivity of scientific and technological measurements by means of its published evaluations and criteria. The responders indicated the publications were helpful to them in meeting their data requirements. Specific uses and benefits were identified. The greatest use of NSRDS publications was in connection with basic research. The results of the survey emphasized that awareness and use of NSRDS compilations are steadily increasing but continued and emphasized promotion is needed, especially among scientists and engineers working on applied technological problems.

APPENDIX IA
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.



APPENDIX IB

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

DEFINITIONS

82 STAT. 340

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

CONTINUING DATA CENTERS IN THE UNITED STATES

As the management office for the NSRDS, the OSRD has certain general responsibilities for coordinating all of the physical science-related data compilation and evaluation activities going on with Federal Government sponsorship. This coordination is not restricted to centers formally supported by OSRD. As a minimum level of "coordination," OSRD seeks to learn about and communicate regularly with all such centers which fall within the following guidelines:

- a) The major objective of the center should be to provide evaluated numerical data within the technical scope of NSRDS.
- b) The center should retrieve, store, and index articles within its scope from the world literature, on a regular basis and in a comprehensive manner.
- c) There should be some reasonable expectation of continuity, as demonstrated by the commitment of the personnel and the stability of the financial support.
- d) The output of the center should be readily available.

Listed below are all the identified data centers in the United States which meet these guidelines. To avoid repetition, centers which have been described in Chapter II are listed by title only, with a reference to the earlier entry. The detailed entries which follow are, accordingly, for those centers which have no formal connection with, and receive no financial support from the Office of Standard Reference Data as of June, 1972.

It is recognized that some groups may have been omitted from this list because of a lack of information on their activities. The Office of Standard Reference Data welcomes suggestions on continuing centers which should be included.

A more detailed description of most of the centers may be found in CODATA-International Compendium of Numerical Data Projects, (Springer-Verlag, New York, Heidelberg, Berlin, 1969). Further information is also given in the Directory of Federally Supported Information Analysis Centers, available from the National Technical Information Service, Springfield, Virginia, as COSATI-70-1 (PB 189300).

Code for Source of Support:

NBS: National Bureau of Standards (other than OSRD)
AEC: Atomic Energy Commission
USAF: United States Air Force

LIST OF CONTINUING DATA CENTERS

Thermodynamic and Transport Properties

1. Title: Chemical Thermodynamics Data Center

(See II A1)

2. Title: Thermodynamics Research Center

(See II A4)

3. Title: Thermophysical Properties Research Center

(See II A20)

4. Title: Cryogenic Data Center

(See II A9)

5. Title: JANAF Thermochemical Tables

Location: Dow Thermal Research Laboratory, Midland, Michigan

Director: Formerly, D. R. Stull, now H. Prophet

Source of Support: USAF

Coverage: 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. Other pertinent properties such as molecular weight, point group, ground state configuration or statistical weight, vibrational frequencies and degeneracies, bond distances and angles, and the product of the moments of inertia are also presented.

Form of Output: JANAF Thermochemical Tables, Second Edition, by D. R. Stull and H. Prophet published in 1971 as NSRDS-NBS 37. Additions and revisions released periodically in data-sheet form.

6. Title: Binary Metal and Metalloid Constitution Data Center

(See II A18)

7. Title: Thermodynamic Properties of Metals and Alloys

Location: Lawrence Radiation Laboratory, University of California, Berkeley, California

Director: Ralph Hultgren

Source of Support: AEC and the American Iron and Steel Institute

Coverage: All elements and binary metallic (alloys) systems. For the elements the following properties are considered: heat capacity,

enthalpy (heat content), entropy, Gibbs energy function (free energy function). Values for enthalpy and entropy of phase changes, for Gibbs energy and enthalpy of vaporization, and for vapor pressure are also given. For alloys, the following data are covered: Gibbs energy, entropy, enthalpy, excess Gibbs energy, and excess entropy of formation. Values for activities and activity coefficients, and for partial molar thermodynamic quantities over a range of compositions are given. Phase diagrams for most of the alloys are included. This project is terminating.

Form of Output: Tables will be published as Selected Values for the Thermodynamic Properties of the Elements; and of Binary Alloys (two volumes) by the American Society for Metals.

8. Title: Contributions to the Data on Theoretical Metallurgy

Location: Thermodynamics Laboratory, Albany Metallurgy Research Center, Albany, Oregon

Director: E. G. King; Project Director: A. D. Mah

Source of Support: Bureau of Mines

Coverage: 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, heat content (enthalpy), high and low temperature heat capacity, heat and free energy of formation and phase change, and vapor pressure.

Form of Output: Published as bulletins of the Bureau of Mines. Some related publications appear as Bureau of Mines "Report of Investigations" series.

9. Title: Thermochemistry for Steelmaking

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

Director: J. F. Elliott

Source of Support: American Iron and Steel Institute

Coverage: Selected elements and compounds involved in the chemistry and technology of steelmaking. The compounds include: carbides, nitrides, oxides, phosphides, silicides, and sulfides. Binary and ternary iron alloys and solutions, complex oxide systems, and slags are also treated. The properties include: heat content (enthalpy) and temperature of phase changes; heat capacity; enthalpy, entropy and Gibbs energy function at 100-degree as appropriate. The following properties, as available, are also given: density, thermal conductivity, electrical resistivity, total and spectral emissivity, viscosity, surface tension, vapor pressure, solubility (including gases), diffusion, and activity coefficients.

Form of Output: Book published commercially by Addison-Wesley Publishing Company in 2 volumes, Thermochemistry for Steelmaking.

10. Title: Molten Salts Data Center

(See II A15)

11. Title: High Pressure Data Center

(See II A19)

Atomic and Molecular Data

1. Title: Atomic Energy Levels Data Center
(See II B2)
2. Title: Atomic Transition Probabilities Data Center
(See II B6)
3. Title: Data Center on Atomic Line Shapes and Shifts
(See II B7)
4. Title: Atomic Collision Cross-Section Information Center
(See II B8)
5. Title: Atomic and Molecular Processes Information Center
(See II B9)
6. Title: X-Ray Attenuation Coefficient Information Center
(See II B12)
7. Title: Diatomic Molecule Spectral Data Center
(See II B13)
8. Title: Microwave Spectral Data Center
(See II B14)
9. Title: Data Center for Atomic and Molecular Ionization Processes
(See II B18)

Chemical Kinetics

1. Title: Chemical Kinetics Information Center
(See II C1)
2. Title: Radiation Chemistry Data Center
(See II C2)

Solid State Data

1. Title: Single Crystal Data Center
(See II D1)
2. Title: Cambridge Crystal Data Centre
(See II D2)
3. Title: Alloy Data Center
(See II D3)
4. Title: Diffusion in Metals Data Center
(See II D4)
5. Title: Superconductive Materials Data Center
(See II D5)
6. Title: Phase Diagrams for Ceramists

Location: Inorganic Materials Division, NBS, Washington, D. C.

Director: Ernest M. Levin

Source of Support: American Ceramic Society; NBS

Coverage: Systems of special interest to ceramists: metal-oxygen and metal oxide systems (including Si), systems with oxygen-containing radical systems containing halides, sulfides, cyanides, alone and with other substances, systems of water with metal oxide and miscellaneous substances. Phase diagrams for one-, two-, three-, temperature, and composition. For some systems, multidiagrams show isothermal and isoplethal sections of phase relations; for others, relations, and base systems of tetrahedra are given. Melting points of metallic oxides, molecular weights of oxides and atomic weights are presented.

Form of Output: Publications of the American Ceramic Society.

Nuclear Data

1. Title: Nuclear Data Project

Location: Oak Ridge National Laboratory, P. O. Box X,
Oak Ridge, Tennessee

Director: Daniel J. Horen

Source of Support: AEC

Coverage: Energy Levels and other properties of all nuclides, with
emphasis on those with $A > 40$.

Form of Output: Nuclear Data Sheets, now published as Section B of the
journal, Nuclear Data, Academic Press.

2. Title: Photonuclear Data Center

(See II E1)

3. Title: Table of Isotopes

(See II E3)

4. Title: National Neutron Cross Section Center

Location: Brookhaven National Laboratory, Upton, New York

Director: S. Pearlstein

Source of Support: AEC

Coverage: All available neutron cross section data for all nuclides
and naturally occurring mixtures of isotopes.

Form of Output: Compilations of cross section data, published as the
"Barn Books", (NBL-325 and BNL-400 series). Answers to specific
inquiries for data in form of listings, tapes, or graphical
displays.

5. Title: Physical Data Group

Location: Lawrence Radiation Laboratory, University of
California, Livermore, California

Group Leader: Robert J. Howerton

Source of Support: AEC

Coverage: 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.

Form of Output: State-of-the-art reviews and data compilations,
published as Lawrence Radiation Laboratory reports and in the
professional journals.

6. Title: Fundamental Particle Data Center

(See II E2)

Colloid and Surface Properties

1. Title: Light Scattering Data Center

Location: Clarkson College of Technology, Potsdam,
New York

Director: Joseph Kratochvil

Source of Support:

Coverage: Light scattering in gases, liquids, and liquid mixtures;
refractive index increments in liquids and solutions.

Form of Output: A critically evaluated data compilation of Rayleigh
ratio and depolarization values for liquids and liquid mixtures is
in preparation.

Appendix III

Publications List

Publications in the National Standard Reference Data Series

- ☐ NSRDS-NBS-1, **National Standard Reference Data System—Plan of Operation**, by E. L. Brady and M. B. Wallenstein, 1964 (15 cents), SD Catalog No. C13.48:1.
- ☐ NSRDS-NBS-2, **Thermal Properties of Aqueous Uni-univalent Electrolytes**, by V. B. Parker, 1965 (45 cents), SD Catalog No. C13.48:2.
- ☐ NSRDS-NBS-3, Sec. 1, **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, Si II, Si III, Si IV**, by C. E. Moore, 1965 (35 cents), SD Catalog No. C13.48:3/Sec. 1.
- ☐ NSRDS-NBS-3, Sec. 2, **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, Si I**, by C. E. Moore, 1967 (20 cents), SD Catalog No. C13.48:3/Sec. 2.
- ☐ NSRDS-NBS-3, Sec. 3, **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, C I, C II, C III, C IV, C V, C VI**, by C. E. Moore, 1970 (\$1), SD Catalog No. C13.48:3/Sec. 3.
- ☐ NSRDS-NBS-3, Sec. 4, **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, N IV, N V, N VI, N VII**, by C. E. Moore, 1971 (55 cents), SD Catalog No. C13.48:3/Sec. 4.
- ☐ NSRDS-NBS-3, Sec. 6, **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, H I, D, T**, by C. E. Moore, 1972 (In press), SD Catalog No. C13.48:3/Sec. 6.
- ☐ NSRDS-NBS-4, **Atomic Transition Probabilities, Vol. I, Hydrogen Through Neon**, by W. L. Wiese, M. W. Smith, and B. M. Glennon, 1966 (\$2.50), SD Catalog No. C13.48:4/Vol. I.
- ☐ NSRDS-NBS-5, **The Band Spectrum of Carbon Monoxide**, by P. H. Krupenie, 1966 (70 cents), SD Catalog No. C13.48:5.
- NSRDS-NBS-6, **Tables of Molecular Vibrational Frequencies, Part 1**, by T. Shimanouchi, 1967. Superseded by NSRDS-NBS-39.
- ☐ NSRDS-NBS-7, **High Temperature Properties and Decomposition of Inorganic Salts, Part 1. Sulfates**, by K. H. Stern and E. L. Weise, 1966 (35 cents), SD Catalog No. C13.48:7/Pt. 1.
- NSRDS-NBS-8, **Thermal Conductivity of Selected Materials**, by R. W. Powell, C. Y. Ho, and P. E. Liley, 1966 (\$3). PB189698*
- ☐ NSRDS-NBS-9, **Tables of Bimolecular Gas Reactions**, by A. F. Trotman-Dickenson and G. S. Milne, 1967 (\$2), SD Catalog No. C13.48:9.
- ☐ NSRDS-NBS-10, **Selected Values of Electric Dipole Moments for Molecules in the Gas Phase**, by R. D. Nelson, Jr., D. R. Lide, Jr., and A. A. Maryott, 1967 (40 cents), SD Catalog No. C13.48:10.
- NSRDS-NBS-11, **Tables of Molecular Vibrational Frequencies, Part 2**, by T. Shimanouchi, 1967. Superseded by NSRDS-NBS-39.
- ☐ NSRDS-NBS-12, **Tables for the Rigid Asymmetric Rotor: Transformation Coefficients from Symmetric to Asymmetric Bases and Expectation Values of P_z^2 , P_z^4 , and P_z^6** , by R. H. Schwendeman, 1968 (60 cents), SD Catalog No. C13.48:12.
- ☐ NSRDS-NBS-13, **Hydrogenation of Ethylene on Metallic Catalysts**, by J. Horiuti and K. Miyahara, 1968 (\$1), SD Catalog No. C13.48:13.
- ☐ NSRDS-NBS-14, **X-Ray Wavelengths and X-Ray Atomic Energy Levels**, by J. A. Bearden, 1967 (40 cents), SD Catalog No. C13.48:14.
- ☐ NSRDS-NBS-15, **Molten Salts: Vol. 1, Electrical Conductance, Density, and Viscosity Data**, by G. J. Janz, F. W. Dampier, G. R. Lakshminarayanan, P. K. Lorenz, and R. P. T. Tomkins, 1968 (\$3), SD Catalog No. C13.48:15/Vol. 1.

- NSRDS-NBS-16, **Thermal Conductivity of Selected Materials, Part 2**, by C. Y. Ho, R. W. Powell, and P. E. Liley, 1968 (\$2), SD Catalog No. C13.48:16/Pt. 2.
NSRDS-NBS-17, **Tables of Molecular Vibrational Frequencies, Part 3**, by T. Shimanouchi, 1968. Superseded by NSRDS-NBS-39.
- NSRDS-NBS-18, **Critical Analysis of the Heat-Capacity Data of the Literature and Evaluation of Thermodynamic Properties of Copper, Silver, and Gold from 0 to 300 K**, by G. T. Furukawa, W. G. Saba, and M. L. Reilly, 1968 (40 cents), SD Catalog No. C13.48:18.
- NSRDS-NBS-19, **Thermodynamic Properties of Ammonia as an Ideal Gas**, by L. Haar, 1968 (20 cents), SD Catalog No. C13.48:19.
- NSRDS-NBS-20, **Gas Phase Reaction Kinetics of Neutral Oxygen Species**, by H. S. Johnston, 1968 (45 cents), SD Catalog No. C13.48:20.
- NSRDS-NBS-21, **Kinetic Data on Gas Phase Unimolecular Reactions**, by S. W. Benson and H. E. O'Neal, 1970 (\$7), SD Catalog No. C13.48:21.
- NSRDS-NBS-22, **Atomic Transition Probabilities, Vol. II, Sodium Through Calcium, A Critical Data Compilation**, by W. L. Wiese, M. W. Smith, and B. M. Miles, 1969 (\$4.50), SD Catalog No. C13.48:22/Vol. II.
- NSRDS-NBS-23, **Partial Grotrian Diagrams of Astrophysical Interest**, by C. E. Moore and P. W. Merrill, 1968 (55 cents), SD Catalog No. C13.48:23.
- NSRDS-NBS-24, **Theoretical Mean Activity Coefficients of Strong Electrolytes in Aqueous Solutions from 0 to 100 °C**, by Walter J. Hamer, 1968 (\$4.25), SD Catalog No. C13.48:24.
- NSRDS-NBS-25, **Electron Impact Excitation of Atoms**, by B. L. Moiseiwitsch and S. J. Smith, 1968 (\$2), SD Catalog No. C13.48:25.
- NSRDS-NBS-26, **Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions**, by J. L. Franklin, J. G. Dillard, H. M. Rosenstock, J. T. Herron, K. Draxl, and F. H. Field, 1969 (\$4), SD Catalog No. C13.48:26.
- NSRDS-NBS-27, **Thermodynamic Properties of Argon from the Triple Point to 300 K at Pressures to 1000 Atmospheres**, by A. L. Gosman, R. D. McCarty, and J. G. Hust, 1969 (\$1.25), SD Catalog No. C13.48:27.
- NSRDS-NBS-28, **Molten Salts: Vol. 2, Section 1. Electrochemistry of Molten Salts: Gibbs Free Energies and Excess Free Energies from Equilibrium-Type Cells**, by G. J. Janz and C. G. M. Dijkhuis; **Section 2. Surface Tension Data**, by G. J. Janz, G. R. Lakshminarayanan, R. P. T. Tomkins, and J. Wong, 1969 (\$2.75), SD Catalog No. C13.48:28/Vol. 2.
- NSRDS-NBS-29, **Photon Cross Sections, Attenuation Coefficients, and Energy Absorption Coefficients from 10 keV to 100 GeV**, by J. H. Hubbell, 1969 (75 cents), SD Catalog No. C13.48:29.
- NSRDS-NBS-30, **High Temperature Properties and Decomposition of Inorganic Salts, Part 2. Carbonates**, by K. H. Stern and E. L. Weise, 1969 (45 cents), SD Catalog No. C13.48:30/Pt. 2.
- NSRDS-NBS-31, **Bond Dissociation Energies in Simple Molecules**, by B. deB. Darwent, 1970 (55 cents), SD Catalog No. C13.48:31.
- NSRDS-NBS-32, **Phase Behavior in Binary and Multicomponent Systems at Elevated Pressures: *n*-Pentane and Methane-*n*-Pentane**, by V. M. Berry and B. H. Sage, 1970 (70 cents), SD Catalog No. C13.48:32.
- NSRDS-NBS-33, **Electrolytic Conductance and the Conductances of the Halogen Acids in Water**, by W. J. Hamer and H. J. DeWane, 1970 (50 cents), SD Catalog No. C13.48:33.
- NSRDS-NBS-34, **Ionization Potentials and Ionization Limits Derived from the Analyses of Optical Spectra**, by C. E. Moore, 1970 (75 cents), SD Catalog No. C13.48:34.
- NSRDS-NBS-35, **Atomic Energy Levels as Derived from the Analyses of Optical Spectra, Vol. I, ¹H to ²³V; Vol. II, ²⁴Cr to ⁴¹Nb; Vol. III, ⁴²Mo to ⁵⁷La, ⁷²Hf to ⁸⁹Ac**, by C. E. Moore, 1971 (Vol. I, \$5; Vol. II, \$4.25; Vol. III, \$4.50), SD Catalog No. C13.48:35/Vols. I, II, and III.
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<p>16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)</p> <p>This is a report on the status of the National Standard Reference Data System as of June 1972. Recent activities of the Office of Standard Reference Data are summarized and future plans are indicated. A complete list of data evaluation projects supported by the Office of Standard Reference Data during Fiscal Year 1972 is included; this list also includes projects which received financial support during an earlier fiscal year, and which are still actively involved in some aspect of data compilation and evaluation, or which are still preparing a product for publication. Progress in data processing and in information services is reviewed. The appendix includes a listing of continuing data centers in the United States and a list of publications resulting from the standard reference data program.</p>			
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