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# NBS TECHNICAL NOTE 553

UNITED STATES  
DEPARTMENT OF  
COMMERCE  
PUBLICATION



## Critical Evaluation of Data In the Physical Sciences— A Status Report on the National Standard Reference Data System

June 1970

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**TECHNICAL NOTE 553**

ISSUED SEPTEMBER 1970

Nat. Bur. Stand. (U.S.), Tech. Note 553, 77 pages (Sept. 1970)  
CODEN: NBTNA

**Critical Evaluation of Data in the Physical Sciences—  
A Status Report on the National Standard Reference  
Data System June 1970**

David R. Lide, Jr., Editor

Office of Standard Reference Data  
National Bureau of Standards  
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.

## PREFACE

The last status report on the National Standard Reference Data System appeared in April 1968 (NBS Technical Note 448). During the past two years the program has proceeded without any major change of direction. The limitations of constant funding have made it difficult to start new projects, except on a very small scale. However, the operation of the existing data centers has been placed on a more routine basis, and the time is in sight when a steady output of evaluated data compilations can be expected. At this stage the greatest need is for additional funds to support new projects in neglected technical areas and to make greater use of the bibliographic resources already developed in the continuing data centers.

The NSRDS-NBS Series, which has been the principal outlet for the evaluated data compilations and critical reviews produced under the program, now stands at 33 titles. In addition, 40 to 50 other data compilations, bibliographies, and descriptions of data-handling techniques have appeared through other publication channels. Current figures show that 60,000 to 70,000 copies of documents in the NSRDS-NBS Series have been distributed. In addition, there has been a significant secondary distribution through reprinting of evaluated data in various handbooks. In spite of this, we feel that many of the potential users of the output of the program are not aware of the availability of NSRDS publications. Strenuous efforts have been made during the last year to publicize the NSRDS publication program, and positive results are beginning to appear.

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.

David R. Lide, Jr.

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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 1970. 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 1970 is included. 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 1970

### 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 serve as the nucleus of the system. These activities 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 also fall outside the program.

Our 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, but equally important aim is to provide feedback into the generation of physical data which will raise the general standards of measurement. That is, by communicating the experience gained in evaluating the world output of data in the physical sciences, it is hoped that experimental techniques will be advanced and the reliability of physical measurements improved.

#### B. Organization of NSRDS

When the National Bureau of Standards was given 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 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.

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 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 is given in Appendix II. It can be seen from this list that their support comes from many sources in addition to OSRD. All of the projects which currently receive financial support from OSRD are described in Chapter II.

### C. Standard Reference Data Legislation

The standard reference data program was established under the general enabling legislation of the National Bureau of Standards. However, 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 this legislation 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. The testimony and debate associated with the Standard Reference Data Act indicate an intention that special services provided to individuals or groups should be largely reimbursable, while data compilations of very general interest are expected to recover only a small percentage of their cost.

Arrangements are being made for commercial publication of several NSRDS compilations which are nearing completion. Publications in the NSRDS-NBS series are now being copyrighted as an interim measure. A general policy on publication and distribution of the NSRDS output will be formulated in the near future.

### D. Advisory Mechanism

In planning 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 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 a reorganization within the NAS-NRC in 1969, the Office of Critical Tables has been replaced by the Numerical Data Advisory Board (NDAB). The scope of the NDAB includes numerical data of concern to all parts of science and technology. Therefore, in addition to its advisory services to NSRDS, the NDAB will be concerned with data outside the physical sciences and with data on less well-defined properties and substances which fall outside the present scope of NSRDS.

The NDAB will continue to administer the advisory panels in each 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 recently been organized in fields such as Mössbauer spectroscopy and interatomic distances. Such meetings sometimes lead to the establishment of new compilation projects or to the recommendation of procedures for obtaining and reporting experimental data in the particular field.

#### E. 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 England, 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. The State Service for Standard and Reference Data (GSSSD) in the Soviet Union supports a broad range of data compilation activities. 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 are exchanged in areas where both countries have a major interest.

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, nine 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.

CODATA has established task groups in special areas such as computer handling of numerical data, key values of thermodynamic properties, rate constants, and fundamental constants. Scientists associated with NSRDS data centers are active in all of these task groups. Particular mention should be given to the task group on key values, which is attempting to reach agreement on uniform values for properties which have a major influence on thermodynamic tables. When this is achieved, it will be possible to use such tables interchangeably without concern for the introduction of errors from inconsistent input data.

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. In addition, OSRD organized a three-day meeting on Thermodynamic Properties of Fluids in November, 1969, at which methods of evaluation were analyzed in some detail and priorities for experimental and compilation work were discussed.

## II. PROGRESS OF THE DATA EVALUATION PROGRAM

The original planning of the NSRDS program envisioned a rapid increase in funds available for the support of data evaluation activities. 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 1967-70. Many of the initial goals have, therefore, not yet been reached. However, a good start has been made in some technical areas, and much experience has been gained in modes of operation of data centers.

The scope of the standard reference data program has been divided into seven technical areas: (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 1970.

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 complete list of continuing data centers in the United States which are recognized as part of NSRDS 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

Since the writing of the previous Status Report early in 1968, ten published monographs have resulted from the program in thermodynamics and transport properties. These cover the following topics:

- Electrical conductance, density and viscosity of molten salts;
- Thermal conductivity of selected materials;
- Heat capacity data and thermodynamic properties of copper, silver and gold from 0 to 300K;
- Thermodynamic properties of ammonia as an ideal gas;
- Theoretical activity coefficients of strong electrolytes in aqueous solution from 0 to 100°C;
- Thermodynamic properties of argon from the triple point to 300K and pressures to 1000 atms;
- Thermodynamic properties from equilibrium-type cells and surface tensions of molten salts;
- High temperature properties and decomposition of inorganic carbonates;
- Thermodynamic properties of elements 35 through 53 in the standard order of arrangement;
- Electrolytic conductance and the conductance of halogen acids in water.

Complete bibliographic listings for these monographs will be found in Appendix III. In addition to these monographs there are several series of publications put out by the major data centers, some with partial support of the Office of Standard Reference Data, some without. These are listed under the activities of the individual data centers. Several research reports on subjects related to data evaluation, originating in data centers supported by the Office of Standard Reference Data, have been published in technical journals.

Additional monographs which have been accepted for publication but have not yet appeared are:

- Phase Behavior in Binary and Multicomponent Systems: n Pentane and Methane-n Pentane, by Virginia M. Berry and Bruce H. Sage, NSRDS-NBS-32
- High Pressure Bibliography 1900-1968, by Leo Merrill
- High Pressure Calibration: A Critical Review, by D.L. Decker, W.A. Bassett, L. Merrill, H.T. Hall and J.D. Barnett

Two other publications might be mentioned. These are products of the GSSSD, the Russian national data system which have been translated into English at the request of the Office of Standard Reference Data. They are:

- Thermophysical Properties of Liquid Air and its Components by A.A. Vasseran and V.A. Rabinovich TT69-55092<sup>(1)</sup>
- Thermophysical Properties of Gases and Liquids No. 1 by V.A. Rabinovich, Editor TT69-55091

(1)The TT numbers are numbers to be used in ordering from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia.

The Office of Standard Reference Data also provides partial support for the Bulletin of Thermodynamics and Thermochemistry, an annual annotated bibliography of the literature in the field and summary of current research. The Bulletin is edited by Professor Edgar F. Westrum of the University of Michigan; major contributions are made by the Chemical Thermodynamics Data Center at NBS and the Thermodynamics Research Center at Texas A & M.

On November 5-7, 1969, a symposium on "The Evaluation of the Thermodynamic Properties of Fluids" was held at Airlie House, Warrenton, Virginia. The symposium 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 primary themes of the symposium were:

- a) The estimation of the reliability of experimental, theoretical, and evaluated data, techniques for data evaluation, and related problems;
- b) Assessment of the needs for evaluated data in science and industry, and discussion of current programs carried out to meet these needs.

A report on the discussions of panels detailed to study data needs, resources and programs in six technical areas is available from the Office of Standard Reference Data.

#### Active Projects:

1. Title: Selected Values of Chemical Thermodynamic Properties

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 the first 53 elements in the standard order of arrangement has been completed and published. Work on an additional set of about 10 elements is well advanced. A table of values of heats, pressures, and temperatures of transition, fusion, and vaporization of selected inorganic substances was prepared for the third edition of the American Institute of Physics Handbook.

Development of automated techniques for data and text handling have continued. In the preparation of the bibliography and subject-property index of the inorganic chemical literature for the 12th annual Bulletin of Thermodynamics and Thermochemistry all sorting, editing, arranging and final master copy preparation were done by computer.

Future Plans: First priority will be given to completion of the evaluation of the thermodynamic properties of inorganic substances. Further automation of data handling techniques will also be carried out.



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

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: Thermodynamic Data on Organic Compounds

Principal Investigator: B.J. Zwolinski

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

Data Initiated: 1964

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

Current Status: A report on thermodynamic and physical properties of the aliphatic alcohols is being prepared for publication. 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.

Future Plans: Selected properties of the halogenated hydrocarbons and of organic oxygen compounds are being evaluated.

4. Title: Low Temperature Heat Capacity

Principal Investigator: G.T. Furukawa

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

Date Initiated: 1963

Objective: The critical analysis of data from the literature on the heat capacities of substances between 0 and 300K, the tabulation of best values, and the calculation and tabulation of derived thermodynamic properties.

Current Status: A preliminary draft of a monograph on the analysis of the heat capacity data for the elements, Cr, Mo, W has been prepared. The analysis of the data on the elements, Pt, Pd, Ir is well advanced.

A revised table on the heat capacities of the elements between 0 and 298K has been prepared for inclusion in the third edition of the AIP Handbook. A file of 12,000 papers essential to the program is

under author index with some under substance and property index. The references to the papers are on punched cards for bibliography preparation. The heat-capacity data on all elements and some compounds to 1967 (and some later) are on punched cards. Computer programs for data analysis and plotting routines have been developed.

Future Plans: Because new responsibilities make it impossible for the principal investigator to continue with the project, it will terminate in its current form.

5. 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: The properties to be considered are the vapor pressures of the pure compounds, the compositions of the coexisting vapor and liquid phases, the vapor pressures of the liquid mixtures, and heat capacities of the coexisting phases and enthalpy and volume changes on mixing where available. A computer assisted program has been developed for applying a modified Antoine Equation to vapor pressure-temperature data for pure components. This program is being applied to appropriate pairs of compounds and the activity coefficients of mixtures of these pairs are being evaluated.

Future Plans: As values of internally consistent thermodynamic properties of mixtures which are compatible with the properties of the pure components are obtained, tables comparing data for chemically related series of mixtures will be developed.

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

Principal Investigator: B.D. Smith

Location: Washington University, St. Louis, Missouri

Date Initiated: 1967

Objective: Preparation of a comprehensive report on the data on the excess free energy of mixing, excess enthalpy of mixing, and excess volume of mixing for liquid mixtures of hydrocarbons containing 5 to 8 carbon atoms.

Current Status: Vapor-liquid equilibrium data, heat of mixing data, and volume change on mixing data are being gathered and will be checked for internal thermodynamic consistency and precision. Excess properties will be obtained.

Future Plans: The project has just been started.

7. Title: Thermodynamic Properties of Nitrogen

Principal Investigator: R.B. Stewart

Location: University of Idaho, Moscow, Idaho

Date Initiated: 1969

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: The thermodynamic data available from the literature have been evaluated, and the temperature values adjusted to the thermodynamic temperature scale. An equation of state has been developed for temperatures from 50K to 1000K with pressures to 1000 atm. Equations have also been determined to represent the ideal gas properties and the vapor pressure data as functions of temperature. The heat capacity and other calorimetric data and the Joule-Kelvin data have been compared with values calculated from the equation of state. A preliminary table of thermodynamic properties is nearly completed.

Future Plans: The equation of state will be extended to lower and higher temperatures, and to pressures to 10,000 atm. The heat capacity and enthalpy data will be used simultaneously with the P-V-T data in the fitting of an equation of state. The consistency of the vapor pressure equation with P-V-T and calorimetric data will be studied further.

8. 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. The properties of the gas at zero density have been finished (NSRDS-NBS-19) and considerable progress has been made on the general PVT surface and the thermodynamic properties at finite density. Correlation techniques have been developed which permit extremely accurate thermodynamic property measurements made at NBS almost 50 years ago to be extrapolated over a wide range of temperature and density.

Future Plans: The PVT surface will be extended into the liquid region and into the higher temperature region where very few experimental data exist.

9. Title: Thermodynamic Properties of Steam Near the Critical Point

Principal Investigator: J.M.H. Sengers

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

Date Initiated: 1970

Objective: A description of the thermodynamic properties of steam in the vicinity of the critical point using scaling laws.

Current Status: The use of scaling laws is a semi-empirical theoretical technique which has had great success in correlating the behavior of various thermodynamic properties in the vicinity of the critical point with a relatively small number of adjustable parameters. A versatile non-linear computer package is being constructed to fit scaled equations to the chemical potential, vapor pressure, and coexisting densities of steam. The resulting equations will then be used to predict other thermodynamic properties over a range of temperatures and densities in the vicinity of the critical point.

Future Plans: The ultimate goal is an accurate fit of the best data in the vicinity of the critical point in terms of a few adjustable parameters. Other existing methods of determining thermodynamic properties in this region either fail or require a large number of adjustable parameters. Successful application of these techniques will make possible simpler, more accurate steam tables.

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

Principal Investigator: M.S. Green

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. The existing data on binary mixtures have been collected and examined with respect to quality of experimental measurement. Where the data are extensive enough they are being examined with respect to conformity to the scaling law equations. This project is coordinated with other related projects being carried out under the sponsorship of the Office of Standard Reference Data and under other sponsorship.

Future Plans: Data on magnetic critical points will also be evaluated and a final report will be prepared.



11. Title: Complex Stability Constants

Principal Investigator: Y. Marcus

Location: Hebrew University, Jerusalem, Israel

Date Initiated: 1968

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 also represents one of the activities of the Commission on Analytical Data of the Analytical Division - IUPAC. The investigators have been systematically studying the principal complexing agents according to chemical type. The alkylphosphoric acids, alkylphosphorates and phosphinates, and the alkylphosphine oxides have been covered so far.

Future Plans: The data for the other major complexary agents will be compiled and selectively evaluated.

12. Title: Thermodynamic Properties of Electrolyte Solutions

Principal Investigator: W.J. Hamer

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

Date Initiated: 1964

Objective: The compilation and critical evaluation of data from the literature on the activity coefficients, electrolytic conductances, ionic mobilities and transference numbers of aqueous electrolytic solutions, and the electrode potentials and electromotive forces of galvanic cells made with aqueous solutions, from the freezing point to the boiling point of the solvent.

Current Status: The results in this project have been reported in some 16 reports to the primary sponsor (NASA) and two monographs - NSRDS-NBS-24 and NSRDS-NBS-33. These consist of critically evaluated conductivities and activities for selected uni-univalent electrolytes and multivalent electrolytes. More comprehensive compilations of these properties for all fully-ionized uni-univalent electrolytes and some multivalent electrolytes are in the later stages of preparation.

Future Plans: Completion of the monographs mentioned above is the primary aim at present.

13. 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

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

Current Status: Data on the densities, viscosities and electrical conductivities of molten salt mixtures have been compiled. Suitable methods for correlating these over a range of temperatures and concentrations are being evaluated.

Data on the above properties as well as the surface tensions of single salt melts and the EMFs of reversible cells are being collected to allow updating of previous reports. Efforts are also being made to mechanize the data and bibliographic files.

Future Plans: A study of mixtures of nitrates should be finished shortly. Studies of other categories of mixtures are also planned.

14. Title: Constitution of Binary Alloys

Principal Investigator: R.P. Elliott

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

Date Initiated: 1967

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

Current Status: Revised updated phase diagrams have been completed for some 300 binary alloys. The alloys are selected on the basis of earliest alphabetical precedence of the individual members.

Future Plans: Phase diagrams for alloys will continue to be revised and updated according to the alphabetical precedence scheme.

15. 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: An annotated bibliography on work in the high pressure field through 1968 is in press. A critical review on high pressure calibration is in the later stages of preparation. The bibliographic files have been automated to such an extent that the bibliography mentioned, as well as a current awareness service, are produced by computer.

Future Plans: A study of data on high pressure polymorphs such as crystal structures, phase diagrams and selected thermodynamic and physical properties where available.



16. Title: Thermal Conductivity of Selected Materials

Principal Investigator: Y.S. Touloukian

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

Date Initiated: 1964

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

Current Status: A report on the thermal conductivities of the elements is in the later stages of preparation. This report will extend and update two previous publications and one unpublished report. Data on the thermal conductivity of the solid oxides and alloys are being evaluated.

Future Plans: Completion of a report on the solid oxides and alloys.

17. 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: Primary attention is being given to the properties of moderately dense gases and their dependence on the nature of inter-molecular interactions. A thorough investigation of the theoretical basis for such measurements has led to the development of correlation techniques which have brought new insight into the detection of possible systematic errors in measurements and improved methods for comparing measurements on different transport properties. These techniques are currently being used for the critical evaluation of the data for several gases.

Future Plans: Current plans call for further development of the techniques mentioned and a series of critical reviews starting with the noble gases.

## B. Atomic and Molecular Data

The NSRDS program has generally followed the priority list which resulted from a meeting of the Advisory Panel on Atomic and Molecular Properties in 1965. Emphasis is placed on providing carefully evaluated data, even though in small quantities, rather than large amounts of unchecked data. Considerable attention is being paid to developing recommended procedures for generating spectral data on widely-used commercial instruments. The Coblenz Society specifications for infrared spectra, published in 1966, have been widely adopted and given the sanction of the Commission on Molecular Structure and Spectroscopy of the International Union of Pure and Applied Chemistry.

The Joint Committee for Atomic and Molecular Physical Data, which was originally formed to compile and publish evaluated infrared spectra, has now expanded its goals to include other spectral areas. As a result, subcommittees on NMR, Laser-Raman, Microwave Spectra, and Mass Spectra have been established to provide criteria for the production of reliable analytical spectra and stimulate their production and distribution. Two projects have been established under OSRD sponsorship to help achieve these goals for Laser-Raman and NMR data. Similarly, other spectral areas will be encouraged to improve the quality of the data being disseminated.

The data evaluation projects in this area continue to emphasize atomic and molecular spectra, collision cross sections, and certain other molecular properties. Publications during the last year include compilations of ionization and appearance potentials, electron collision cross section data, and X-ray attenuation coefficients. Funding limitations prevented the start of major new projects. However an ad hoc panel on interatomic distances was held which developed plans for an international effort to revise the publication, "Interatomic Distances", edited by L.E. Sutton. Work on this project is expected to begin during the next year.

The charter of the standard reference data program permits the support of experimental determination of data to which a particularly high importance is attached. Such "benchmark" data could 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 started on the measurement of the absolute cross section for excitation of helium by electron impact. It is hoped that this experiment will provide a definitive value of the cross section, with a reliable estimate of the limits of systematic error; in addition, it should lead to criteria for making cross section measurements of other types.

### Active Projects:

1. Title: Atomic Energy Levels Data Center

Principal Investigators: W.C. Martin, C.M. Sitterly

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: A semi-automated system involving edge-punched cards for storage and classification of bibliographic information has been developed. Four bibliographies, entitled "The Analyses of Optical Atomic Spectra," Sections 1-4, and a compilation entitled, "Partial Grotrian Diagrams of Astrophysical Interest," NSRDS-NBS 23, have been published. A compilation of ionization potentials and additional sections of NSRDS-NBS 3 "Selected Tables of Atomic Spectra," are in preparation.

Future Plans: Publication of Volume 4 of "Atomic Energy Levels," and eventually, of revised Volumes 1-3 is planned. Revised multiplet tables and energy levels of selected atoms will be published as sections of NSRDS-NBS-3. Bibliographies will be issued as needed.

2. Title: Spectroscopy of Two-Electron Atoms

Principal Investigator: C.L. Pekeris

Location: Weizmann Institute of Science, Rehovoth, Israel

Date Initiated: 1968

Objective: The objective is to provide very accurate solutions of the Schroedinger 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.

Current Status: Calculations of the  $f$  values for transitions from ground state to  $2^1P$ ,  $3^1P$ ,  $4^1P$ , and  $5^1P$  states for atoms  $Z = 2$  through 10 have been completed. Additionally, selected  $f$  values for transitions  $m^1S-n^1P$  and  $m^3S-m^3P$  for  $m, n = 2, 3, 4, 5$  for He, Li<sup>+</sup> and Be<sup>2+</sup> are complete and have been compared with previous work.

Future Plans: Calculation of  $f$  values will be continued for the transitions in the cases  $Z = 5, 6, \dots 10$ .

3. 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

Objective: The objective is to calculate spectral energy levels for the transition groups and rare earth elements and theoretically predict their spectra.

Current Status: Theoretical spectral interpretations have been partially completed for the first spectra of Ce I, Gd I and Yb I. In addition, similar results have been obtained for the second spectra of La II, the third spectra of Pr III, the fourth spectra of Er IV and the second spectra of Th II. The effects of some magnetic interactions on the levels were also calculated.

Future Plans: The plan calls for continued efforts to calculate spectra of the rare earths.

4. 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

Objective: The objective of the project will be 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 spectral energy levels.

Current Status: The work on erbium has progressed well. The work on holmium is not as easily susceptible to classification.

Future Plans: The effort will continue for another two-year period, after which a final report on the results will be published.

5. Title: Atomic Collision Cross Section Information Center

Principal Investigator: L.J. Kieffer

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

Data Initiated: 1963

Objective: The objective is to compile, evaluate and disseminate low energy atomic collision cross section data. Automated procedures are used to prepare and maintain a literature file on the pertinent data and a current data bank.

Current Status: Recent publications include bibliographies on photoabsorption cross section data, ion-molecule reaction rates, and low-energy electron cross section data. Compilations of electron-collision cross section data have appeared as JILA Reports and in Atomic Data. Reviews on excitation and ionization of atoms by electron impact have been published in Rev. Mod. Phys.

6. Title: Atomic and Molecular Processes Data Center

Principal Investigator: C.F. Barnett

Location: Oak Ridge National Laboratory, Oak Ridge, Tennessee

Data Initiated: 1965



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, has been published by John Wiley & Sons, Inc. Five other reviews are in varying stages of publication.

Future Plans: The five monographs will be completed in the next two-year period.

7. 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

Objective: This project is 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 will be given to data describing the production and destruction of long-lived and metastable excited species.

Current Status: The book is in process of being written following the compilation and evaluation of the data. Five chapters are in rough draft.

Future Plans: The monograph will be completed and published.

8. Title: Compilation and Verification of X-ray Wavelength

Principal Investigator: J.A. Bearden

Location: Johns Hopkins University, Baltimore, Maryland

Date Initiated: 1966

Objective: The objective of this project is to remeasure the wavelength ratios between the  $W K\alpha$ , 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  $Al K\alpha$  doublet.

Current Status: Tabulations of selected x-ray wavelengths and a reevaluation of x-ray energy levels have been published. The various remeasurements have also been completed.

Future Plans: 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 will be published.

9. 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. Three additional contributions by the principal investigator have been published elsewhere.

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

10. Title: Diatomic Molecule Spectral Data Center

Principal Investigator: P.H. Krupenie

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

Date Initiated: 1967

Objective: The objective is to maintain a literature file of spectroscopic information from which the molecular constant data on specific molecules are extracted, compiled, evaluated and disseminated.

Current Status: A library of 4,000 documents covering the years 1900 to 1965 have been collected; 3,000 have been catalogued by molecule. A critical review of the spectral data on O<sub>2</sub> is nearing completion.

Future Plans: The critical review on O<sub>2</sub> will be published. Another monograph on N<sub>2</sub> will be undertaken.

11. Title: Microwave Spectral Data Center

Principal Investigator: W.H. Kirchhoff

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

Date Initiated: 1967

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 32 compounds, consisting of more than 2,000 reported transitions, have been evaluated and transferred to punched cards for subsequent storage in the computer. Three supplements to



NBS Monograph 70 have been issued. Volume III, IV and V are entitled: Microwave Spectral Tables, Polyatomic Molecules with Internal Rotation; Microwave Spectral Tables, Polyatomic Molecules without Internal Rotation; Microwave Spectral Tables, Spectral Line Listing.

Future Plans: Future efforts will involve continued compilation and evaluation using automated techniques for easy storage and retrieval.

12. Title: Fundamental Vibration Frequencies of Molecules

Principal Investigator: T. Shimanouchi

Location: University of Tokyo, Japan

Date Initiated: 1964

Objective: The objective of this project is to compile and evaluate the fundamental vibrational frequencies of important molecules. Experimental infrared and Raman spectral data and the results of normal coordinate calculations are taken into consideration in arriving at selected values of the fundamental frequencies. Tables are prepared with these selected values plus representative infrared and Raman data and important references.

Current Status: A new group of 50 tables has been completed and submitted for review. These will be combined with revised tables for approximately 150 molecules previously published in the NSRDS-NBS series to form a consolidated volume.

Future Plans: Evaluation will continue on the next group of about 50 molecules, which emphasizes simple compounds of nitrogen, boron, sulfur, silicon and germanium,

13. Title: NMR Data Compilation Project

Principal Investigator: B.L. Shapiro

Location: Texas A & M University, College Station, Texas

Date Initiated: 1969

Objective: The objective of the program is to establish criteria for the generation of high quality NMR spectra. This would lead to the compilation of tables of evaluated data of parameters such as chemical shift, coupling constants, and frequency values for protons and other elements of interest.

Current Status: A sample mixture has been produced to intercompare, among selected laboratories, the ability of present instruments to generate high quality proton spectra. This will be followed by the establishment of criteria for NMR spectral measurements. Work on other nuclei has focused on carbon-13, whose use is rapidly expanding. Meetings and discussions with leaders in the field have resulted in tentative new

referencing and standardization procedures.

Future Plans: The intercomparison and criteria writing projects will be followed by compilation and evaluation efforts.

14. Title: Parameters for Presentation of Laser-Raman Spectra

Principal Investigator: E.R. Lippincott

Location: University of Maryland, College Park, Maryland

Date Initiated: 1970

Objective: The objective of this project is to investigate the operating parameters for presenting Laser-Raman spectra in standard format. The areas to be examined are the physical presentation of the spectra, instrument operating parameters, presentation of depolarization data, intensity and frequency standards, and influence of activating source on Raman intensities.

Current Status: The project has just been initiated.

Future Plans: Each of the areas named will be investigated. The study of these parameters will serve as the basis for developing criteria for presenting Laser-Raman spectra.

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

Principal Investigator: Coblenz Society Inc., C.L. Angell, President

Location: Union Carbide and Carbon, New York

Date Initiated: 1965

Objective: The Board of Management is to advise 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 adopted and published by the IUPAC. Volume 6 of the NSRDS-Coblenz Society series, containing 1,000 evaluated IR spectra, has been published.

Future Plans: Additional volumes of NSRDS-Coblenz Society evaluated IR spectra will be published when ready.

16. Title: Infrared Bibliography

Principal Investigator: C.N.R. Rao

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1969

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 bibliographic references for 1960 have now been collected and indexed.

Future Plans: References will be compiled until sufficient material has been collected to issue a publication.

17. Title: Mass Spectrometry Data Center

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.

Future Plans: Work is underway to collect and abstract data for the period 1966 to present. A revision of NSRDS-NBS-26 is planned.

### C. Chemical Kinetics

A meeting of the NAS-NRC Advisory Panel in Chemical Kinetics was convened in May 1969, to review the progress made by the OSRD in this area and to offer advice on future program activities. The Panel confirmed the philosophy, which it had expressed previously, that the office should sponsor critical reviews in kinetics which emphasis on rate constant data. It endorsed the existing program and recommended expansion into solution kinetics and heterogeneous kinetics as soon as funds are available.

A number of reviews have been published on selected gas phase reactions; some of these are pertinent to research on environmental problems. This type of review will continue to receive emphasis. Two reviews covering other gas phase reactions encountered in the atmosphere have been initiated. Close cooperation is maintained with the Leeds group in the United Kingdom, which is conducting a similar program.

The two data centers sponsored by the OSRD have grown in capability and are able to supply bibliographic material to potential reviewers. In addition, they can respond to specific questions put to them by the scientific public. Bibliographies have also been published on selected topics. The Radiation Chemistry Center also issues a current awareness bulletin on radiation chemical literature. Some thought is being given to establishing a data center covering solution kinetics and another for ion-molecule reactions.

#### Active Projects:

##### 1. Title: Chemical Kinetics Data Center

Principal Investigator: David Garvin

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

Date Initiated: 1964

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 to be compiled, evaluated and issued as critical reviews.

Current Status: Approximately 20,000 documents have been indexed and are retrievable by reference, author, title and subject matter. A non-critical collection of gas phase rate constant data was issued as NBS Report 9884. A bibliography on the reactions of nitrogen, oxygen, ozone and nitrogen oxide has been issued. A critical evaluation of the rates of dissociation of fluorine and chlorine has been prepared. Eight short bibliographies on special topics in kinetics are available for distribution.

Future Plans: The evaluation on rate constants for dissociation and combination reactions will be continued. The assembly of a comprehensive automated index to research on kinetics will continue.



2. Title: Radiation Chemistry Data Center

Principal Investigator: A. Ross

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

Date Initiated: 1966

Objective: The project will develop an automated literature reference file of data on "G" values and other constants pertinent to radiation chemistry. The center will compile, evaluate and disseminate reviews on selected topics.

Current Status: The automated storage and retrieval file is in operation. A weekly current awareness listing of papers in radiation chemistry and related topics is being issued. Three bibliographies have been published. A state-of-the-art monograph on gaseous ammonia is in preparation.

Future Plans: The ammonia review will be published. Two additional reviews on ethane and ethanol are in progress. A table of rate constants for H, OH, HO<sub>2</sub> and e<sup>-</sup> in aqueous solution is being updated. A table of rate constants for e<sub>solv</sub><sup>-</sup> in polar solvents is being prepared.

3. Title: A Critical Evaluation of the Gas Phase Reaction Kinetics of the Hydroxyl Radical

Principal Investigator: Wm. E. Wilson, Jr.

Location: Battelle Memorial Institute, Columbus, Ohio

Date Initiated: 1969

Objective: The objective of this critical review is to examine some of the more important reaction rate constants of the OH radical in the gas phase and recommend "best" values. The review will include discussions of experimental technique and its validity in terms of the value sought. The four principal reactions covered are OH+OH, CO+OH, H<sub>2</sub>+OH and CH<sub>4</sub>+OH.

Current Status: A preliminary draft has been written and is now being corrected to conform to reviewers' comments.

Future Plans: This report, when completed, will be published in the NSRDS-NBS series.

4. 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 O<sup>-</sup> reactions. Optical absorption, acid dissociation constants, and other properties will also be discussed.

Current Status: The literature is being scanned and a comprehensive bibliography on all pertinent reactions is being compiled.

Future Plans: The monograph will be published in the NSRDS-NBS series when it is completed.

5. Title: A Critical Review on Dissociation-Recombination Reaction Rate Constants of  $H_2$ ,  $N_2$ ,  $NO$ ,  $HNO$  and  $NO_2$

Principal Investigator: F. Kaufman

Location: University of Pittsburgh, Pittsburgh, Pennsylvania

Date Initiated: 1970

Objective: A critical review is to be written on the dissociation-recombination reactions of  $H_2$ ,  $N_2$ ,  $NO$ ,  $HNO$ , and  $NO_2$ . Reaction rate constants will be recommended after each reaction has been examined for experimental technique, measurement error, etc., in the context of rate theory.

Current Status: This project has just been initiated.

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

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

Principal Investigator: K. Schofield

Location: AC Electronics, Defense Research 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  $CO$ ,  $SO_2$ ,  $SO_3$ ,  $H_2S$ ,  $NH_3$ ,  $CH_4$ ,  $C_2H_6$ ,  $NO$ ,  $NO_2$ ,  $N_2O$ ,  $N_2O_4$  and the atoms and radicals  $H$ ,  $O$ ,  $SO$ ,  $HS$ ,  $NH_2$ ,  $CH_3$  and  $C_2H_5$ .

Current Status: This project has just been initiated.

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



#### D. Solid State Data

The effort devoted to this program area has remained small. Under the funding priorities previously assigned, the project receiving the most emphasis has been the publication of the third edition of Crystal Data Determinative Tables. Inasmuch as the procedure employed for producing this work is unique, i.e. by computer composition of very complex material, considerable difficulty and delay was encountered in establishing the necessary error-free programs. This problem has now been overcome and the two volume publication will soon enter the production stage.

An updated compilation of superconductive materials has been issued. In view of the recent observation of superconductivity up to a temperature of 21 K, increased research activity is predicted in this field. Another publication now in preparation will describe metallic shifts in the nuclear magnetic resonance of alloys. A report describing the activities of the Alloy Data Center was issued. Several bibliographies are in various stages of preparation.

An ad-hoc advisory panel on Mössbauer data was convened to suggest a program of activity which would yield a standard reference material against which measurements could be calibrated. This was expected to lead to criteria for obtaining high quality data.

An examination of the data on static dielectric constants and energy gaps in semiconductors has been initiated, with the view of producing tables of evaluated data on a limited range of materials. Other efforts on phase transformations in solids and defect properties in crystals are also underway.

#### Active Projects:

##### 1. Title: Crystal Data Center

Principal Investigator: H.M. Ondik

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

Date Initiated: 1964

Objective: The objective is to provide and maintain a semi-critical compilation of crystallographic data. This includes collecting and maintaining a literature reference file of the data.

Current Status: Computer programs for checking and evaluating the data and for converting the evaluated data into an automatic typesetting format are complete and functioning. The third edition of Crystal Data Determinative Tables by J.D.H. Donnay, et al. is nearing completion.

Future Plans: The book will be completed and published. The data center's activity will continue.

2. Title: Production of Text Crystal Data

Principal Investigator: J.D.H. Donnay

Location: Johns Hopkins University, Baltimore, Maryland

Date Initiated: 1965

Objective: This subproject of the Crystal Data Center program has been established to assist the editor, by providing the professional services for editing and correcting the data entries which are to be included in the third edition of the book Crystal Data Determinative Tables.

Current Status: Most of the data entries have been examined and edited for inclusion in the book.

Future Plans: This project will be concluded upon the publication of the book.

3. Title: Compilation of Crystal Data on Organic Compounds

Principal Investigator: O. Kennard

Location: University of Cambridge, Cambridge, England

Date Initiated: 1964

Objective: This subproject of the Crystal Data Center program provides input material for the revision of Crystal Data. Specifically, this involves scanning of the literature for inorganic and organic compounds, and abstracting and updating the data relevant to carbon containing compounds, excluding proteins.

Current Status: To date, the literature for the years 1968-1970 have been scanned and treated as described above.

Future Plans: This effort will continue to compile and submit data on organic compounds to the Crystal Data Center.

4. Title: Computer Assisted Crystal Data Correlations

Principal Investigator: G.G. Johnson, Jr.

Location: Pennsylvania State University, University Park, Pennsylvania

Date Initiated: 1968

Objective: This subproject of the Crystal Data Center program has the objective of ascertaining the accuracy and consistency of the Linofilm keyboarded data entries of the book Crystal Data. The data are manipulated by computer using special programs developed by the principal investigator. In addition, the data are being refined by use of the Takada and Donnay cell reduction computer program.

Current Status: The computer programs are all completed and have been used to check about 20,000 entries for inclusion in the book. Some have required several passes through the program to make them error free. An additional 5,000 entries will be checked for the first time.

Future Plans: The project will conclude with the publication of the book Crystal Data.

5. Title: Alloy Data Center

Principal Investigator: G.C. Carter

Location: Metallurgy Division, NBS, 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 reference system has been made operative. A technical note, NBS-Tech Note 464, describing the system and its contents, has been issued. A book on metallic shifts in nuclear magnetic resonance is in preparation; this will include tables of evaluated Knight shift data in metallic materials. Two bibliographies describing the data center's holdings are in publication.

Future Plans: The three publications will be issued. The data center's activities will continue with emphasis on the preparation of a critical compilation of soft x-ray spectroscopy data.

6. Title: Diffusion in Metals Data Center

Principal Investigator: J.R. Manning

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

Date Initiated: 1964

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

Current Status: The reference file is complete. A critical analysis of diffusion data on copper and its alloys is in progress.

Future Plans: The literature reference file will be maintained and the critical analysis of the data continued.

7. 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: The first publication on superconductive materials data has been updated in NBS Tech Note 482.

Future Plans: The assigned activities of the center will continue.

8. Title: Compilation of Thermal Expansion Data

Principal Investigator: R.K. Kirby

Location: Inorganic Materials Division, NBS, 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, who will furnish bibliographic assistance and other data information, so that a selection of "best" values of linear expansion and expansivity can be made.

Current Status: This project is in its initial stages. An exchange of information between the principals has begun.

Future Plans: A tabulation of thermal expansion data will be published.

9. Title: Compilation of Energy Gap Data

Principal Investigator: R.F. Blunt

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

Date Initiated: 1970

Objective: The objective of this project is to collect numerical data of the energy gap of semiconductors and insulators, primarily from optical measurements but supplemented by results from electrical measurement. The energy data will be tabulated as a function of absorption coefficient ( $\propto$ ). Temperature and pressure dependencies will be given. Where applicable, the absorption coefficient will be plotted as a function of energy to show the shape of the absorption edge.

Current Status: The project is in its initiative stage. Using the AIP Handbook tables as a data base, the literature is being compiled and a data file established.

Future Plans: Following the bibliographic search the data will be compiled, evaluated and published.

10. Title: Compilation of Static Dielectric Constants

Principal Investigator: K.F. Young

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

Date Initiated: 1970

Objective: The objective of this project is to enlarge and improve the American Institute of Physics Handbook tables for 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  $\epsilon''$  or  $\tan \delta$  (losses) will be included.

Current Status: This project has just been initiated. The literature is now being searched and a file of data is being established.

Future Plans: Following the bibliographic search, the data will be compiled, evaluated and published.



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

Principal Investigator: S.C. Jain

Location: Solid State Physics Laboratory, Ministry of Defense, New Delhi, India

Date Initiated: 1967

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: The optical properties of the transition metal ions in halide crystals have been compiled. Tables giving the point defect, its optical transition, absorption band and half width and, in some instances, oscillator strength, are being assembled for all of the materials examined. A bibliography on impurity centers in alkali halides has also been produced.

Future Plans: The primary effort will be directed toward finishing the optical properties work, after which work will start on the energy values for the defects in crystals.

12. Title: Phase Transformation in Solids

Principal Investigator: C.N.R. Rao

Location: Indian Institute of Technology, Kanpur, India

Date Initiated: 1969

Objective: This project will survey the literature on phase transformation in solids with a view toward preparing bibliography and data 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: Data on phase transformations in binary halides and oxides are being collected. A survey of the data for the alkali halides, silver halides and copper halides is complete.

Future Plans: A monograph on the phase transformations in the halides mentioned above will be prepared. Another similar monograph on the oxides will be written.

## E. Nuclear Data

Almost from the start of the applications of nuclear physics twenty-five years ago, for both historical and practical reasons, a great deal of effort has been expended in the compilation and evaluation of nuclear data. The Atomic Energy Commission, from its inception, has encouraged the support of data activities through its operating divisions. For this reason the nuclear data area is in many respects more advanced and more highly organized than most of the other technical areas discussed in this report. A thorough discussion of nuclear data activities in the United States and their relation to international efforts was given in the previous NSRDS Status Report (NBS Tech. Note 448).

As reported previously, a journal, Nuclear Data, has appeared as a mechanism for the dissemination of appropriate compilations or evaluations of nuclear properties. Section A, edited by Katherine Way, contains a wide variety of types of information, including data that have been included as Appendices to the Nuclear Data Sheets, e.g., the recently published "Table of Nuclear Moments" by Fuller and Cohen. Section B of the journal is the publication mechanism for the data sheets of the Nuclear Data Project of Oak Ridge National Laboratory.

Recently, the OSRD has been able to contribute to the support of the Elementary Particle Data Center, located at Lawrence Radiation Laboratory, Berkeley. A similar arrangement will begin in FY 1971 with the Table of Isotopes Group, also at Lawrence Radiation Laboratory. Both centers had been supported by the Division of Research of the Atomic Energy Commission as part of the research activity of the laboratory. To demonstrate the national and international significance of these compilation groups, the Division of Research has decided to recognize them as separate activities which will be jointly supported with OSRD and possibly other agencies.

### Active Projects:

#### 1. Title: Photonuclear Data

Principal Investigator: E.G. Fuller

Location: Linac Radiation Division, NBS, Washington, D.C.

Date Initiated: 1963

Objective: To maintain file 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: NBS Special Publication 322, the second supplement to the Photonuclear Data Index (NBS Miscellaneous Publication 277) has just been issued. This annotated guide covers the literature from January 1965, to January 1970. Procedures for digitizing graphical data from the literature have been developed and about 200 curves have been entered into the files.

Future Plans: The digitized data file will be expanded. Plans are being made to publish compilation of "best available" cross section data for various groups of nuclei. Critical reviews of important reactions are under consideration.

2. Title: Fundamental Particle Data

Principal Investigator: Arthur H. Rosenfeld

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

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

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

Current Status: The regular activities of the center include the collection and indexing of the literature of high-energy physics and the preparation of the semi-annual "Review of Particle Properties". In addition, compilations of cross sections for various classes of particle reactions are being prepared. Two of these, on  $K^*N$  and  $YN$  reactions, were issued in 1969.

Future Plans: The regular activities will continue. Additional cross section reports will be prepared.

## F. Colloid and Surface Properties

Two monographs of importance in the area of colloid and surface properties have been published. These are:

Hydrogenation of Ethylene on Metallic Catalysts by J. Horiuti and  
K. Miyahara  
NSRDS-NBS-13

Surface Tension Data which is Section 2 of Molten Salts Vol. 2 by  
G.J. Janz, G.R. Lakshminarayanan, R.P.T. Tomkins and J. Wong  
NSRDS-NBS-28

A further monograph:

Critical Micelle Concentrations of Aqueous Surfactant Systems by  
Pasupati Mukerjee and Karol J. Mysels has been approved for publication.

Although it has been necessary to limit the program on colloid and surface properties rather drastically, several other reports are in the final stages of preparation.

### Active Projects:

#### 1. Title: Properties of Importance in Phase Transformation Kinetics

Principal Investigator: G.M. Pound

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: Reports have been received on coefficients of evaporation and condensation, homogeneous nucleation and equilibrium distribution coefficients from liquidus curves. Work is progressing on the remainder of the topics.

Future Plans: It is planned to complete the reviews of the various topics currently underway and to prepare a final report.

#### 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: Data have been compiled in all areas mentioned and a first critical selection and discussion has been made in all areas save one. The nature of the field involved makes the criteria for selection and evaluation very important. Discussions of these criteria are in preparation.

Future Plans: Preparation of the final evaluations and discussions leading to a final report.

G. Mechanical Properties

From the inception of its program, the Office of Standard Reference Data has recognized the value and importance of mechanical properties data to the industrial and engineering community. However, financial considerations have precluded the initiation of an effort in the field. Recently, a pilot study was undertaken to examine which properties and materials lend themselves to an evaluative process and should be included in the NSRDS program when resources permit. The results of this study are expected to provide the basis for evaluation projects in the mechanical properties area.

### III. RESEARCH IN DATA PROCESSING

The Data Systems Design Group (DSDG) is engaged in computer programming, systems design, and application, as well as data correlation. The DSDG's earlier experience gained in design and application of a number of general-purpose computing programs like OMNITAB 1/ is now providing guidelines for the preparation of general-purpose computer programs for data 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 can be grouped into three 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 NSRD System.

Among the projects in which the Data Systems Design Group is engaged or is promoting are the following:

(1) Computer-Assisted Text Preparation and Editing. 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.

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1/ Hilsenrath, J., Ziegler, Guy G., Messina, Carla G., Walsh, Philip J., and Herbold, Robert J., OMNITAB: A Computer Program for Statistical and Numerical Analysis, NBS Handbook 101. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, Price \$3.00.

The first release in this series is REFORM, an independent program with which it is possible to manipulate and edit files containing as many as nine different fixed-field card formats. It can select or abridge information from any of the cards and print that information, or reformat new cards in any desired order or arrangement. Provision is made for introducing as many as 26 arbitrary strings of characters, each of which may be up to 79 characters in length, thereby permitting the insertion of labels, headings, or comments into the file. The program and its characteristics are described in NBS Tech. Note #444 2/.

The second release in this series is called EDPAC and is described in NBS Tech. Note #470 3/. It contains five programs that have been used extensively at NBS over the last four years. These are called JUSTIFY, SCRAMBLE, SEARCH, BLOCKSEARCH, and SUBSTITUTE. These programs perform transformations on alphanumeric data. They have been written in FORTRAN, with care taken to make them as system- and machine-independent as possible, permitting their use on many different computers. This reflects the authors' view that the best way to attack the problem of compatibility and interchangeability of data cards or tapes is to provide a series of utility programs that will transform, translate, transpose, and transcribe information from one format to another.

SCRAMBLE scans an input file for specified characters, which it replaces by different characters. SUBSTITUTE similarly replaces strings of characters by other strings. SEARCH and BLOCKSEARCH scan for the occurrence of certain strings and list the lines or blocks, respectively, in which they occur.

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2/ McClenon, R.C., and Hilsenrath, J., REFORM: A General-Purpose Program for Manipulating Formatted Data Files, NBS Tech. Note #444. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, Price 40 cents.

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



JUSTIFY produces text for printing on a card-controlled typewriter or on an extended character printer which has been left and right-justified between specified margins. The REFORM and EDPAC programs have been put on magnetic tape and are being distributed by the CFSTI 4/.

Other programs in varying stages of production are:

- (a) A general-purpose program for manipulating formatted data file.
- (b) A general-purpose program for editing structured but unformatted data files.
- (c) A program to generate indexes for books and reports.

(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," was 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 handset and placed on a transparent film. The film is laid over each table, in turn, as the negatives are made.

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4/ PB-183 142, Computer Programs for Editing of Text and Data Files. Available from the Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 22151, Price \$100.

SETLST and KWIND are the first programs to be 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 photo-compositions. These programs and their characteristics are described in NBS Tech. Note #500 5/.

(3) Input Devices and Line Printers. A major problem in the extension of computer techniques to the processing of scientific manuscripts -- either for editing and automatic typesetting or for storage and retrieval -- is the limited number of characters on the ordinary computer printer, card punch, and typewriter.

Recent developments in hardware and programming should soon provide a capability to handle text with scientific notations, such as subscripts, superscripts, Greek letters, mathematical and logic symbols, and diacritical marks present in some languages.

It is neither economical, nor necessary, for computer printers to provide authors with the nearly 1000 symbols available to printers who specialize in scientific publications. A computer line-printer component with 240 distinct characters and having provision for half-line spacings offers enough flexibility to cope with all but the most specialized situations.

In 1969, the Office of Standard Reference Data gained access to such a device. This line-printer has 188 distinct characters, is able to provide half-line spacing for subscripts and superscripts, and is able to print several characters in the same position (e.g., / imposed over 0 gives  $\emptyset$ ). (See NSRDS News February 1970)

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5/ Messina, C.G., and Hilsenrath, J., Edit-Insertion Programs for Automatic Typesetting of Computer Printout. NBS Tech. Note #500 available from Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, Price 60 cents.

While extended character printers have been in use for some time, they have not yet achieved their full potential. This results largely from the fact that the printing speed is reduced by having a greater variety of characters. Each group felt constrained, therefore, to limit the number of special characters. Thus, there is little, if any compatibility between the existing extended character trains or the software to support them.

Three NSRDS Data Centers in the Physical Chemistry Division, NBS are now using, on a production basis, an automated text processing system for manipulating complex chemical notations. This system is based on the General Purpose Scientific Document Image Code. It accepts machine records from a variety of input devices: keypunch paper tape typewriters, and photocomposition machines. It includes a facile line editing routine and can produce records for archival storage, line printers and photocomposition.

Important advances during the year include the installation of a line printer with the full capability for printing GPSDIC records and the development of programs for using these records to drive a Linotron photocomposition machine.

The routines in this system are written in FORTRAN and are currently being used on a UNIVAC 1108. A parallel system is being developed at the National Library of Medicine.

The illustrations which follow show some of the results achieved by the programs and keyboarding systems developed by the DSDG and certain of the NSRDS Data Centers.

```

CALL NUMFND(SCAN,A,80,START,GOOF)
IF((A.GE.79).OR.(GOOF.LE.0)) CALL EXIT
CALL NUMFND(SCAN,A,80,STOP,GOOF)
IF(GOOF.LE.0) CALL EXIT
READ(5,1) (SCAN(A), A=1,80)
DO 7 A=1,72
IF(SCAN(A).NE.BLANK) GO TO 8
7 CONTINUE
9 WRITE(6,10)
10 FORMAT('ONO OR POOR SKIPCC CARD. RUN ABORTED.')
CALL EXIT
8 DO 11 B=1,6
IF(SCAN(A).NE.CHK(B)) GO TO 9
11 A=A+1
DO 12 B=A,80
IF(SCAN(B).NE.BLANK) GO TO 13
12 CONTINUE
GO TO 14
13 SKIP=SCAN(B)
14 READ(5,1) (SCAN(A),A=1,80)
19 READ(7,1,END=20) (TAPE(A), A=1,80)
DO 16 B=START,STOP
IF(SCAN(B).EQ.SKIP) GO TO 16
IF(TAPE(B).NE.SCAN(B)) GO TO 19
16 CONTINUE
WRITE(6,17) (TAPE(A), A=1,80)
17 FORMAT(17X,80A1)
GO TO 19
18 CALL EXIT
20 D=D+1
GO TO 15
END

```

Figure 1. A portion of a program listing phototyped at the Government Printing Office from a tape produced by SETLST from the original program deck, using the control cards shown in Figure 2.



```

ABCDEF GHI JKLMNOPQRST UVWXYZ0123456789 / \
  1   0   80   0   5   8
FIELD 1 GOES FROM 1 TO 80
THE FOLLOWING 1 CARDS CONTAIN THE INSERT STRINGS.

```

```

!F1
0

```

```

SUBROUTINE AMATCH INPUT

```

```

  4 '
>>
FINIS$
ABCDEF GHI JKLMNOPQRST UVWXYZ0123456789'/(*)=,$.+
  5 6 3
  0>< 0
  0>< 1
  /!F1/          /!F1/
  /A/            />A/
  /B/            />B/
  /C/            />C/
  /D/            />D/
  :              :
  /X/            />X/
  /Y/            />Y/
  /Z/            />Z/
  /+/            />8/
  /=/            />9/
  /*/            />0/
  /// ★          />//
  /(/            />,/
  /)/            />./
  /@/            />2/
  /#/            />1/
  /&/            />-/
  /:/            />3/
  /!/            /// ★
  /?/            />?/
FINIS

```

Figure 2. A printout supplied at the end of a SETLST run of the control cards used to produce Figure 1. The substitution table was entered in free-field format. The program lined it up for readability.

	—	ff	fl	(	)	ff	—	&	!	fi	fl	/
Shift	$\frac{1}{4}$	#	@	→	$\frac{1}{4}$	←	—	$\frac{1}{2}$	+	=	*	/
Unshift	%	1	2	3	4	5	6	7	8	9	0	!
	1	2	3	4	5	6	7	8	9	10	11	12
	Q	W	E	R	T	Y	U	I	O	P	?	
Shift	Q	W	E	R	T	Y	U	I	O	P	?	
Unshift	q	w	e	r	t	y	u	i	o	p	\$	
	13	14	15	16	17	18	19	20	21	22	23	
	A	S	D	F	G	H	J	K	L	:	'	
Shift	A	S	D	F	G	H	J	K	L	:	"	
Unshift	a	s	d	f	g	h	j	k	l	;	'	
	24	25	26	27	28	29	30	31	32	33	34	
	Z	X	C	V	B	N	M	,	.	*		
Shift	Z	X	C	V	B	N	M	(	)	&		
Unshift	z	x	c	v	b	n	m	,	.	<small>EM DASH</small>		
	35	36	37	38	39	40	41	42	43	44		

Figure 3. The layout of characters on the monowidth grid used to typeset Figure 1. Note the connection between the layout of the graphics and the substitution table in the previous figure. Because other typefaces have different distributions of characters in the shift and unshift position, it is a great advantage to define the locations of the character via a substitution table rather than in the program proper. The advantage of this grid is that it contains all of the characters on a model 26 key punch. The use of most other grids for typesetting of computer listings require time consuming grid changes.

55Ba5 P. S. Baranov, V. U. Gol danskii; Zhur. Eksp. i Teoret. Fiz. 28, 746, (1955); Soviet Phys. JETP 1, 613 (1955)  
 55Bu1 J. L. Burkhardt; Phys. Rev. 100, 192 (1955)  
 55Ca2 J. H. Carver, H. J. Hay, E. W. Titterton; Phil. Mag. 46, 841 (1955)  
 55Er1 P. Erdos, P. Jordan, P. Stoll; Helv. Phys. Acta 28, 322 (1955)  
 55Gl1 H. Glattli, E. Loepfe, P. Stoll; Helv. Phys. Acta 28, 366 (1955)  
 55Go1 F. K. Goward, J. J. Wilkins; Proc. Roy. Soc. (London) A228, 376 (1955)

+55'BA5 'P. 'S. 'BARANOV, 'V. 'U. 'GOL DANSKII\$ 'ZHUR. 'EKSP. I 'TEORET. )  
 -'FIZ. 28, 746, (1955)'(\$ 'SOVIET 'PHYS. 'J'ETP 1, 613 (1955)'( )  
 +55'BU1 'J. 'L. 'BURKHARDT\$. 'PHYS.. 'REV. 100, 192 (1955)'( )  
 +55'CA2 'J. 'H. 'CARVER, 'H. 'J. 'HAY, 'E. 'W. 'TITTERTON\$ 'PHIL. 'MAG. )  
 155'CA2 -46, 841 (1955)'( )  
 +55'ER1 'P. 'ERDOS, 'P. 'JORDAN, 'P. 'STOLL\$ 'HELV. 'PHYS. 'ACTA 28, 322 )  
 155'ER1 -(1955)'( )  
 +55'GL1 'H. 'GLATTLI, 'E. 'LOEPFE, 'P. 'STOLL\$ 'HELV. 'PHYS. 'ACTA 28, )  
 155'GL1 -366 (1955)'( )  
 +55'GO1 'F. 'K. 'GOWARD, 'J. 'J. 'WILKINS\$ 'PROC. 'ROY. 'SOC. ('LONDON)'( )  
 155'GO1 -A228, 376 (1955)'( )

Figure 4. The upper half is from a bibliography, NBS Spec. Pub 322, Photonuclear Data Index, phototypeset from a magnetic tape prepared by the program SEILST from an existing card deck shown in the lower half. The \$ sign is defined in this character stream as a semicolon. In this example the capitalization was controlled by the authors through the use of the apostrophe as a shift symbol because an earlier version of this bibliography was produced on a card controlled typewriter.





CUPRIC	ACETATE(1968)
AMMONIUM	ACETATE(1968)
ETHYL	ACETATE(1968)
R RIGID POLYVINYL CHLORIDE VINYL	ACETATE)COMPOUNDS(1966)
R RIGID POLYVINYL CHLORIDE-VINYL	ACETATE)PLASTIC SHEET(1967)
IT UNDERWEAR EXCLUSIVE OF RAYON,	ACETATE, AND NYLON(1955)
ON FOR PHOTOGRAPHIC GRADE, SODIUM	ACETATE, ANHYDROUS(1964)
MOLDINGS + EXTRUSIONS-CELLULOSE	ACETATE, GENERAL PURPOSE(1954)
FICATIONS FOR PHOTOGRAPHIC GRADE	ACETIC ACID GLACIAL(1964)
ITRILE-BUTADIENE-STYRENE PIPE BY	ACETIC ACID IMMERSION(1967)
IFICATION FOR PHOTOGRAPHIC GRADE	ACETIC ACID TWENTY-EIGHT PERCENT
SAFE HANDLING AND USE OF	ACETIC ACID(1951)
PHENYL	ACETIC ACID(1957)
GLACIAL	ACETIC ACID(1968)
ARD METHOD OF COPPER-ACCELERATED	ACETIC ACID-SALT SPRAY(FOG)TEST
STANDARD METHOD OF	ACETIC ACID-SALT SPRAY(FOG) TES
S OF TEST FOR HYDROXYL GROUPS BY	ACETIC ANHYDRIDE ACETYLATION(1967)
SAFE HANDLING AND USE OF	ACETIC ANHYDRIDE(1962)
OF TEST FOR PERMANGANATE TIME OF	ACETIC ANHYDRIDE(1968)
STANDARD METHOD OF TEST FOR	ACETONE AND METHANOL(1967)
CS/TENTATIVE METHOD OF TEST FOR	ACETONE EXTRACT IN BLACK PIGMEN
	ACETONE EXTRACTION AND IGNITION

Figure 6. A listing showing the condition of the records which were used by the program KWIND to produce the results shown in the previous figure. See Figure 7 for the control cards and the substitution table which achieved this transformation.

Figure 7.

ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789

0 120 7 8  
0 0 2 53 54 107 108 116

!I01  
!I02  
!I03  
!I04  
!I05  
!I06  
!I07  
!I08

\$ '

.....  
.....

U. S. DEPT. OF COMMERCE STANDS  
TITLE WORD INDEX \$

FINISS

ABCDEFGHIJKLMNOPQRSTUVWXYZ0123456789 /

0 5 3  
← 0  
← 1

/(SRD/ / (→S→D→R/  
/PVC/ / (→P→V→C/  
/(PE)/ / (→P→E)/  
/ PR/ / →P→R)/  
/ PR / / →P→R /  
/ SDR/ / →S→D→R/  
/ DWV/ / →D→W→V/  
/ IPS/ / →I→P→S/  
/ ABS / / →A→B→S /  
/ USA/ / →U→S→A/  
/ AND / / AND →/  
/ OR / / OR →/  
/ FOR / / FOR →/  
/ TO / / TO →/  
/ OF / / OF →/  
/ WITH / / WITH →/  
/ II/ / →I→I/  
/ III/ / →I→I→I/  
/ IV/ / →I→V/  
/ VI/ / →V→I/  
/ VII/ / →V→I→I/  
/ VIII/ / →V→I→I→I/  
/ IX/ / →I→X/  
/ XI/ / →X→I/  
/ XII/ / →X→I→I/  
/ XIII/ / →X→I→I→I/  
/ XIV/ / →X→I→V/  
/ XV/ / →X→V/  
/ XVI/ / →X→V→I/  
/ XVII/ / →X→V→I→I/

/ XVIII/ / →X→V→I→I→I/  
/ XIX// →X→I→X/  
/ XX/ / →X→X/  
/!I03A/ /!I03→A/  
/!I03B/ /!I03→B/  
/!I03C/ /!I03→C/  
/!I03D/ /!I03→D/  
/!I03E/ /!I03→E/  
/!I03X/ /!I03→X/  
/!I03Y/ /!I03→Y/  
/!I03Z/ /!I03→Z/  
/!I06A/ /!I06→A/  
/!I06B/ /!I06→B/  
/!I06C/ /!I06→C/  
/!I06D/ /!I06→D/  
/!I06E/ /!I06→E/  
/!I06X/ /!I06→X/  
/!I06Y/ /!I06→Y/  
/!I06Z/ /!I06→Z/  
/'A/ /'→A/  
/'B/ /'→B/  
/'C/ /'→C/  
/'D/ /'→D/  
/'E/ /'→E/  
/'X/ /'→X/  
/'Y/ /'→Y/  
/'Z/ /'→Z/

Continued

Figure 7 Concluded

/S / /S →/	/+A/ /!G2!T3←U!G1!T1→A/
/ A/ / →A/	/+B/ /!G2!T3←U!G1!T1→B/
/ B/ / →B/	/+C/ /!G2!T3←U!G1!T1→C/
/ C/ / →C/	/+D/ /!G2!T3←U!G1!T1→D/
/ D/ / →D/	<del>/+E/ /!G2!T3←U!G1!T1→E/</del>
<del>/ E/ / →E/</del>	/+X/ /!G2!T3←U!G1!T1→X/
/ X/ / →X/	/+Y/ /!G2!T3←U!G1!T1→Y/
/ Y/ / →Y/	/+Z/ /!G2!T3←U!G1!T1→Z/
/ Z/ / →Z/	/=A/ /!G2!T3→:!G1!T1→A/
/(A/ / (→A/	/=B/ /!G2!T3→:!G1!T1→B/
/(B/ / (→B/	/=C/ /!G2!T3→:!G1!T1→C/
/(C/ / (→C/	/=D/ /!G2!T3→:!G1!T1→D/
/(D/ / (→D/	<del>/=E/ /!G2!T3→:!G1!T1→E/</del>
<del>/(E/ / (→E/</del>	/=X/ /!G2!T3→:!G1!T1→X/
/(X/ / (→X/	/=Y/ /!G2!T3→:!G1!T1→Y/
/(Y/ / (→Y/	/=Z/ /!G2!T3→:!G1!T1→Z/
/(Z/ / (→Z/	/'S! / 'S! /
/-A/ /-→A/	/+ /!G2!T3←U!G1!T1/
/-B/ /-→B/	/=/ /!G2!T3→:!G1!T1/
/-C/ /-→C/	FINIS
/-D/ /-→D/	
<del>/-E/ /-→E/</del>	
/-X/ /-→X/	
/-Y/ /-→Y/	
/-Z/ /-→Z/	
./A/ ./→A/	
./B/ ./→B/	
./C/ ./→C/	
./D/ ./→D/	
./E/ ./→E/	
<del>./W/ ./→W/</del>	
./X/ ./→X/	
./Y/ ./→Y/	
./Z/ ./→Z/	

Figure 7. Control cards and substitution table for transforming the character stream in Figure 7 to that shown in Figure 6. Note that four sets of alphabet cards are needed to capitalize characters following: a space, a right parenthesis, a hyphen, and the locator !I03 inserted by the program at the middle gutter. The other substitution cards override these and achieve the desired exceptions.

#### IV. INFORMATION SERVICES

There are four basic units of activity within the Information Services operation: Data File, Compilation Publication Services, Inquiry Services, and Analysis and User Relations.

Data File: The mission of the Data File is to acquire known world-wide data compilations and other reference documents and publications within the scope of the mission of the NSRDS and to organize the collection systematically. The Data File houses a collection of about 1300 reference data compilations, critical reviews, bibliographies, and other ancillary reference works. It has been judged as one of the most extensive collections of its kind in the world. An Annotated Listing of the documents in this collection is in preparation and will be published in the near future as an NBS Technical Note.

Compilation Publication Services: This activity serves as the editorial intermediary between the Office of Standard Reference Data and the associated data centers of the NSRDS and other individuals and groups producing data compilations, on the one hand, and publishers on the other hand. The publishers are the Government Printing Office, commercial publishers, and the Clearinghouse for Federal Scientific and Technical Information. One of the functions of the Compilation Publication Services is to produce the monthly newsletter, the NSRDS News, which has a mailing list of more than 5000. This newsletter contains general information on data evaluation, news of specific projects, and announcements of new publications.

The program has produced, thus far, 31 publications in the NSRDS series of critically evaluated data compilations; 12 other compilations of data; 21 non-data publications from NSRDS related projects, as well as a number of publications published under the aegis of various of its associated data centers.

Inquiry Services: This unit provides replies to inquiries received by the Office of Standard Reference Data. At present, due to limited resources, information and data provided in response to queries are usually limited to that which is available within NSRDS and related publications. However, inquiries are frequently referred to competent sources in the NBS or elsewhere. At times, references are provided; if available, copies of publications or excerpts therefrom containing the requested information is provided. Inquiries have steadily been increasing from about 200 in 1966 to more than 1000 in 1969, with less than 30 in the latter instance receiving negative replies because of lack of information or the inability to refer the correspondent to a likely source of information.

Analysis and User Relations: The mission of this unit is to provide the Office understanding of requirements, both present and future, of the NSRDS's actual and potential users. Among its efforts to determine user needs and means for developing feedback mechanisms have been several surveys. The most recent was a pilot survey in the form of an interview/questionnaire aimed at providing information on technical reference data use patterns of NBS scientists. This pilot



study revealed that 42, or 84%, of a representative sample of 50 NBS scientists use physical properties data. The scientists, on the average, spend approximately 1 hour of their working day in seeking data or discussing their data requirements. One of the results of this pilot study is a revised interview/questionnaire suitable for survey of similar information by other organizations. In preparation are two surveys, one on the knowledge by special librarians of the NSRDS and how they use NSRDS publications. The other is a survey on how purchasers of NSRDS publications use these publications in their everyday work.



**APPENDIX I:**

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

**An Act**

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

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

Standard Reference Data Act.

**DECLARATION OF POLICY**

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

82 STAT. 339  
82 STAT. 340

**DEFINITIONS**

Sec. 2. For the purposes of this Act—

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

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

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

Collection and publication of standard reference data.

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

Standards, etc. Publication in Federal Register.

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

Sale of reference data. Cost recovery.

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

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

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

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

Appropriation.

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

Short title.

Sec. 8. This Act may be cited as the "Standard Reference Data Act."  
**Approved July 11, 1968.**

LEGISLATIVE HISTORY:

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

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

CONGRESSIONAL RECORD:

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

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

June 27, House concurred in Senate  
amendments.

## APPENDIX II:

### CONTINUING DATA CENTERS IN THE UNITED STATES

The distinction between continuing data centers and "one-shot" evaluation projects was discussed in Chapter I. B. An attempt has been made to identify the continuing centers in the United States which fall within the technical scope of the NSRDS program. The following guidelines have been used in drawing up this list:

- 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.

It should be emphasized that many of the data centers listed here have no formal connection with, and receive no financial support from the Office of Standard Reference Data. This office is directly involved with only those centers for which NBS-OSRD is indicated as a Source of Support. In the case of some centers receiving joint support, OSRD is involved with only one part of the center's activities.

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.

The following list gives brief information on the coverage and form of output of each center. 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 Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, as COSATI-70-1 (PB 189300).

#### Code for Source of Support:

NBS:	National Bureau of Standards
NBS-OSRD:	Office of Standard Reference Data
AEC:	Atomic Energy Commission
ARPA:	Advanced Research Projects Agency (Dept. of Defense)
NAVORD:	Naval Ordnance Systems Command
ONR:	Office of Naval Research
USAF:	United States Air Force



LIST OF CONTINUING DATA CENTERS

Thermodynamic and Transport Properties

1. Title: Chemical Thermodynamics Data Center

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

Director: D.D. Wagman; Project Director: William Evans

Source of Support: NBS-OSRD

Coverage: All elements, inorganic compounds, C<sub>1</sub> and C<sub>2</sub> organic compounds, aqueous solutions of important acids, bases, and salts, and some gaseous and aqueous ions. Data are grouped in two series. Series I includes standard state values at 25°C for heat (enthalpy), Gibbs energy and logarithm of equilibrium constant of formation, entropy, and heat capacity, and for a few substances, values for heat of formation at 0°K. For solutions of important salts, thermodynamic properties are given at concentrations from near saturation to infinite dilution. Series II gives change-of-phase values, i.e., temperature, heat and entropy of transition, fusion, vaporization, or sublimation, heat capacity, and some vapor pressure values.

Form of Output: NBS Circular 500, Selected Values of Chemical Thermodynamic Properties was issued in 1952. It is being revised in sections. Updated parts are issued when ready in the NBS Technical Note 270 series. NSRDS-NBS-2, Thermal Properties of Aqueous Uni-univalent Electrolytes was issued in NSRDS-NBS series. Annual annotated index to thermodynamic studies of inorganic substances is prepared for and published in the Bulletin of Thermodynamics and Thermochemistry.

2. Title: Thermodynamics Research Center

Location: Department of Chemistry, Texas A & M University, College Station, Texas

Director: Bruno J. Zwolinski

Source of Support: NBS-OSRD; American Petroleum Institute; Gulf Oil Foundation; Texas A & M Research Foundation

Coverage: Thermodynamic and other physico-chemical properties; infrared, far infrared, ultraviolet, Raman, mass, and nuclear magnetic resonance spectral data; special emphasis on all classes of organic compounds, including hydrocarbons, sulfur and nitrogen derivatives of hydrocarbons, organic oxygen and halogenated compounds, as well as other organic materials.

Form of Output: Tables of Selected Physical and Thermodynamic Property Data: (a total of 3600 loose-leaf data sheets in 11 volumes) API Research Project 44 Tables of Numerical Data--48 tables of properties with 410,000 numerical entries covering 167 classes of hydrocarbons, sulfur,

and nitrogen derivatives of hydrocarbons; and TRC (formerly MCA) Data Project Tables of Numerical Data--18 tables of properties with 43,000 numerical entries covering 235 classes of inorganic and organic compounds of interest to the chemical industries. Catalogs of Selected Spectroscopic Data (a total of 10,400 loose-leaf spectral data sheets in 31 separate volumes): Infrared (including Far Infrared)--API Research Project 44--3,000 spectra, and TRC Data Project--600 spectra; Ultraviolet--API Research Project 44--1,200 spectra, and TRC Data Project--200 spectra; Raman--API Research Project 44--500 spectra, and TRC Data Project--200 spectra; Mass (standard, matrix, and element-maps formats)--API Research Project 44--2,600 spectra, and TRC Data Project--400 spectra; and Nuclear Magnetic Resonance (60 and 100 MHz)--API Research Project 44--800 spectra, and TRC Data Project--800 spectra. All new spectral supplements include the Wiswesser Line Notation. A computer-generated index entitled "Comprehensive Index of API44-TRC Selected Data on Thermodynamics and Spectroscopy" allows rapid access to the 8,000 compounds in the twelve publications. The first volume in a series of special handbooks entitled "Vapor Pressures and Heats of Vaporization of Hydrocarbons" will be available late in 1970.

All inquiries regarding publications should be directed to TRC Data Distribution Office, F.E. Box 130, College Station, Texas 77843.

3. Title: Thermophysical Properties Research Center

Location: Purdue University, West Lafayette, Indiana

Director: Y.S. Touloukian

Source of Support: NBS-OSRD; USAF Materials Laboratory; NASA; NSF; ONR; Private Industry

Coverage: Thermophysical properties of all matter covering the following 16 properties: Thermal conductivity, accommodation coefficient, thermal contact resistance, thermal diffusivity, specific heat, viscosity, emissivity, reflectivity, absorptivity, transmissivity, absorptance to emittance ratio, Prandtl number, diffusion coefficient, thermal linear expansion, thermal volumetric expansion coefficient, and surface tension. Thermophysical properties are keyed to representative groups such as slags, scales, ceramics, oxides, glasses, mixtures, solutions, metals, nonmetals, numerals, compounds, coatings, cermets, pharmaceuticals, cosmetics, toiletries, petroleum products, animal and vegetable substances, fabrics, yarns, rubbers, plastics, resins, polymers, paper and wood products, and building materials.

Form of Output: A critically evaluated compilation entitled, Thermal Conductivity of the Elements has been published in NSRDS-NBS Series. Additionally, the TPRC Data Series, under the umbrella title, Thermophysical Properties of Matter is published commercially by the Plenum Publishing Corporation. This consists of 13 volumes in its first edition, ten

volumes to be published in 1970 and the remainder by 1972. Other major publications include the six volume handbook entitled, Thermophysical Properties of High Temperature Solid Materials (MacMillan) and a set of three books entitled, Thermophysical Properties Research Literature--Retrieval Guide, published by the Plenum Corporation. The annual volume listing, Master's Theses in the Pure and Applied Sciences continues to be compiled by the Center and is currently published and disseminated by the University Microfilms Library Services, Ann Arbor, Michigan.

4. Title: Cryogenic Data Center

Location: Cryogenics Division, NBS, Boulder, Colorado

Director: Victor J. Johnson

Source of Support: NBS-OSRD; NASA; AEC; American Gas Assoc.; Reimbursable

Coverage: Cryogenic fluids and selected solids. The fluids include helium, hydrogen, neon, nitrogen, oxygen, air, carbon monoxide, fluorine, argon, methane, LNG, xenon, krypton, and mixtures of these fluids. Solids include metallic elements, selected alloys, plastics, elastomers and element dielectrics. Emphasis is on properties useful in engineering applications to cryogenic systems. Properties of fluids include pressure-volume-temperature relations, vapor pressure, saturation densities, isothermal compressibility, volume expansivity, entropy, enthalpy, internal energy, specific heats, velocity of sound, thermal conductivity, viscosity, Prandtl number, diffusion coefficients; thermal diffusion coefficients, dielectric constant, refractive index, dielectric breakdown, electrical resistivity, surface tension, magnetic properties, and optical properties. For solids, properties include electrical resistivity, dielectric constant, thermal conductivity, thermal expansion, specific heat, and enthalpy.

Form of Output: A large number of publications have been issued within the various NBS series, NBS Technical Notes, Monographs in the NSRDS-NBS series, some as journal articles and thermodynamic charts. Some compendia of properties were issued as Air Force reports and are available through the CFSTI. A current awareness bulletin is also published, as well as a Quarterly survey of the literature on superconducting devices and materials and a Quarterly survey of the literature on LNG. Numerous bibliographies are prepared from the data bank of some 65,000 documents; accessioned into the automated storage and retrieval system.

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, Be, Br, C, Cl, Co, Cu, F, Fe, H, Hg, I, K, Li, Mg, Mo, N, Na, O, P, Pb, S, Si, Ti, 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, heat content (enthalpy), heat of formation, and Gibbs energy of formation for the ideal gas, liquid or solid state as appropriate. 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: Tables published on 22x28 cm loose-leaf sheets and collated in loose-leaf binders. Available through Clearinghouse for Federal Scientific and Technical Information. First set PB 168-370 published in 1965; supplements and addendums PB 168-370-1, PB 168-370-2, PB 168-370-3 issued periodically. All tables available also on magnetic tape.

6. Title: Binary Metal and Metalloid Constitution Data Center

Location: IIT Research Institute, Chicago, Illinois

Director: Rodney P. Elliott

Source of Support: NBS-OSRD; AEC; USAF

Coverage: Binary combinations of metallic elements, excluding binaries with halogens and those which are not metal related. Properties covered are solidus, liquidus, solubility, crystal structure, and lattice parameters. Parameters included are temperature and composition.

Form of Output: Data published commercially by McGraw-Hill in 1958 as Constitution of Binary Alloys by M. Hansen and K. Anderko. First supplement by R.P. Elliott published in 1965; Second supplement by F.A. Shunk in 1969. Revision in progress.

7. Title: Thermodynamic Properties of Metals and Alloys

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

Director: Ralph Hultgren

Source of Support: AEC

Coverage: All metallic elements and binary alloy systems. For the elements the following properties are considered: heat capacity, enthalpy (heat), entropy, Gibbs energy (free energy). 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, 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.



Form of Output: Tables published as Selected Values for the Thermodynamic Properties of Metals and Alloys by John Wiley and Sons. New and revised data sheets issued at intervals.

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: NBS-OSRD; 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 (enthalpy) and temperature of phase changes; heat capacity; enthalpy, entropy and Gibbs energy function at 100-degree intervals; and enthalpy, Gibbs energy, and  $\log K_p$  of formation 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, activity, 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

Location: Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York

Director: George J. Janz

Source of Support: NBS-OSRD

Coverage: Inorganic compounds in the molten state. Properties included are: electrical conductance, viscosity, density, surface tension, and emf.

Form of Output: The center produces critically evaluated compendia of data published in the NSRDS-NBS series. A non-critical compendium, Molten Salts Handbook, was published by Academic Press. Bibliographies appear as Rensselaer Polytechnic Institute publications.

11. Title: High Pressure Data Center

Location: Brigham Young University, Provo, Utah

Director: H. Tracy Hall; Assistant Director : Leo Merrill

Source of Support: NBS-OSRD

Coverage: All pressure studies from 1 kbar up to the megabar range.

Thermodynamic variables of interest are pressure, temperature, latent heats, specific heat, and triple points.

Form of Output: Two-volume bibliography of high pressure field covering period 1900-1968 is being distributed by Federal Clearinghouse. Critical reviews on phase transition points are in progress.

## Atomic and Molecular Data

### 1. Title: Atomic Energy Levels Data Center

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

Director: William C. Martin

Source of Support: NBS-OSRD

Coverage: Atomic spectra and atomic energy levels for both neutral and ionic species.

Form of Output: Evaluated compilations of data on atomic energy levels, multiplet tables, selected tables of atomic spectra, and bibliographies. These have appeared in the NSRDS-NBS series and as other NBS publications.

### 2. Title: Atomic Transition Probabilities Data Center

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

Director: W.L. Wiese

Source of Support: ARPA, NBS-OSRD

Coverage: Radiative transition probabilities of atoms and atomic ions in the gas phase. All elements are covered.

Form of Output: Two critical compilations of atomic transition probabilities covering the first twenty elements have appeared in NSRDS-NBS series and others are in progress; bibliographies in the NBS Special Publications Series; critical compilation on Ba I and II appeared as NBS Tech. Note.

### 3. Title: Diatomic Molecule Spectral Data Center

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

Director: Paul H. Krupenie

Source of Support: NBS-OSRD

Coverage: Spectroscopic data for diatomic molecules, with emphasis on the optical region, and molecular parameters derived from spectroscopic measurements.

Form of Output: Detailed reviews of spectroscopic data on important diatomic molecules are published in NSRDS-NBS series.

### 4. Title: Microwave Spectral Data Center

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

Director: William H. Kirchhoff

Source of Support: NBS-OSRD

Coverage: Microwave absorption spectra of gases, including transition frequencies and intensities as well as molecular constants derived from the spectral data.

Form of Output: Tables of observed microwave frequencies of molecules will be published as supplements to NBS Monograph 70, Microwave Spectral Tables.

5. Title: JILA Information Analysis Center

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

Director: L.J. Kieffer

Source of Support: NBS-OSRD; ARPA

Coverage: Cross sections (low energy range) for collision of electrons and photons with atoms, ions, and small molecules. Emphasis on data of interest in astrophysics, aeronomy, and plasma physics.

Form of Output: Critical reviews and data compilations (NSRDS-NBS series, Reviews of Modern Physics, Atomic Data); bibliographies (JILA Information Center Reports and NSRDS Clearinghouse Series).

6. Title: Atomic and Molecular Processes Information Center

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

Director: C.F. Barnett

Source of Support: NBS-OSRD; AEC

Coverage: Atomic and small molecule collisions, specifically: heavy particle-heavy particle atomic collision cross sections, particle interactions with quasistatic electric and magnetic fields, particle penetration into macroscopic matter, and energetic particle interactions with surfaces.

Form of Output: Critical monographs on various classes of heavy particle interactions. The first monograph, Ion-Molecule Reactions, is being published by John Wiley and Sons, Inc. Ten bibliographies and a directory of workers in the field published as AMPIC publications.

7. Title: Charged-Particle Cross-Section Information Center

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

Director: F.K. McGowan

Source of Support: AEC

Coverage: Nuclear cross-section data for charged-particle-induced reactions of the type  $A(a,b)B$ , where  $M_a \geq$  one nucleon mass.

Form of Output: First two compilations of data published as AEC reports; since 1966 compilations published in Section A of the journal, Nuclear Data Tables, published by Academic Press.

8. Title: Mass Spectrometry Data Center

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

Director: Henry M. Rosenstock

Source of Support: NBS-OSRD

Coverage: Ionization and appearance potentials and the properties of excited ionic states--the energetics of gaseous ionization. All atomic and molecular species are included.

Form of Output: Tabular compilation of evaluated data on ionization potentials, appearance potentials, and ionic heats of formation has appeared as an NSRDS-NBS publication; bibliography in the NBS Tech Note series.

9. Title: X-Ray Attenuation Coefficient Information Center

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

Director: J.H. Hubbell

Source of Support: NBS-OSRD

Coverage: Attenuation coefficients for high energy photon (X-ray, gamma-ray) interaction with matter, including Compton and Rayleigh scattering, atomic photo-effect, and electron-positron pair production.

Form of Output: Several journal papers discussing theoretical calculations have appeared in professional journals. Some numerical data compilations have been published as parts or sections of larger works; also a critical compilation published in the NSRDS-NBS series.



## Solid State Data

### 1. Title: Crystal Data Center

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

Director: J.D.H. Donnay, Chief, Editor; Helen M. Ondik, Inorganic Editor; O. Kennard, Organic Editor; Mary E. Mrose, Mineral Editor; Sten Samson, Intermetallic Editor; Murray V. King, Protein Editor

Source of Support: NBS-OSRD; American Crystallographic Association

Coverage: Tables for the identification of crystalline substances by means of cell constants and auxiliary properties such as axial ratios, space group, formula units per cell, and measured and calculated specific gravities. Other properties included are: melting point, color, pleochroism, twinning, cleavage, crystal habit, indices of refraction, optic axial angle, and optical orientation. Full literature references for the data are given.

Form of Output: Crystal Data Determinative Tables in 2 volumes of approximately 30,000 entries for the identification of crystalline substances to appear as an NSRDS publication.

### 2. Title: Alloy Data Center

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

Director: G.C. Carter

Source of Support: NBS-OSRD

Coverage: Substances of interest are: metals, semi-metals, intermetallic compounds, and alloys, consisting of two, three and sometimes more components. Properties covered include: electronic transport, magnetic, mechanical (density, internal structure, acoustical), nuclear magnetic resonance (NMR) and other resonances (e.g., electron paramagnetic resonance (EPR), Mössbauer effect, etc.), quantum description of solids (electronic structure of metals), electromagnetic radiation, superconductivity, thermodynamics and soft X-ray spectroscopy. Emphasis at present is on NMR (Knight or metallic shifts) and soft X-ray data.

Form of Output: Bibliographies in NBS Special Publication Series and in NSRDS series of Bibliographies published through the Clearinghouse for Federal Scientific and Technical Information. NBS Tech Note 464 describes the Alloy Data Center, its holdings and its services. A critical compilation on Metallic Shifts in NMR will appear in Progress in Materials Science.

### 3. Title: Diffusion in Metals Data Center

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

Director: John R. Manning

Source of Support: NBS-OSRD

Coverage: Diffusion properties of pure metals and binary alloys--diffusion coefficients and activation energies. Two types of diffusion are of particular interest: tracer diffusion--(radioactive tracer atoms diffuse into a homogeneous crystal)--and chemical interdiffusion--(atoms from bulk specimens in contact intermingle).

Form of Output: Critical evaluation of data is in progress.

4. Title: Superconductive Materials Data Center

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

Director: B.W. Roberts

Source of Support: NBS-OSRD

Coverage: Properties of superconductive materials, i.e., critical temperatures, critical magnetic fields, crystallographic parameters, critical magnetic fields of high field superconductors and some thermodynamic data.

Form of Output: Noncritical data compilations published in NBS Technical Note series and entitled Superconductive Materials and Some of Their Properties.

5. 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-, and multicomponent systems are given involving variables of pressure, 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.

## Chemical Kinetics

1. Title: Chemical Kinetics Information Center

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

Director: David Garvin

Source of Support: NBS-OSRD; NAVORD

Coverage: Rates of homogeneous chemical reactions in gaseous, liquid and solid phases, photochemistry, and inelastic scattering. Among properties of concern are rate constants, frequency factors, heats, energies, and entropies of activation.

Form of Output: NBS Circulars and Monographs on Tables of Chemical Kinetics. Bibliographies on kinetic data published as NBS Lists of publications. Specialized bibliographies in response to requests from individuals and organizations.

2. Title: Radiation Chemistry Data Center

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

Director: Milton Burton; Supervisor: Alberta Ross

Source of Support: NBS-OSRD; AEC

Coverage: Radiation yields and kinetic data on elementary processes in irradiated substances (organic and inorganic, aqueous and nonaqueous solutions, solids, and gases); changes in physical properties on irradiation. Property scope includes: specific rates, equilibrium constants, decay time, entropy of activation, cross section, or probability, activation energy and other Arrhenius parameters; G (yield in molecules/100eV) or M/N (molecules/ion pair); properties of transients including absorption and emission bands, extinction coefficients, and half-lives; parameters describing interactions of radiation and matter. Species are limited to chemically defined systems, excepting metals, including solid, liquid, gas, and heterogeneous systems made up of organic and inorganic compounds, in the pure state or as mixtures containing two or more components.

Form of Output: Specific bibliographies upon request and current awareness bulletin. Data sheets, data reviews, and compilations in preparation.

## 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  $A \geq 40$ .

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

2. Title: Table of Isotopes

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

Director: J.M. Hollander

Source of Support: AEC; NBS-OSRD

Coverage: All nuclear species, stable and unstable. Among properties  
included are: energy levels; spin; moments; alpha, beta, and gamma radia-  
tion data; and decay schemes.

Form of Output: Tables of data originally published in Reviews of Modern  
Physics. The sixth edition of the Table of Isotopes was published  
by John Wiley and Sons, Inc., 1967. A revision is in progress.

3. Title: Photonuclear Data Center

Location: Linac Radiation Division, NBS, Washington, D. C.

Director: Everett G. Fuller

Source of Support: NBS-OSRD

Coverage: Interactions of high energy electromagnetic radiation with  
nuclei. The energy range of primary interest is 5 to 150 MeV.

Form of Output: Publishes Photonuclear Data Index with supplements in  
the NBS Special Publications series.

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", (BNL-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: Berkeley Particle Data Center

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

Director: Arthur H. Rosenfeld

Source of Support: AEC; NBS-OSRD

Coverage: Properties and interactions of leptons, mesons, and baryons.

Form of Output: Reviews as particle properties published annually in Reviews of Modern Physics; compilations of cross section data appear as UCRL reports. Also distributes publications of CERN/HERA.



## Colloid and Surface Properties

1. Title: Light Scattering Data Center

Location: Clarkson College of Technology, Potsdam, New York

Director: Joseph Kratochvil

Source of Support: NBS-OSRD

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 to be  
published in the NSRDS series is in preparation.

# Publications List

## Publications Issued in the NSRDS Series

NSRDS-NBS-1, (C13.48:1) **National Standard Reference Data System—Plan of Operation**, by E. L. Brady and M. B. Wallenstein, 1964 (15 cents).

NSRDS-NBS-2, (C13.48:2) **Thermal Properties of Aqueous Uni-univalent Electrolytes**, by V. B. Parker, 1965 (45 cents).

NSRDS-NBS-3, Sec. 1, (C13.48:3/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).

NSRDS-NBS-3, Sec. 2, (C13.48:3/Sec. 2) **Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, Si I**, by C. E. Moore, 1967 (20 cents).

NSRDS-NBS-4, (C13.48:4/Vol. I) **Atomic Transition Probabilities, Vol. I, Hydrogen Through Neon**, by W. L. Wiese, M. W. Smith, and B. M. Glennon, 1966 (\$2.50).

NSRDS-NBS-5, (C13.48:5) **The Band Spectrum of Carbon Monoxide**, by P. H. Krupenie, 1966 (70 cents).

NSRDS-NBS-6, (C13.48:6/Pt. 1) **Tables of Molecular Vibrational Frequencies, Part 1**, by T. Shimanouchi, 1967 (40 cents).

NSRDS-NBS-7, (C13.48:7/Pt. 1) **High Temperature Properties and Decomposition of Inorganic Salts, Part 1. Sulfates**, by K. H. Stern and E. L. Weise, 1966 (35 cents).

NSRDS-NBS-8, (PB189698) **Thermal Conductivity of Selected Materials**, by R. W. Powell, C. Y. Ho, and P. E. Liley, 1966 (\$3.00).

NSRDS-NBS-9, (C13.48:9) **Tables of Bimolecular Gas Phase Reactions**, by A. F. Trotman-Dickenson and G. S. Milne, 1967 (\$2.00).

NSRDS-NBS-10, (C13.48:10) **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).

NSRDS-NBS-11, (C13.48:11/Pt. 2) **Tables of Molecular Vibrational Frequencies, Part 2**, by T. Shimanouchi, 1967 (30 cents).

NSRDS-NBS-12, (C13.48:12) **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).

NSRDS-NBS-13, (C13.48:13) **Hydrogenation of Ethylene on Metallic Catalysts**, by J. Horiuti and K. Miyahara, 1968 (\$1.00).

NSRDS-NBS-14, (C13.48:14) **X-Ray Wavelengths and X-Ray Atomic Energy Levels**, by J. A. Bearden, 1967 (40 cents).

NSRDS-NBS-15, (C13.48:15/Vol. 1) **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 (\$3.00).

NSRDS-NBS-16, (C13.48:16/Pt. 2) **Thermal Conductivity of Selected Materials, Part 2**, by C. Y. Ho, R. W. Powell, and P. E. Liley, 1968 (\$2.00).

NSRDS-NBS-17, (C13.48:17/Pt. 3) **Tables of Molecular Vibrational Frequencies, Part 3**, by T. Shimanouchi, 1968 (30 cents).

NSRDS-NBS-18, (C13.48:18) **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).

NSRDS-NBS-19, (C13.48:19) **Thermodynamic Properties of Ammonia as an Ideal Gas**, by L. Haar, 1968 (20 cents).

NSRDS-NBS-20, (C13.48:20) **Gas Phase Reaction Kinetics of Neutral Oxygen Species**, by H. S. Johnston, 1968 (45 cents).

NSRDS-NBS-21, (C13.48:21) **Kinetic Data on Gas Phase Unimolecular Reactions**, by S. W. Benson and H. E. O'Neal, 1970 (\$7.00).

NSRDS-NBS-22, Volume II, (C13.48:22/Vol. II) **Atomic Transition Probabilities, Vol. II, Sodium Through Calcium**, by W. L. Wiese, M. W. Smith, and B. M. Miles, 1969 (\$4.50).

NSRDS-NBS-23, (C13.48:23) **Partial Grotrian Diagrams of Astrophysical Interest**, by C. E. Moore and P. W. Merrill, 1968 (55 cents).

NSRDS-NBS-24, (C13.48:24) **Theoretical Mean Activity Coefficients of Strong Electrolytes in Aqueous Solutions from 0 to 100°C**, by Walter J. Hamer, 1968 (\$4.25).

NSRDS-NBS-25, (C13.48:25) **Electron Impact Excitation of Atoms**, by B. L. Moisewitsch and S. J. Smith, 1968 (\$2.00).

NSRDS-NBS-26, (C13.48:26) **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 (\$4.00).

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NSRDS-NBS-28, (C13.48:28/Vol. 2) **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 Chr. 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).

NSRDS-NBS-29, (C13.48:29) **Photon Cross Sections, Attenuation Coefficients, and Energy Absorption Coefficients From 10 keV to 100 GeV**, by J. H. Hubbell, 1969 (75 cents).

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NSRDS-NBS-33, (C13.48:33) **Electrolytic Conductance and the Conductances of the Halogen Acids in Water**, by Walter J. Hamer and Harold J. DeWane, 1970 (50 cents).

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#### Other NBS Compilations of Data

NBS Tech Note 270-3, (C13.46:270-3) **Selected Values of Chemical Thermodynamic Properties, Tables for the First Thirty-Four Elements in the Standard Order of Arrangement**, by D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey, and R. H. Schumm, 1968 (\$1.25).

NBS Tech Note 270-4, (C13.46:270-4) **Selected Values of Chemical Thermodynamic Properties, Tables for Elements 35 Through 53 in the Standard Order of Arrangement**, by D. D. Wagman, W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey, and R. H. Schumm, 1969 (\$1.25).

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NBS Misc. Publ. 281, (C13.10:281) **Bibliography on Flame Spectroscopy, Analytical Applications, 1800 to 1966**, by R. Mavrodineanu, 1967 (\$2.00).

NBS Misc. Publ. 289, (C13.10:289) **Bibliography of Low Energy Electron Collision Cross Section Data**, by L. J. Kieffer, 1967 (50 cents).

NBS Tech Note 290, (C13.46:290) **Information Handling in the National Standard Reference Data System**, by F. L. Alt, 1966 (25 cents).

NBS Tech Note 291, (C13.46:291) **A Bibliography on Ion-Molecule Reactions, January 1900 to March 1966**, by F. N. Harlee, H. M. Rosensstock, and J. T. Herron, 1966 (30 cents).

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NBS Tech Note 464, (C13.46:464) **The NBS Alloy Data Center: Function, Bibliographic System, Related Data Centers, and Reference Books**, by G. C. Carter, L. H. Bennett, J. R. Cuthill, and D. J. Kahan, 1968 (\$1.25).

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NBS Special Publication 306-1, (C13.10:306-1) **Bibliography on the Analyses of Optical Atomic Spectra, Section 1  $^1\text{H}$ - $^{23}\text{V}$** , by Charlotte E. Moore, 1968 (\$1.00).

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**Coblentz Society Specifications for Evaluation of Infrared Reference Spectra**, by Board of Managers, Coblentz Society, *Analytical Chemistry* 38, No. 9 (August 1966).

Kieffer, L. J. and Dunn, Gordon H., **Electron Impact Ionization Cross-Section Data For Atoms, Atomic Ions, and Diatomic Molecules: I. Experimental Data**, *Rev. Mod. Phys.* 38, No. 1, 1-35 (1966).

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NBS Special Publication 322, (C13.10:322) **Photonuclear Data Index, January 1965 through January 1970**, prepared by the Photonuclear Data Group, 1970 (75 cents). (To accompany NBS Miscellaneous Publication 277. Supersedes Supplement 1 to Miscellaneous Publication 277).

NBS-OSRDB-70-1-I, (PB191174) **High Pressure Bibliography 1900-1968, Vol. I, Section I-Bibliography and Section II-Author Index**, by L. Merrill, 1970 (Microfiche 65¢, Paper Copy \$7.00).

NBS-OSRDB-70-1-II, (PB191175) **High Pressure Bibliography 1900-1968, Vol. II, Subject Index**, by L. Merrill, 1970 (Microfiche 65¢, Paper Copy \$7.00).

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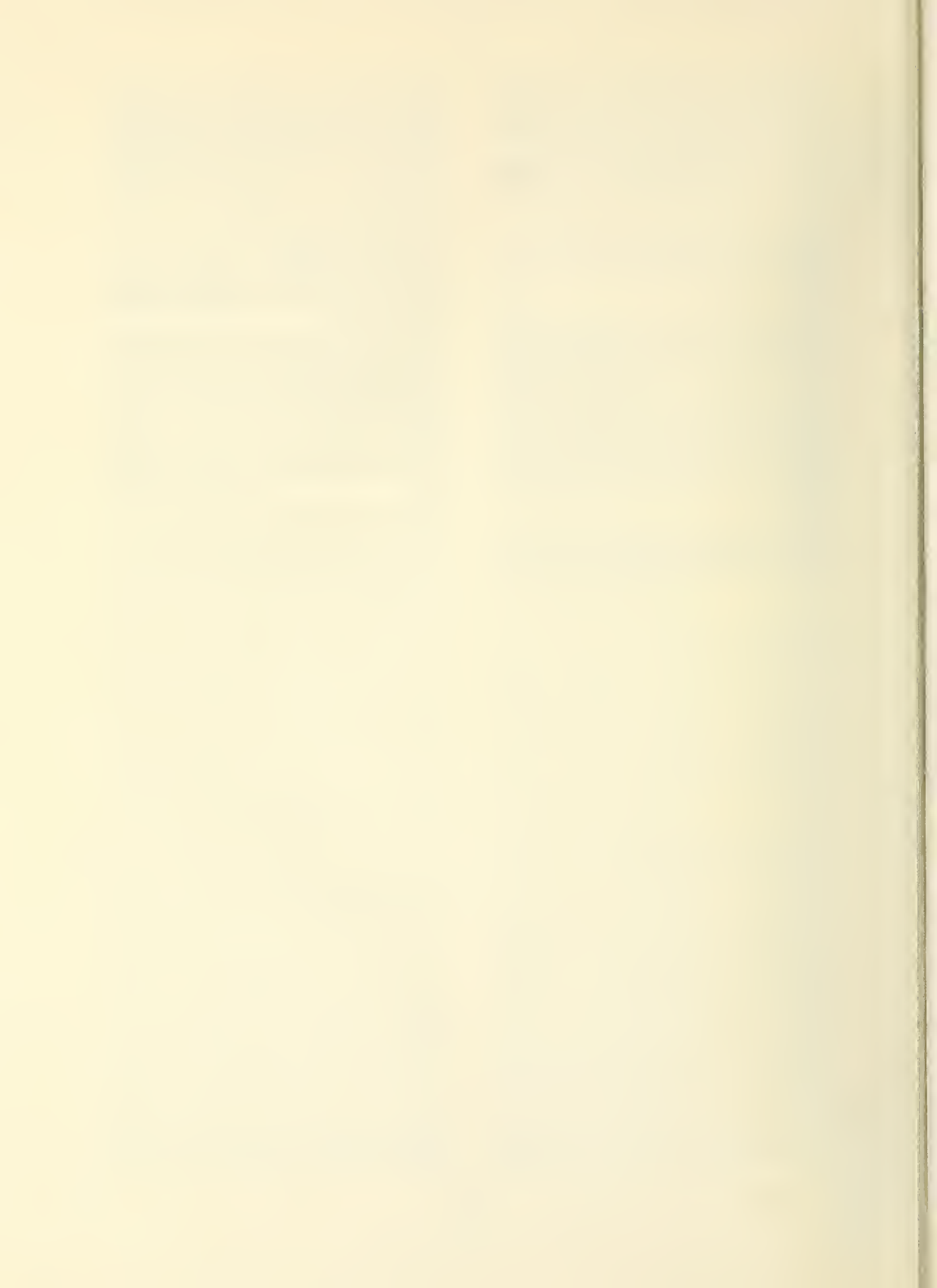
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